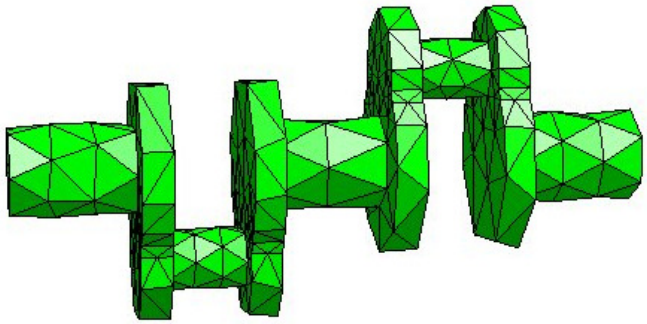
Applied Mathematics Foundations

(winter term 2021/22)



Lecture Notes

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Chapter 0

Introduction

The aim of this lecture is to provide the necessary mathematical foundations for the master studies Computational Science and Engineering.

The main focus is to introduce the fundamental concepts of vector calculus, line and surface integrals, integral transformations, (partial) differential equations, calculus of variations and complex analysis. Apart from the precise theoretical statements, the aim is to present possible (physical) applications and examples of the theory.

These lecture notes are based on the assumption that the reader is familiar with concepts of

- analysis: real and complex numbers, functions, series and limits, continuity, differentiation and integration in one variable;
- linear algebra: basic set theory, vectors (in $\mathbb{R}^n$) and matrices, solution of linear systems of equations, computation of eigenvalues.

Since this lecture is concerned with differentiation and integration in more variables, a short introduction into the 1D-concepts are given to recall the basics and fix notations.

The lecture notes draw material from the books

- *Mathematical Methods for Physics and Engineering* (by Riley, Hobson and Bence)
- *Higher Mathematics for Physics and Engineering* (by Shima, Nakayama)

as well as from some basic mathematics lectures at TU Wien. The books mentioned above actually contain way more information and many interesting examples and applications for the interested reader.

This is version 2 of the lecture notes, which were originally written during the winter term 2020/21.

Chapter 1

Vector, Banach and Hilbert spaces

1.1 Scalars

We call real or complex numbers α scalars. We use the notation $\mathbb{K}$, to denote either the real numbers $\mathbb{R}$ or the complex numbers $\mathbb{C}$, when both choices are possible.
Moreover, we call functions f mapping into $\mathbb{K}$ scalar valued or scalar functions.

1.2 Vector spaces

In the following, we introduce the abstract concept of vector spaces.

Definition 1.1 (Vector space). *A set V is called a* **vector space***, if the following three properties hold:*

1. *There is an operation $+$ such that $x + y \in V$ for all $x, y \in V$ and*
$$x + y = y + x.$$
2. *There exists an identity vector in V (denoted by 0 and also sometimes called neutral element) that satisfies*
$$x + 0 = 0 + x = x.$$
3. *For every $x \in V$ and scalar $\alpha \in \mathbb{K}$ (either in $\mathbb{R}$ or $\mathbb{C}$), we have $\alpha x \in V$. Moreover, for all $x, y \in V$ we require*
$$\alpha(\beta x) = (\alpha\beta)x \qquad 1(x) = x$$
$$\alpha(x + y) = \alpha x + \alpha y \qquad (\alpha + \beta)x = \alpha x + \beta x.$$

The elements of a vector space are called **vectors***. If scalars are taken from $\mathbb{K} = \mathbb{R}$ we speak of real vector spaces, if scalars are allowed to be complex, i.e., $\mathbb{K} = \mathbb{C}$ we speak of complex vector spaces.*

We note that (see the following example) the Euclidean space $\mathbb{R}^n$ (often visualized with geometric

arrows also called "vectors") is an example of a vector spaces. The concept of vector spaces is more general as a set with an algebraic structure.

Example.

1. The space $\mathbb{R}^n$ of real (column) n-tuples

$$x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$$

is a vector space, where the operation $+$ is the componentwise addition and $\alpha x = \begin{pmatrix} \alpha x_1 \\ \vdots \\ \alpha x_n \end{pmatrix}$ for real scalars $\alpha \in \mathbb{R}$.

2. In the same way is the space $\mathbb{C}^n$ of complex n-tuples a vector spaces, where the scalars α can also be chosen from $\mathbb{C}$.

3. The set of all real polynomials of fixed degree $n \in \mathbb{N}$

$$P_n := \left\{ a_n x^n + a_{n-1} x^{n-1} + \cdots + a_0 \ : \ a_i \in \mathbb{R} \ \forall i = 0, \ldots, n \right\}$$

is a real vector space. ■

1.3 Banach and Hilbert spaces

In many applications (and theoretical results) it is required to have a quantitative measure of the size of objects or the distance between two objects. In the space $\mathbb{R}^n$ this is usually done by using the absolute value $|x| := \sqrt{x_1^2 + \cdots + x_n^2}$. In order to generalize this concept to other vector spaces, we introduce the concept of *norms* to measure lengths.

Definition 1.2. *A norm is a scalar-valued function $\| \cdot \| : V \to \mathbb{R}$, which acts on a vector space V, and satisfies*

1. $\|\alpha x\| = |\alpha| \, \|x\|$.
2. $\|x + y\| \leq \|x\| + \|y\|$.
3. $\|x\| \geq 0$ *for all* $x \in V$ *and* $\|x\| = 0 \iff x = 0$.

A vector space V together with a norm $\| \cdot \|$ is called a normed vector space $(V, \| \cdot \|)$.

Property 1 is called homogeneity, Property 2 is called triangle inequality and Property 3 is called definiteness.

Norms allow the measurement of lengths, but not of angles, for which the concept of *inner products*, which generalizes the scalar product $x \cdot y = x_1 y_1 + \cdots + x_n y_n$ in $\mathbb{R}^n$, can be used.

Definition 1.3. *An inner-product (also called scalar-product) is a scalar-valued function* $(\cdot,\cdot): V \times V \to \mathbb{K}$*, which acts on tuples of vectors of a vector space* V*, and satisfies*

1. $(x,y) = (y,x)^* = \overline{(y,x)}$ *(Here* * *and* $\overline{\ }$ *are two different notations for the complex conjugation).*
2. $(\alpha x + \beta y, z) = \alpha(x,z) + \beta(y,z) \qquad \alpha, \beta \in \mathbb{K}.$
3. $(x,x) \geq 0$ *for all* $x \in V$ *and* $(x,x) = 0 \Longleftrightarrow x = 0.$

A vector space V *together with an inner-product* $(\cdot,\cdot)$ *is called an inner-product space* $(V,(\cdot,\cdot))$*.*

Property 1. is called conjugate symmetry and for real vector spaces with scalars $\alpha, \beta \in \mathbb{R}$ inner products are by definition symmetric. Property 2. is called linearity and Property 3. is called positive-definiteness.

An inner-product always induces a norm by defining

$$\|x\| := (x,x)^{1/2}.$$

However, not all norms are induced by an inner-product.

Example. On the space $\mathbb{R}^n$, we already mentioned a norm induced by an inner-product, the absolute value $|\cdot|$, which is also called the Euclidean norm (or 2-norm)

$$\|x\|_2 := |x| = \sqrt{x_1^2 + \cdots + x_n^2} \quad x \in \mathbb{R}^n,$$

which is induced from the Euclidean scalar product

$$(x,y)_2 := x_1 y_1 + \cdots + x_n y_n.$$

A norm that is not induced by a scalar product is the maximum-norm defined by

$$\|x\|_\infty := \max\{|x_1|, |x_2|, \ldots, |x_n|\}.$$

We also mention that on $\mathbb{R}^n$ all norms are equivalent, i.e., for two different norms $\|\cdot\|_a, \|\cdot\|_b$, we have constants $0 < c \leq C$ such that

$$c\|x\|_a \leq \|x\|_b \leq C\|x\|_a \qquad \forall x \in \mathbb{R}^n.$$

In theoretical results the Euclidean norm $\|\cdot\|_2$ is commonly used. However, in many applications the maximum norm $\|\cdot\|_\infty$ is used, since e.g. engineers are more interested in the "worst case" error (so the maximal error) rather than a mean error. ■

On inner product spaces we have (additionally to the ones of Definition 1.2) several important geometric properties. In the following, let $(V,(\cdot,\cdot))$ be an inner product space.

- Parallelogram law:
  For all $x, y \in V$, we have

$$\|x+y\|^2 + \|x-y\|^2 = 2(\|x\|^2 + \|y\|^2).$$

- Schwarz inequality:
  For all $x, y \in V$, we have

  $$|(x, y)| \leq \|x\| \cdot \|y\|$$

  and

  $$|(x, y)| = \|x\| \cdot \|y\| \qquad \Longleftrightarrow \qquad x = cy.$$

- Measuring of angles:
  For all $x, y \in V$, we can define the angle α between the vectors x, y by

  $$\cos \alpha = \frac{(x, y)}{\|x\| \cdot \|y\|},$$

  which generalizes the formula in the Euclidean space by using the (general) inner product and norm.

  Schwarz inequality implies $(x, y) \leq \|x\|\|y\|$, which gives $\cos(\alpha) \in [-1, 1]$, so the formula for α is well-defined (up to the periodicity of the cosine).

- Orthogonality:
  Let $x, y \in V$. We call x, y **orthogonal**, if

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

  Note that using that in the above formula for the angle gives $\cos(\alpha) = 0$ or $\alpha = \frac{\pi}{2}$, which coincides with the geometric interpretation of orthogonality as vectors which span an angle of 90 degrees.

The concept of orthogonality is an important one in inner product spaces, as it allows us to establish so called orthonormal bases that span the inner product space. We call a set of $n \in \mathbb{N}$ vectors $\{x_1, \ldots, x_n\}$ **orthonormal**, if

$$(x_i, x_j) = \delta_{ij},$$

where δ_{ij} is the Kronecker delta defined by $\delta_{ij} = 0$ if $i \neq j$ and $\delta_{ij} = 1$ if $i = j$.
An example of a set of orthonormal vectors in the Euclidean space $\mathbb{R}^3$ is given by the unit vectors e_i, $i = 1, 2, 3$, give by $e_1 = (1, 0, 0)^T$, $e_2 = (0, 1, 0)^T$, $e_3 = (0, 0, 1)^T$.

Note that an orthonormal set is always **linearly independent**, which means that from

$$\alpha_1 x_1 + \alpha_2 x_2 + \cdots + \alpha_n x_n = 0$$

follows that $\alpha_1 = \alpha_2 = \cdots = \alpha_n = 0$.

Example. The vectors $\left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 2 \\ 0 \end{pmatrix} \right\}$ are not linearly independent, since

$$2 \begin{pmatrix} 1 \\ 0 \end{pmatrix} - 1 \begin{pmatrix} 2 \\ 0 \end{pmatrix} = 0,$$

but $\alpha_1 = 2$ and $\alpha_2 = 1$ are not zero.

The vectors $\left\{ \begin{pmatrix} 2 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 3 \end{pmatrix} \right\}$ are linearly independent, since

$$\alpha_1 \begin{pmatrix} 2 \\ 0 \end{pmatrix} + \alpha_2 \begin{pmatrix} 0 \\ 3 \end{pmatrix} = 0$$

means that $2\alpha_1 = 0$ (first component) and $3\alpha_2 = 0$ (second component), so $\alpha_1 = \alpha_2 = 0$. ■

Linear independency means that there is no "redundant" vector in the set $\{x_1, \ldots, x_n\}$ in the sense that this vector can be computed from the other vectors by simple scalar multiplications and additions.

Definition 1.4 (Basis of a finite dimensional vector space). *A* **basis** *of the vector space V is a set of linearly independent vectors $\{b_i : i = 1, \ldots, n\} \subset V$ such that every $x \in V$ can be written as a linear combination of the basis vectors, i.e.,*

$$x = \sum_{i=1}^{n} \alpha_i b_i.$$

The $\alpha_1, \ldots, \alpha_n$ are called the (unique) coordinates of the vector x with respect to the given basis and n is called the **dimension** *of the space V.*
If the basis $\{b_i : i = 1, \ldots, n\}$ is an orthonormal set, we call it an **orthonormal basis**.

Remark. With the help of the so-called Gram-Schmidt process, one can always construct an orthonormal basis out of a given basis. The Gram-Schmidt process works as follows: Let $\{b_1, \ldots, b_n\}$ be a set of linearly independent vectors of an inner-product space $(V, (\cdot, \cdot))$. Then, one can construct an orthonormal set $\{v_1, \ldots, v_n\}$ by the following algorithm:

$$\begin{aligned}
v_1 &= \frac{b_1}{\|b_1\|} \\
v_2 &= \frac{w_2}{\|w_2\|} \qquad \text{with } w_2 = b_2 - (v_1, b_2)v_1 \\
v_3 &= \frac{w_3}{\|w_3\|} \qquad \text{with } w_3 = b_3 - (v_1, b_3)v_1 - (v_2, b_3)v_2 \\
&\vdots \\
v_n &= \frac{w_n}{\|w_n\|} \qquad \text{with } w_n = b_n - \sum_{i=1}^{n-1} (v_i, b_n)v_i.
\end{aligned}$$

Example.

1. In $\mathbb{R}^n$, the set of unit vectors $\{e_i : i = 1, \dots, n\}$ given by $e_i = (0, \dots, 0, 1, 0, \dots, 0)^T$ are an orthonormal basis. However, orthonormal bases are not unique. For example, in $\mathbb{R}^2$ both the unit vectors $e_1 = (1, 0)^T$ and $e_2 = (0, 1)^T$ and the vectors $b_1 = \frac{1}{\sqrt{5}}(2, 1)^T$ and $b_2 = \frac{1}{\sqrt{5}}(-1, 2)^T$ form orthonormal bases.

2. On the space P_n of polynomials of maximal degree n, a basis is given by the monomials $\{1, x, \dots, x^n\}$. Using the square-integral inner-product on $(0, 1)$, i.e,

$$(p, q)_{L^2} = \int_0^1 p(x)q(x)dx,$$

one can easily verify that the monomials are not orthogonal. Applying the Gram-Schmidt process to the set $\{1, x, \dots, x^n\}$ produces a set of orthogonal polynomials, the so called Legendre polynomials (exercise!). ■

By definition, every set of n linearly independent vectors is a basis of a finite dimensional vector space spanned by these vectors (here, spanned means the set of all linear combinations).

Not all vector spaces have a *finite* basis (i.e., there exists $n \in \mathbb{N}$ and n linearly independent vectors that span the whole space). Those who do not, are called **infinite-dimensional**. In this lecture, we are also concerned with **countably infinite-dimensional spaces**, for which we introduce the concept of completeness. For finite dimensional spaces, the completeness of an orthonormal set may be characterized by the fact that it is not contained in any larger orthonormal set. For infinite-dimensional spaces, completeness is determined via the Cauchy-criterion[1].

Definition 1.5 (Complete normed space (Banach space)). *A normed space $(V, \|\cdot\|)$ is called complete, if every Cauchy sequence in the space is convergent in V.*

Note that inner product spaces are also normed spaces, which gives rise to the following definition.

Definition 1.6 (Hilbert space). *A complete inner product space $(V, (\cdot, \cdot))$ is called a* **Hilbert space**.

In the following, we present some examples of infinite-dimensional Hilbert spaces and also present an incomplete inner product space.

Example.

1. The space $\mathbb{R}^n$ (or $\mathbb{C}^n$) with the Euclidean inner-product $(\cdot, \cdot)_2$ is a Hilbert space. In fact, any finite-dimensional inner-product space is a Hilbert space.

2. The set of all square summable series $(x_n)_{n\in\mathbb{N}}$ with $x_n \in \mathbb{C}$, i.e.,

$$\sum_{n\in\mathbb{N}} |x_n|^2 < \infty$$

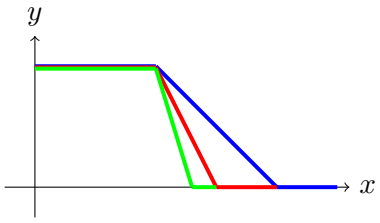
[1]Reminder: A Cauchy sequence is a sequence $(x_m)_{m\in\mathbb{N}}$ of elements $x_m \in V$ such that for all $\varepsilon > 0$ there exists a $N_0 \in \mathbb{N}$ such that $\|x_n - x_m\| < \varepsilon \qquad \forall m, n \geq N_0$.

is usually denoted by $\ell^2(\mathbb{N})$ and is a Hilbert space with the inner product

$$((x_n)_{n\in\mathbb{N}}, (y_n)_{n\in\mathbb{N}})_{\ell^2} := \sum_{n\in\mathbb{N}} x_n \overline{y_n}.$$

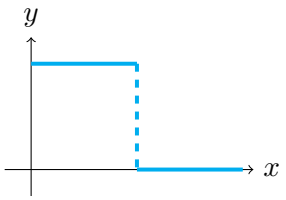
3. We also give an example of an incomplete inner product space V given by all real-valued continuous functions on $[0,1]$ with the inner-product $(\cdot,\cdot)_{L^2}$. Defining the sequence

$$f_n(x) = \begin{cases} 1 & \text{if } 0 \le x \le \frac{1}{2} \\ 1 - 2n(x - \frac{1}{2}) & \text{if } \frac{1}{2} < x \le \frac{1}{2n} + \frac{1}{2} \\ 0 & \text{if } \frac{1}{2n} + \frac{1}{2} < x \le 1 \end{cases}$$



then one can easily check that $(f_n)_{n\in\mathbb{N}}$ is a Cauchy sequence, but it converges (pointwise) to the function

$$f(x) = \begin{cases} 1 & \text{if } 0 \le x \le \frac{1}{2} \\ 0 & \text{if } \frac{1}{2} < x \le 1 \end{cases}$$



which is not continuous and hence not in V!

Similarly to Definition 1.4 we want to define a basis for general (infinite-dimensional) Hilbert spaces (in fact, one can prove that every Hilbert space has an orthonormal basis). The crucial ingredient here is the completeness of a given (infinite dimensional) set.

Definition 1.7. *We call an infinite set $\{b_i\}$ in a Hilbert space V* **complete***, if the only vector in V that is orthogonal to all b_i is the zero vector.*

A complete orthonormal set $\{b_i\}$ in a Hilbert space $(V,(\cdot,\cdot))$ is called a basis of V. For any $x \in V$, we have

$$\|x\|^2 = (x,x) = \sum_{i=1}^{\infty} |(b_i, x)|^2 .$$

This formula is also called Parseval identity.

Finally, we present some important properties and results for Hilbert spaces.

1. Pythagoras identity: Let $x, y \in V$ be orthogonal (i.e., $(x,y) = 0$), then

$$\|x+y\|^2 = \|x\|^2 + \|y\|^2.$$

2. Best approximation (closest point projection): Let S be a nonempty closed convex subset of an Hilbert space V and $x \in V$ be arbitrary. (S is convex $\Leftrightarrow$ for all $x, y \in S$: every convex combination $tx + (1-t)y \in S$ is in S for all $t \in [0,1]$). Then, there exists a unique point $y \in S$ that minimizes the distance (norm) between x and all points in S, i.e.,

$$\operatorname{dist}(x, S) := \min\{\|x - z\| \, : \, z \in S\} = \|x - y\|.$$

If S is a complete sub space of V, then y is characterized by the property $x - y \perp z$ for all $z \in S$.

The name "best approximation" comes from the following idea: Take a finite dimensional subspace $V_n \subset V$, then for a given $x \in V$ there is $x_n \in V_n$ with minimal distance ("error"), so you can approximate the space V by V_n. Since computers can only cope with finite dimensional problems, this basic idea of general approximation techniques (e.g. for PDEs in the next semester) is very useful.

3. Similarly as for a finite dimensional space, the inner product allows us to derive "coordinates" with respect to a given basis e_i of the Hilbert space.

In $\mathbb{R}^3$ an orthogonal basis is given by the unit vectors $e_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, e_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, e_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$.
Then, for a given vector $u \in \mathbb{R}^3$, we can obtain its i-th coordinate u_i by multiplication $u_i = u \cdot e_i$ with the i-th unit vector, e.g., for $u = \begin{pmatrix} 7 \\ 4 \\ 2 \end{pmatrix}$, we have

$$u_2 = 4 = \begin{pmatrix} 7 \\ 4 \\ 2 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 7 \cdot 0 + 4 \cdot 1 + 2 \cdot 0.$$

Note that we have the representation $u = \sum_{i=1}^{3} u_i e_i$. This idea directly translates to general inner-product spaces and bases, since we can write

$$f = \sum_{i=1}^{\infty} (f, b_i) b_i$$

and $f_i := (f, b_i)$ is the i-th coordinate of f with respect to the basis b_i and the inner-product $(\cdot, \cdot)$.

Chapter 2

Differentiation and Integration

In this chapter, we recall differentiation and integration in one variable as well as generalize both concepts to functions in multiple variables. Finally, we consider a different definition of integration, so called Lebesgue integrals.

2.1 Differentiation in one variable

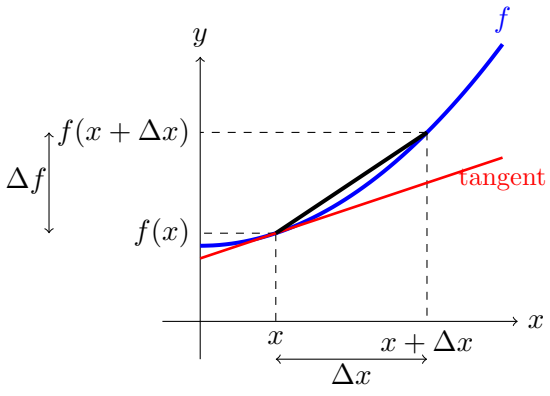
In this subsection, we consider scalar valued functions $f : \mathbb{R} \to \mathbb{R}$.

Definition 2.1. *The* **derivative** *of f at a fixed point $x_0 \in \mathbb{R}$ is defined as limit of the so called difference quotient*

$$f'(x_0) = \frac{df(x)}{dx}\Big|_{x_0} = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}, \tag{2.1}$$

where Δx denotes a small perturbation of the input around x_0. We call f differentiable at x_0, if the limit in (2.1) exists and we call a function **differentiable**, *if it is differentiable at every point, and write f' for the corresponding derivative (as a function).*

Note that we allow Δx to be positive or negative. In literature, oftentimes signs are fixed and the limit is either taken from the left- or the right-hand side, and a function there is called differentiable if the left- and right-limit both exist and are equal.



Defining $\Delta f := f(x + \Delta x) - f(x)$, we observe that close to x, the change Δf the results from a small change Δx can be written as

$$\Delta f \approx \frac{df(x)}{dx}\Delta x.$$

Taking the limit, i.e. making the change Δx infinitesimally small, which is denoted by dx, we obtain the **differential**

$$df = \frac{df(x)}{dx}dx,$$

which relates the infinitesimally small changes of the function df to the infinitesimally small changes in the argument dx (Note: this should be seen as notation).
If a function $f : \mathbb{R} \to \mathbb{R}$ is differentiable at x_0, we can approximate it (closely to x_0) by the linear function $g(x) = f(x_0) + f'(x_0)(x - x_0)$ (its tangent, see the drawing above). In fact, we can see

$$f(x_0 + \Delta x) - g(x_0) = f(x_0 + \Delta x) - (f(x_0) + f'(x_0)\Delta x) = \Delta x \underbrace{\left(\frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x} - f'(x_0)\right)}_{\to 0 \text{ for } \Delta x \to 0},$$

so the approximation gets better the smaller Δx gets (and the speed of convergence is at least Δx).

In the same way, we can derive higher-order derivatives inductively by applying the limit of the difference quotient to the derivative f', i.e.,

$$f''(x_0) = \lim_{\Delta x \to 0} \frac{f'(x_0 + \Delta x) - f'(x_0)}{\Delta x},$$

and we use the notation $f' = f^{(1)}$, $f'' = f^{(2)}$, ...

Example.

1. The function $f(x) = x^2$ is differentiable in every point $x \in \mathbb{R}$ since

   $$\lim_{\Delta x \to 0} \frac{(x + \Delta x)^2 - x^2}{\Delta x} = \lim_{\Delta x \to 0} \frac{2x\Delta x + (\Delta x)^2}{\Delta x} = \lim_{\Delta x \to 0} 2x + \Delta x = 2x$$

   and we have $f'(x) = 2x$.

2. The function $f(x) = |x|$ is not differentiable at $x = 0$ (on every other point it is differentiable), since taking at first only $\Delta x > 0$ (denoted by the limit going to 0^+), we get

   $$\lim_{\Delta x \to 0^+} \frac{f(0 + \Delta x) - f(0)}{\Delta x} = \lim_{\Delta x \to 0^+} \frac{|\Delta x|}{\Delta x} = \lim_{\Delta x \to 0^+} \frac{\Delta x}{\Delta x} = 1.$$

   However, taking only $\Delta x < 0$ (denoted by the limit going to 0^-) we obtain

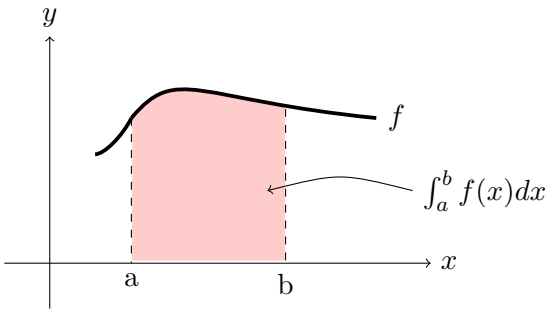
   $$\lim_{\Delta x \to 0^-} \frac{f(0 + \Delta x) - f(0)}{\Delta x} = \lim_{\Delta x \to 0^-} \frac{|\Delta x|}{\Delta x} = \lim_{\Delta x \to 0^-} \frac{-\Delta x}{\Delta x} = -1.$$

   Since the limits from these both directions are not equal, the function is not differentiable at $x = 0$. ■

Many dynamical processes in physics can be described by derivatives or equations containing derivatives (so called differential equations). The most classical example is, when $f(t)$ denotes the position of a particle at time t. Then, the derivative $\frac{df}{dt}$ describes the velocity of the particle and the second derivative $\frac{d^2f}{dt^2}$ describes the acceleration of the particle.

2.2 Integration in one variable

In this subsection, we are concerned with integration in one variable. The interpretation of the integral in one variable $\int_a^b f(x)dx$ as area under the curve f should be familiar.



In the following, we give a formal definition of this heuristic statement, which results in the definition of the Riemann integral. For many applications the "classical" Riemann integral should be applicable since the considered functions are continuous. However, in more involved cases, e.g. in advanced subjects in mathematical physics, one may encounter highly irregular functions for which we introduce the concept of Lebesgue integration later on.

Let $I = [a, b]$ be a given interval, which we divide into small subintervals $\Delta x_k = [x_k, x_{k+1}]$ such that

$$a = x_1 < x_2 < \cdots < x_{n+1} = b.$$

The finite set of points $\{x_i : i = 1, \ldots, n+1\}$ is called a partition P of I. Then, we can define the so called upper sum U_P and lower sum L_P of a function f by

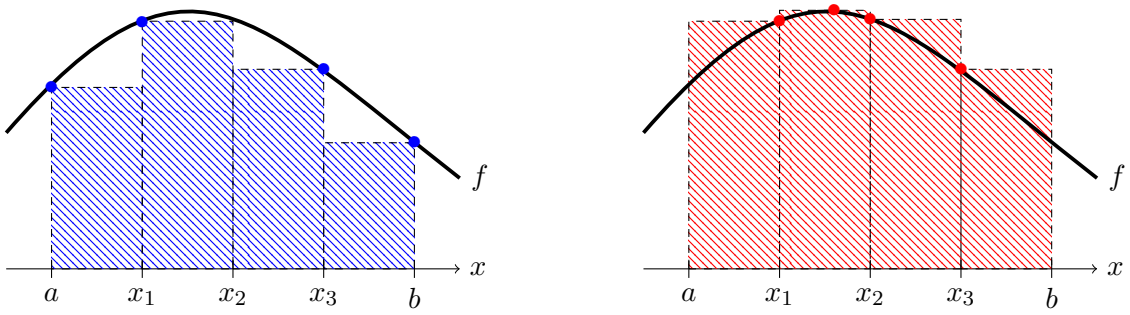
$$U_P(f) = \sum_{k=1}^{n} M_k(x_{k+1} - x_k), \qquad M_k := \sup_{[x_k, x_{k+1}]} f$$
$$L_P(f) = \sum_{k=1}^{n} m_k(x_{k+1} - x_k), \qquad m_k := \inf_{[x_k, x_{k+1}]} f.$$

If f is bounded on I, we obviously have $L_P(f) \leq U_P(f)$. If we now make the partition more and more fine, we can define the limit

$$U(f) = \liminf_{n\to\infty} U_P(f) = \inf\{U_P(f) : P \text{ is a partition of } I\},$$
$$L(f) = \limsup_{n\to\infty} L_P(f) = \sup\{L_P(f) : P \text{ is a partition of } I\},$$

where all possible choices of partitions P are taken into account.
If both the limits are equal, we call the limit the Riemann integral of f on I and write

$$\int_a^b f(x)dx = U(f) = L(f).$$



One can prove that the Riemann integral exists (i.e, $U(f) = L(f)$), if either

1. f is continuous in I;
2. f has only a finite number of discontinuities in I.

Example.

1. We show that the integral $\int_0^1 x\ dx$ exists with the definition of upper and lower sum. Let $0 < x_1 < \cdots < x_n = 1$ an uniformly spaced partition of $[0, 1]$, i.e., $x_k = k/n$. Then, since the function $f(x) = x$ is monotone increasing, the minimum on each interval $[x_i, x_{i+1}]$ is obtained on the left endpoint and the maximum is obtained on the right endpoint. We therefore compute

$$L_P(f) = \sum_{k=1}^{n} x_k(x_{k+1} - x_k) = \frac{1}{n}\sum_{k=1}^{n} \frac{k}{n} = \frac{n(n+1)}{2n^2} \longrightarrow \frac{1}{2},$$
$$U_P(f) = \sum_{k=1}^{n} x_{k+1}(x_{k+1} - x_k) = \frac{1}{n}\sum_{k=1}^{n} \frac{k+1}{n} = \frac{n(n+2)}{2n^2} \longrightarrow \frac{1}{2},$$

   so in the limit $n \to \infty$ (i.e. making the partition infinitesimally small), we obtain the value of the integral $\int_0^1 x\,dx = \frac{1}{2}$.

2. Let $I = [0, 1]$ and $g(x) = \begin{cases} 1 & \text{if } x \in \mathbb{Q} \\ 0 & \text{if } x \in \mathbb{R}\backslash\mathbb{Q} \end{cases}$. Since any partition consists of intervals that all include both rational and irrational numbers, we have

$$m_k = 0 \qquad \text{and} \qquad M_k = 1$$

   and therefore $U(g) = 1$ and $L(g) = 0$, so the Riemann integral does not exist! ■

We stress that the formal definitions for differentiation and integration are rather clumsy to work with. Thankfully, for many functions (such as polynomials, trigonometric functions, rational functions, etc.), there are rules to compute the derivatives and integrals that always hold true (such as $(x^n)' = nx^{n-1}$ or $\int x^n dx = \frac{x^{n+1}}{n+1}$) and should be known from previous lectures.

We finish the section on 1D-integration with the so called fundamental theorem of calculus, which states that integration and differentiation are (essentially - up to constants) inverse operations.

Theorem 2.2. *Let f be a continuous function on the interval $I = [a, b]$. Let F be defined as*

$$F(x) = \int_a^x f(s)\, ds \qquad \forall x \in I.$$

Then, F is continuous on I and differentiable on (a, b) with

$$F'(x) = f(x) \qquad \forall x \in (a, b).$$

2.3 Differentiation in more variables

We now generalize the concept of derivatives to functions in more variables. For simplicity, we start with the case of a function in two variables, i.e., $f = f(x, y) : \mathbb{R}^2 \to \mathbb{R}$. Analyzing formula (2.1) shows that we need to be more precise in the definition of the perturbation Δx. Taking only perturbations in one variable and keeping the other variable fixed leads to so called **partial derivatives** at the point (x_0, y_0) defined as

$$\frac{\partial f}{\partial x}(x_0, y_0) = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x, y_0) - f(x_0, y_0)}{\Delta x}$$

and

$$\frac{\partial f}{\partial y}(x_0, y_0) = \lim_{\Delta y \to 0} \frac{f(x_0, y_0 + \Delta y) - f(x_0, y_0)}{\Delta y}.$$

Oftentimes, the short notation $\partial_x f$ and $\partial_y f$ are used for the partial derivatives.

Definition 2.3. *The vector consisting of the partial derivatives*

$$\nabla f := \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right)^T$$

is called the **gradient** *of f (as differential operator this is also called the nabla operator).*

Similar to the case of one variable, second order and higher order derivatives can be defined inductively, and we write

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

The following theorem, called Schwarz's theorem, shows that the mixed second order derivatives are equal.

Theorem 2.4. *Let f be a two times differentiable function and all partial derivatives of second order be continuous. Then,*

$$\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right) = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right).$$

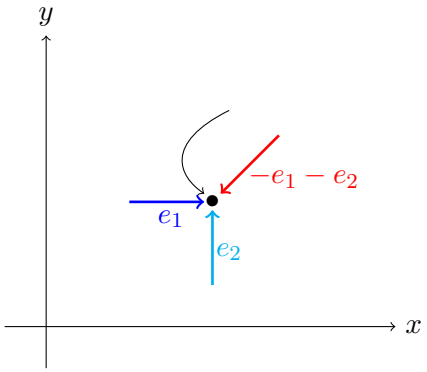
Example. We verify Schwarz theorem for the function $f(x,y) = 2x^3y^2 + y^3$.
Differentiation in x and y gives

$$\frac{\partial f}{\partial x} = 6x^2y^2$$
$$\frac{\partial f}{\partial y} = 4x^3y + 3y^2$$

and hence,

$$\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right) = \frac{\partial}{\partial y}(6x^2y^2) = 12x^2y = \frac{\partial}{\partial x}(4x^3y + 3y^2) = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right).$$

Partial derivatives only describe the rate of change of f into one fixed direction (either in the x or y direction). However in $\mathbb{R}^2$ there are infinitely many different directions leading to a point (see the drawing below).



Definition 2.5. *Fixing an arbitrary vector $v \in \mathbb{R}^2$ (also called direction), the* **directional derivative** *in direction v of a function $f : \mathbb{R}^2 \to \mathbb{R}$ is defined by*

$$\frac{\partial f}{\partial \nu} = \partial_\nu f = \lim_{h\to 0} \frac{f((x_0,y_0) + h\nu) - f(x_0,y_0)}{h}.$$

We note that the value of the limit depends on the length $|v|$, so it is convenient to work with unit vectors (i.e. $|v| = 1$). Comparing the definition of the directional derivative and the partial derivatives, we can see that

$$\frac{\partial f}{\partial e_1} = \frac{\partial f}{\partial x} \qquad \text{and} \qquad \frac{\partial f}{\partial e_2} = \frac{\partial f}{\partial y}$$

with the Cartesian basis vectors e_1, e_2.

In higher dimensions, one can also ask the question similar to the approximation of a function by its tangent: is it is also possible to approximate a function $f(x,y)$ by a linear function, which leads to the following definition.

Definition 2.6. *A function $f : \mathbb{R}^2 \to \mathbb{R}$ is called* **(totally) differentiable** *in the point $(x_0, y_0)^T$, if there exists a linear function*

$$g(x, y) = f(x_0, y_0) + df \cdot \left[\begin{pmatrix} x \\ y \end{pmatrix} - \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} \right],$$

where $df \in \mathbb{R}^2$ is a vector (depending on x_0, y_0) that approximates f close to (x_0, y_0), i.e.,

$$\lim_{|z| \to 0} \frac{f((x_0, y_0) + z) - g((x_0, y_0) + z)}{|z|} = 0.$$

If a function is totally differentiable, then

$$df = \nabla f(x_0, y_0),$$

and the directional derivative can then also be written as

$$\frac{\partial f}{\partial \nu} = \nabla f \cdot \nu = \nu_1 \frac{\partial f}{\partial x} + \nu_2 \frac{\partial f}{\partial y}.$$

However, there are functions (see the following example), where every partial derivative exists, but there exists no linear approximation to f! This shows that total differentiability is a stronger concept than partial differentiability in the sense that for total differentiability all possible directions need to be taken into account (not only those along the coordinate axes).

Example. The function

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

is differentiable everywhere aside from the point $(0, 0)$. There, we compute the partial derivatives

$$\frac{\partial f}{\partial x}(0, 0) = \lim_{\Delta x \to 0} \frac{f(0 + \Delta x, 0) - f(0, 0)}{\Delta x} = \lim_{\Delta x \to 0} \frac{0}{\Delta x} = 0,$$
$$\frac{\partial f}{\partial y}(0, 0) = \lim_{\Delta y \to 0} \frac{f(0, 0 + \Delta y) - f(0, 0)}{\Delta y} = \lim_{\Delta y \to 0} \frac{0}{\Delta y} = 0,$$

so the partial derivatives exist. However, the directional derivative along the direction $\nu = (1, 1)^T$ does not exist, since

$$\frac{\partial f}{\partial \nu}(0, 0) = \lim_{h \to 0} \frac{f(0 + h\nu_1, 0 + h\nu_2) - f(0, 0)}{h} = \lim_{\Delta x \to 0} \frac{h^2}{2h^2} \frac{1}{h} = \infty.$$

In fact, this example fails, since f is not continuous at the origin along directions that are not Cartesian unit vectors. However, there are other examples of continuous functions that have partial derivatives but are not totally differentiable. ■

The following theorem is very useful, since it presents a criterion, when a function is totally differentiable by only studying the partial derivatives.

Theorem 2.7. *Let $f : \mathbb{R}^2 \to \mathbb{R}$ and assume that all partial derivatives exist and are continuous at a point $(x_0, y_0)^T$. Then, f is totally differentiable at $(x_0, y_0)^T$.*

The above definitions and results can be directly transfered to the case of functions in n-variables, $f : \mathbb{R}^n \to \mathbb{R}$. In that case, the partial derivative with respect to the variable x_i is defined as

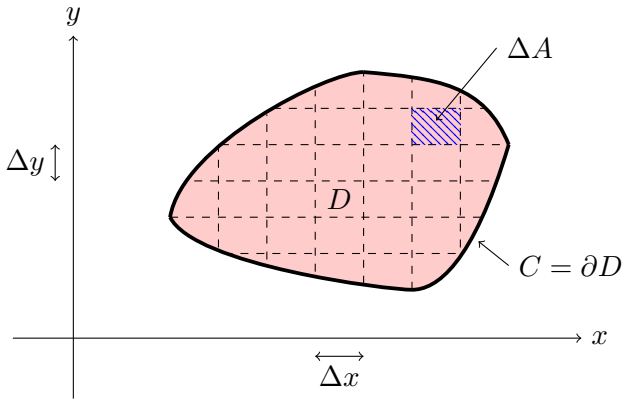
$$\frac{\partial f(x_1, \ldots, x_n)}{\partial x_i} = \lim_{\Delta x_i \to 0} \frac{f(x_1, \ldots, x_i + \Delta x_i, \ldots, x_n) - f(x_1, \ldots, x_i, \ldots, x_n)}{\Delta x_i}.$$

2.4 Multiple integrals

We now look at integration in multiple variables.

2.4.1 Double integrals

Let D be a given region in $\mathbb{R}^2$ with the boundary $C = \partial D$.



As in the 1D-case we divide D into N-subregions D_k with area ΔA_k for $k = 1, \ldots, N$ and let (x_k, y_k) be a point in D_k. For a function $f : \mathbb{R}^2 \to \mathbb{R}$, we define the sum

$$S = \sum_{k=1}^{N} f(x_k, y_k) \Delta A_k.$$

Taking the limit $N \to \infty$ (which means convergence of the areas $\Delta A_k \to 0$) gives a definition of the double integral: If the limit exists, it is called the double integral of f on D and we denote it by

$$\int_D f(x, y)\, dA.$$

Here, dA stands for the element of area in the xy-plane. If we choose for example small axis-parallel rectangles, we have $\Delta A = \Delta x \Delta y$ and taking the limit $\Delta x, \Delta y \to 0$ motivates writing

$$\int_D f(x, y)\, dA = \int \int_D f(x, y)\, dxdy.$$

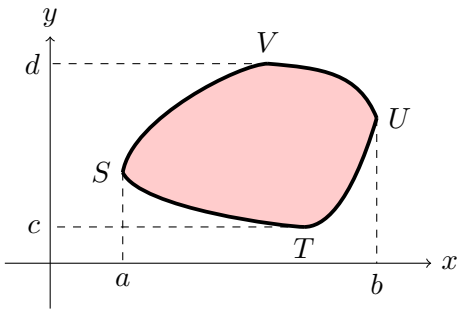
One way to evaluate the above integral is first to sum up contributions in a horizontal direction and then combine these contributions to make up the whole region D. This leads to

$$I = \int_{y=c}^{y=d} \left(\int_{x=x_1(y)}^{x=x_2(y)} f(x,y)\, dx \right) dy,$$

where $x_1(y)$ and $x_2(y)$ describe the boundary of the region D. (In the image curves connecting TSV and TUV). Similarly by switching the roles of x and y, we may write

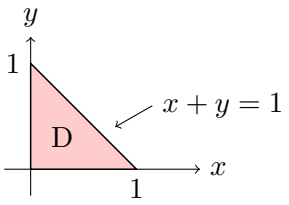
$$I = \int_{x=a}^{x=b} \left(\int_{y=y_1(x)}^{y=y_2(x)} f(x,y)\, dy \right) dx,$$

where $y_1(x)$ and $y_2(x)$ describe the boundary of the region D (in the image the curves STU and SVU).



Example. Let D be the triangle bounded by the lines $x = 0, y = 0, x + y = 1$. We want to evaluate

$$I = \int_D x^2 y\, dA.$$



We compute

$$I = \int_0^1 \int_0^{1-x} x^2 y\, dy dx = \int_0^1 \frac{x^2 y^2}{2}\Big|_0^{1-x} dx = \int_0^1 \frac{x^2(1-x)^2}{2} dx = \frac{1}{60}.$$

Similarly, switching the roles of x, y, we get

$$I = \int_0^1 \int_0^{1-y} x^2 y\, dx dy = \int_0^1 \frac{x^3 y}{3}\Big|_0^{1-y} dy = \int_0^1 \frac{(1-y)^3 y}{3} dy = \frac{1}{60}.$$

2.4.2 Triple integrals

The same ideas for double integrals can also be applied for multiple integrals. Triple integrals are commonly used for computations of volumes.
Taking a region D and subdividing it into small volumes ΔV_k, the limit of the Riemann sum

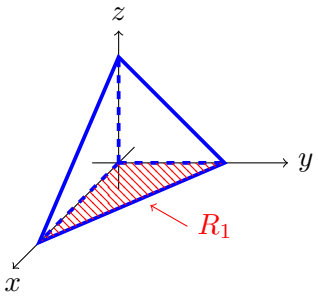
$$S = \sum_{k=1}^{N} f(x_k, y_k, z_k)\Delta V_k$$

(if it exists) defines the triple integral

$$\int_D f(x,y,z)\, dV = \int\int\int_D f(x,y,z)\, dxdydz.$$

For the evaluation, we can use the same idea as for the case of the double integrals.

Example. We want to compute the volume of a tetrahedron bounded by the surfaces $x = 0, y = 0, z = 0$ and the plane $\frac{x}{a} + \frac{y}{b} + \frac{z}{c} = 1$.



To obtain the volume, we integrate the function $f(x, y, z) = 1$ over the tetrahedron, which gives

$$\begin{aligned} V &= \int_{R_1} \left(\int_0^{c(1-y/b-x/a)} 1 dz \right) dA = \int_0^a \int_0^{b-bx/a} \int_0^{c(1-y/b-x/a)} 1\, dzdydx \\ &= \int_0^a \int_0^{b-bx/a} c\left(1 - \frac{y}{b} - \frac{x}{a}\right) dydx = \frac{abc}{6}. \end{aligned}$$

2.5 The Lebesgue integral

The Riemann integral is very useful for many practical applications in physics and engineering as most of the time continuous functions are studied. However, e.g. in statistical physics, highly irregular functions, such as the characteristic function of the rational numbers in a previous example may appear, for which the Riemann integral does not exist. This example motivates the need for a different definition of integration to give meaning to the integral of such functions.

The mathematical problem of the previous example is that the length of the set of rational numbers is not well-defined. The main idea of the so called Lebesgue integral is to "generalize" the length of an interval (or area, volume in higher dimensions).

In order to do this, we define a so called measure (which essentially is a function acting on sets that generalizes the length of the set).

Definition 2.8. *A measure is a real valued function μ (that can also be ∞) that acts on sets, i.e., $\mu = \mu(X)$, where X is a set of points (e.g. an interval) that satisfies*

1. *There holds $\mu(X) \geq 0$ and, if $X = \emptyset$, we have $\mu(X) = 0$.*
2. *The measure of two non-overlapping sets is equal to the sum of the measure of the sets, i.e.,*

$$\mu(X_1 \cup X_2) = \mu(X_1) + \mu(X_2), \qquad X_1 \cap X_2 = \emptyset.$$

We give some simple examples of measures in the following. An example of a measure in physics is given by the spatial distribution of mass.

Example.

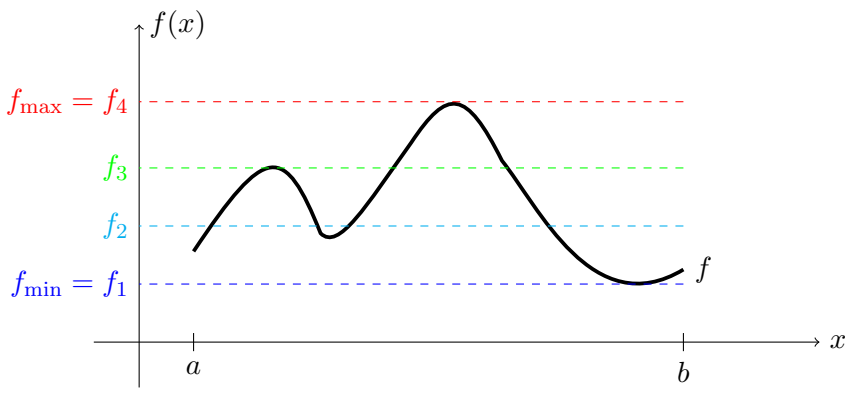
1. Point mass at 0: The function $\delta_0(X) := \begin{cases} 1 & \text{if } 0 \in X \\ 0 & \text{otherwise} \end{cases}$ defines a measure.
2. The counting measure: $\mu(X) = \begin{cases} \#X & \text{if } X \text{ is finite} \\ \infty & \text{otherwise} \end{cases}$.

   Here, $\#X$ denotes the number of elements in the finite set X.
3. Gaussian probability measure: The Gaussian measure of a set $X \subset \mathbb{R}$ is given by the integral

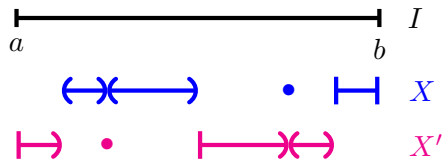
$$\mu(X) = \frac{1}{\sqrt{2\pi}} \int_X \exp(-x^2/2)\, dx.$$

■

The idea of the Lebesgue integral is rather than finding a partition of the x-axis (the input values of the function), we take a partition of y-axis (the function values), see the drawing below. Therefore, the essential task is finding a measure for sets of arguments of a function f that produce similar values. In particular, if a set consists of too many points of discontinuity (of the given function), we also need to give it a proper measure.

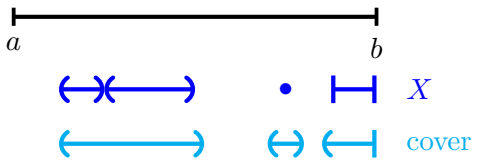


As a simple example, we consider the interval $I = [a, b]$ of length $L = b - a$. Now, let X be a set consisting of a union of some points (this can be a union of intervals and single points) and write $X' = I \setminus X$ for the complementary set (i.e, all points of I that are not in X).



In the following, we want to introduce the so called Lebesgue measure of a set $X \subset [a, b]$. For this we need to cover X by non-overlapping (semi-)open intervals (closed only at a or b) $\Lambda_i \subset [a, b]$ such that

$$X \subset \Lambda_1 \cup \Lambda_2 \cup \dots .$$



Now, let ℓ_i be the length of Λ_i. Then, we have $0 \leq \sum_i \ell_i \leq L$. The value of the sum $\sum_i \ell_i$ obviously depends on the cover $\{\Lambda_i\}$. Taking the "smallest" cover, i.e., we infimize the sum, leads to the so called outer measure of X and is denoted by

$$\mu_{\text{out}}(X) = \inf_{\text{covers}} \sum_i \ell_i.$$

For the complimentary set X', we can do the same and compute $\mu_{\text{out}}(X')$. Using this, we can define the inner measure of X by

$$\mu_{\text{in}}(X) = L - \mu_{\text{out}}(X').$$

There always holds $0 \leq \mu_{\text{in}}(X) \leq \mu_{\text{out}}(X)$, and if there holds equality, we have the value of the Lebesgue measure.

Definition 2.9. *A set X is called* **Lebesgue measurable**, *if $\mu_{\text{in}}(X) = \mu_{\text{out}}(X)$, and the value*

$$\mu(X) := \mu_{\text{in}}(X) = \mu_{\text{out}}(X)$$

is called the **Lebesgue measure** *of X.*

We note that points $X = \{x_0\}$ with $x_0 \in I$ are measurable since

$$\mu_{\text{in}}(\{x_0\}) = 0 = \mu_{\text{out}}(\{x_0\})$$

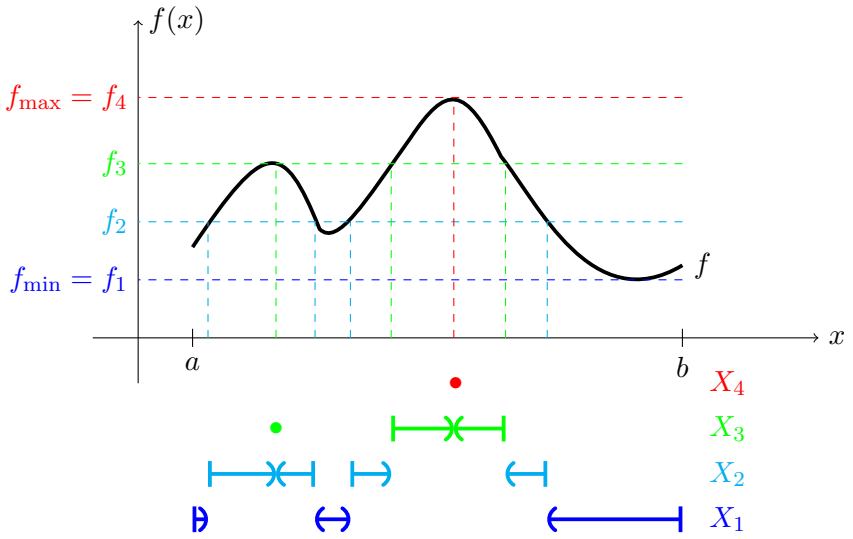
and intervals $X = (c, d)$ have its length as Lebesgue measure $\mu(X) = d - c$.

Now, we can define the Lebesgue integral. Let f be a bounded non-negative function, i.e., $0 \leq f_{\min} \leq f(x) \leq f_{\max}$. As explained in the drawing below, in comparison with the Riemann-integral,

we – this time – partition the y-axis, i.e., the function values, rather than the x-axis. Taking values $\{f_k \ : \ k = 1, \ldots, n\}$ with $f_1 = f_{\min}$ and $f_n = f_{\max}$, there exist sets $X_i \subset [a, b]$ such that

$$f_k \leq f(x) < f_{k+1} \qquad \forall x \in X_k, \qquad 1 \leq k \leq n-1$$

and a set X_n with $f(x) = f_n = f_{\max}$.



For each X_k, we use the Lebesgue measure to define the size of X_k and add up the products of the function value with the measure to obtain the Lebesgue sum

$$\sum_{k=1}^{n} f_k \cdot \mu(X_k).$$

Now, if we infinitesimally refine the partition f_k of the y-axis such that $\max |f_k - f_{k+1}| \to 0$, the limit of the Lebesgue sum defines the Lebesgue integral.

Definition 2.10. *Let f be a non-negative function and $\{f_k\}$ be an arbitrary partition of $[f_{\min}, f_{\max}]$. Then, if the limit*

$$\lim_{\max|f_k - f_{k+1}| \to 0} \sum_{k=1}^{n} f_k \cdot \mu(X_k) =: \int_X f d\mu$$

over all possible partitions exists, we call the function f **Lebesgue integrable** *and the value of the limit the* **Lebesgue integral** $\int_X f d\mu$.

Some important properties of Lebesgue integrals are:

1. If $\mu(X) = 0$ then $\int_X f(x)d\mu = 0$ (by definition since all Lebesgue sums are zero).

2. If f is not non-negative, then we can define

$$\int_X f d\mu := \int_X f^+ d\mu - \int_X f^- d\mu,$$

where $f^+(x) := \max\{f(x), 0\}$ and $f^-(x) := -\min\{f(x), 0\}$, and both integrals on the right-hand side contain non-negative functions.

3. Monotone convergence theorem: Let $(f_n)_{n\in\mathbb{N}}$ be a sequence of functions $0 \leq f_n \leq f_{n+1}$ for all $n \leq 1$ and $f(x) := \lim_{n\in\mathbb{N}} f_n(x)$. Then,

$$\lim_{n\in\mathbb{N}} \int_X f_n \, d\mu = \int_X \lim_{n\in\mathbb{N}} f_n \, d\mu = \int_X f \, d\mu.$$

4. Dominated convergence theorem: Let $(f_n)_{n\in\mathbb{N}}$ be a sequence of functions and $f(x) := \lim_{n\in\mathbb{N}} f_n(x)$. Assume that there exists a non-negative function g that is Lebesgue integrable such that $|f_n(x)| \leq g$ for all $n \in \mathbb{N}$. Then,

$$\lim_{n\in\mathbb{N}} \int_X f_n \, d\mu = \int_X \lim_{n\in\mathbb{N}} f_n \, d\mu = \int_X f \, d\mu.$$

Hence, much weaker conditions are needed to interchange the limit and the integral compared to Riemann integrals.

Remark. Since single points have Lebesgue measure 0, by 1. of the above properties, we have that the value of the Lebesgue integral does not change, when one changes the function f at a single point. Therefore, in the sense of Lebesgue integration, functions that only differ on countably many points are equal, which in literature is denoted as the concept of equality almost everywhere.

Example.

1. If a function f is Riemann integrable on $[a, b]$, it is also Lebesgue integrable and the value of the integrals are the same.

2. We now can give meaning to the integral over the characteristic function of the rational numbers of the previous subsection. Since every point has Lebesgue measure zero and $\mu(X_1 \cup X_2) = \mu(X_1) + \mu(X_2)$, we get that every countable (infinite) set of points has measure 0, which tells us that $\mu(\mathbb{Q}) = 0$.

   The definition of the Lebesgue sum directly gives with $X_1 = [0, 1]\backslash\mathbb{Q}$ and $X_n = \mathbb{Q}$ and $X_k = \emptyset$ for any arbitrary partition of $[f_{\min}, f_{\max}] = [0, 1]$ that

$$\sum_{k=1}^{n} f_k \cdot \mu(X_k) = 0 \cdot \mu(X_1) + 1 \cdot \mu(X_n) = 0 \cdot 1 + 1 \cdot 0 = 0.$$

■

Example. The set of square integrable functions (w.r.t. the Lebesgue-integral) on $[a, b]$, i.e., all functions satisfying

$$\|f\|_{L^2}^2 := \int_a^b |f(x)|^2 \, d\mu < \infty$$

is denoted by $L^2([a, b])$ and is a Hilbert space with the inner product

$$(f, g)_{L^2} := \int_a^b f(x)g(x)d\mu.$$

This can be proven with the help of the monotone convergence theorem. ■

Chapter 3

Vector calculus

In the previous chapter, we introduced differentiation and integration of scalar valued functions. In the following, we want to generalize the previous results to vector valued functions. Therefore, we now focus on vector quantities and present several geometric tools.
Before we start, we recall some basic computational rules for vectors. We recall the scalar product in $\mathbb{R}^3$ (previously denoted by $(\cdot,\cdot)_2$), which we will abbreviate with the notation $\cdot$ as

$$x \cdot y = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \cdot \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = x_1y_1 + x_2y_2 + x_3y_3.$$

Additionally, we introduce the cross product

$$x \times y = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \times \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} x_2y_3 - x_3y_2 \\ x_3y_1 - x_1y_3 \\ x_1y_2 - x_2y_1 \end{pmatrix}.$$

There hold the computational rules

$$\begin{aligned} x \times x &= 0 \\ x \times y &= -(y \times x) \\ x \times (y + z) &= x \times y + x \times z \\ x \cdot (y \times z) &= y \cdot (z \times x) = z \cdot (x \times y). \end{aligned}$$

3.1 Differentiation and integration of vector fields

A vector valued function

$$f : \mathbb{R}^n \to \mathbb{R}^m, \quad f(x) = \begin{pmatrix} f_1(x_1, \ldots, x_n) \\ \vdots \\ f_m(x_1, \ldots, x_n) \end{pmatrix}$$

is called vector field and consists of m scalar valued coordinate functions f_m. Vector field commonly appear in physics, e.g., as force fields or velocity fields, when physical effects appear in multiple coordinate directions.

In the same way as for scalar valued functions, we can define partial derivatives and the total derivative of a vector field by working with the component functions. We illustrate the idea for $n = 1$ and $m = 3$, so we take a function $f : \mathbb{R} \to \mathbb{R}^3$. As in the case for scalar functions, we can define the derivative of f by

$$\frac{df}{dx} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

and call the function differentiable if the limit exists. Here, $f(x + \Delta x) - f(x)$ is a vector in $\mathbb{R}^3$ and the difference and quotient are taken componentwise. Writing $f(x) = f_1(x)e_1 + f_2(x)e_2 + f_3(x)e_3$ with the Cartesian unit vectors e_i, we see that

$$\frac{df}{dx} = \sum_{i=1}^{3} \frac{df_i}{dx} e_i.$$

The following computational rules hold for the derivatives of vector valued functions in one variable. Let $\phi(x)$ be a scalar function and $f(x), g(x)$ be vector valued functions. Then, we have

$$\begin{aligned}
\frac{d}{dx}(\phi f) &= \phi \frac{df}{dx} + \frac{d\phi}{dx} f \\
\frac{d}{dx}(f \cdot g) &= f \cdot \frac{dg}{dx} + \frac{df}{dx} \cdot g \\
\frac{d}{dx}(f \times g) &= f \times \frac{dg}{dx} + \frac{df}{dx} \times g.
\end{aligned}$$

Moreover, if f depends on $\phi(x)$, hence $f(\phi(x))$, the classical chain rule gives

$$\frac{d}{dx}\left[f(\phi(x))\right] = \frac{df}{d\phi}\frac{d\phi}{dx}.$$

Example.

1. The simplest application of the above theory is finding the velocity (and acceleration) of a particle in space. Let t be a parameter (time) and

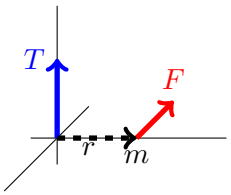
   $$r(t) = x_1(t)e_1 + x_2(t)e_2 + x_3(t)e_3$$

   be the location for a fixed t. Then, the velocity of the particle is given by

   $$\frac{dr}{dt} = \frac{dx_1}{dt}e_1 + \frac{dx_2}{dt}e_2 + \frac{dx_3}{dt}e_3.$$

2. A mass particle m at the point r (relative to 0) experiences a force F that creates some movement at 0 given by $T = r \times F$. The angular movement of m at 0 is given by $L = r \times mv$, where mv is the momentum. Then, the change of L is equivalent to T as

   $$\frac{d}{dt}L = \frac{d}{dt}(r \times mv) = \frac{dr}{dt} \times (mv) + r \times \frac{d(mv)}{dt}.$$



Newton's second law now gives $\frac{d(mv)}{dt} = F$ and using that $\frac{dr}{dt} = v$ and that $v \times (mv) = 0$, we get

$$\frac{d}{dt}L = v \times (mv) + r \times F = T.$$

■

The same concepts also apply to functions $f : \mathbb{R}^n \to \mathbb{R}^m$ in several variables, as we can define the partial derivatives

$$\frac{\partial f}{\partial x_i} = \sum_{\ell=1}^{m} \frac{\partial f_\ell}{\partial x_i} e_\ell.$$

For scalar valued functions (i.e. $m = 1$) this is consistent with the definition of the gradient $\nabla f = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \ldots, \frac{\partial f}{\partial x_n}\right)^T$. The generalization of the gradient to the case $m > 1$ is called the **Jacobi matrix** (or Jacobian) $Df \in \mathbb{R}^{n \times m}$ given by

$$(Df)_{ij} := \frac{\partial f_j}{\partial x_i},$$

hence for the case $m = n = 3$ the Jacobi matrix (sometimes also called Jf) is given by

$$Df = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_2}{\partial x_1} & \frac{\partial f_3}{\partial x_1} \\ \frac{\partial f_1}{\partial x_2} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_3}{\partial x_2} \\ \frac{\partial f_1}{\partial x_3} & \frac{\partial f_2}{\partial x_3} & \frac{\partial f_3}{\partial x_3} \end{pmatrix},$$

so one can see that the i-th column of the Jacobi matrix is the gradient ∇f_i of the component functions of f_i and the i-th row is the partial derivative $\frac{\partial f}{\partial x_i}$.

Theses ideas can also be applied on differentials, then the infinitesimal change of the function f is given by

$$df = \sum_{j=1}^{n} \frac{\partial f}{\partial x_j} dx_j.$$

Integration of vector valued functions (in one variable) follows more or less by the same rules as for scalar valued functions, we only have to keep in mind that the integrals and the constants that

might appear (seeing integration as the inverse action of differentiation) must be the same nature as the vector field, i.e., for $f : \mathbb{R} \to \mathbb{R}^2$ with $f(x) = \frac{dF(x)}{dx}$, we have

$$\int f(x)dx = F(x) + c \qquad \text{with } \ c \in \mathbb{R}^2$$

and

$$\int_a^b f(x)dx = F(b) - F(a).$$

For other - more involved - problems concerning integration, we refer to the following subsections.

3.2 Vector operators

In the following, we introduce certain differential operators (mainly in $\mathbb{R}^3$) that are widely used in physical sciences.

Remark. An **operator** is a function that acts on functions. An example is the (scalar) differential operator $\frac{d}{dx}$ that takes a function $f : \mathbb{R} \to \mathbb{R}$ as input and produces a function $\frac{d}{dx}f : \mathbb{R} \to \mathbb{R}$. Operators that involve differentiation are called **differential operators**.

Previously, we already introduced the gradient, which is recalled in the following definition.

Definition 3.1. *The* **gradient***, also called nabla operator,* ∇ *is given by*

$$\nabla := \sum e_i \frac{\partial}{\partial x_i}.$$

For scalar valued functions $\phi : \mathbb{R} \to \mathbb{R}^3$ *this reads as*

$$\nabla\phi = (\partial_{x_1}\phi, \partial_{x_2}\phi, \partial_{x_3}\phi)^T.$$

Moreover, we also introduced the directional derivative $\nabla\phi \cdot \nu$ in direction ν, which represents the change of the function in one given direction ν (and therefore is a scalar).

Definition 3.2. *Let* $\psi : \mathbb{R}^n \to \mathbb{R}^n$ *be a given vector field. The* **divergence** *of* ψ *is given by*

$$\operatorname{div} \psi = \nabla \cdot \psi = \frac{\partial \psi_1}{\partial x_1} + \frac{\partial \psi_2}{\partial x_2} + \cdots + \frac{\partial \psi_n}{\partial x_n}$$

hence

$$\operatorname{div} = \sum_{i=1}^{n} \frac{\partial (\cdot)_i}{\partial x_i}.$$

The divergence operator plays, for example, an important role in fluid dynamics as the velocity field u and the density ρ of a fluid have the relation

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho u) = 0,$$

which corresponds to the conservation of mass and will be derived more precisely later on.

Now, let the vector field ψ be given as the gradient of a scalar function, i.e., $\psi = \nabla\phi$, then we have

$$\operatorname{div}(\psi) = \operatorname{div}(\nabla\phi) = \frac{\partial^2\phi}{\partial x_1^2} + \frac{\partial^2\phi}{\partial x_2^2} + \cdots + \frac{\partial^2\phi}{\partial x_n^2}.$$

The right-hand side contains a very famous operator.

Definition 3.3. *The Laplace operator Δ is given by*

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

For a scalar function $\phi : \mathbb{R}^3 \to \mathbb{R}$ this reads as

$$\Delta\phi = \frac{\partial^2\phi}{\partial x_1^2} + \frac{\partial^2\phi}{\partial x_2^2} + \frac{\partial^2\phi}{\partial x_3^2}$$

and for vector valued functions we have the application of the Laplace operator to each (scalar) component function.

It plays an important role in many equations governed by physical laws, such as diffusion processes, heat transfer, motion of waves, etc.

Definition 3.4. *The* **curl operator** *(sometimes also called* rot*) is given by*

$$\operatorname{curl} = \nabla\times$$

For a vector field $\psi : \mathbb{R}^3 \to \mathbb{R}^3$ this reads as

$$\operatorname{curl}\psi = \nabla \times \psi = \begin{pmatrix} \partial_{x_1} \\ \partial_{x_2} \\ \partial_{x_3} \end{pmatrix} \times \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} = \left(\frac{\partial\psi_3}{\partial x_2} - \frac{\partial\psi_2}{\partial x_3}, \frac{\partial\psi_1}{\partial x_3} - \frac{\partial\psi_3}{\partial x_1}, \frac{\partial\psi_2}{\partial x_1} - \frac{\partial\psi_1}{\partial x_2} \right)^T.$$

The curl operator appears for example in electromagnetics when studying the Maxwell equations or in fluid dynamics, where it measures the angular velocity of a fluid.

Remark. In contrast to the gradient, divergence and Laplace operator, the curl operator is previously only defined for vector fields in $\mathbb{R}^3$ since it uses the cross product. However, it is also possible to define the curl operator in $\mathbb{R}^2$ for $\psi : \mathbb{R}^2 \to \mathbb{R}^2$ by setting

$$\operatorname{curl}\psi = \frac{\partial\psi_2}{\partial x_1} - \frac{\partial\psi_1}{\partial x_2},$$

which is a scalar function. ■

Example.

- Let $\phi(x, y, z) = xy^2z^3$, then

$$\nabla\phi = (y^2z^3, 2xyz^3, 3xy^2z^2)^T$$

and

$$\begin{aligned}\Delta\phi = \operatorname{div}(\nabla\phi) &= \operatorname{div}\left((y^2z^3, 2xyz^3, 3xy^2z^2)^T\right) \\ &= 2xz^3 + 6xy^2z\end{aligned}$$

- Let $\psi(x, y, z) = (x^2y^2, y^2z^2, x^2y^2)^T$, then

$$\operatorname{div}\psi = 2xy^2 + 2yz^2$$

and

$$\operatorname{curl}\psi = (2x^2y - 2y^2z, -2xy^2, -2x^2y).$$

■

For the presented operators many identities hold. Two important ones are

$$\begin{aligned}\operatorname{curl}(\nabla\psi) = \nabla \times \nabla\psi &= 0 \\ \operatorname{div}(\operatorname{curl}\psi) &= 0.\end{aligned}$$

The first one will appear again in the next section when evaluating path integrals.
Moreover, as all operators are differential operators, we have the standard product and chain rules. For example, for scalar functions ϕ, ζ and a vector valued function ψ, we have

$$\begin{aligned}\nabla(\phi\zeta) &= \nabla\phi\zeta + \phi\nabla\zeta \\ \operatorname{div}(\phi\psi) &= \phi\operatorname{div}(\psi) + \nabla\phi \cdot \psi.\end{aligned}$$

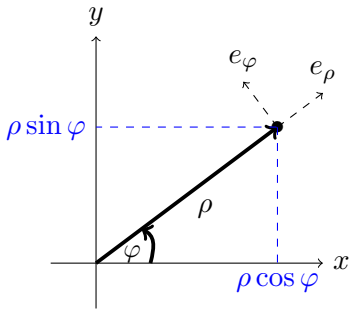
3.3 Non-cartesian coordinate systems

The operators of the previous chapter are all defined with respect to the Cartesian coordinate system. Here, we implicitly used the crucial property that the coordinate system is constant at every point. However, in many physical applications a different coordinate system is used, such as polar, cylindric or spherical coordinates.

Polar coordinates

We start with the 2D-case of polar coordinates. For every point $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \in \mathbb{R}^2$ there exists a unique magintude ρ (radius) and direction φ (angle) such that

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \rho \begin{pmatrix} \cos\varphi \\ \sin\varphi \end{pmatrix} = \rho\cos\varphi\, e_1 + \rho\sin\varphi\, e_2.$$



The previous drawing shows that the point x can also be written with respect to the unit vectors e_ρ, e_φ given by

$$\begin{aligned} e_\rho &= \cos\varphi\, e_1 + \sin\varphi\, e_2 \\ e_\varphi &= -\sin\varphi\, e_1 + \cos\varphi\, e_2. \end{aligned}$$

From these definitions one can see that Polar coordinates act differently than Cartesian coordinates: When the point x changes its position, hence φ and ρ change, also the unit vectors change! This has an impact when defining the vector operators of the previous section as we need to apply the chain rule.
For example, the gradient in polar coordinates reads as

$$\nabla_{\rho\varphi} f(\rho, \varphi) = \frac{\partial f}{\partial \rho} e_\rho + \frac{1}{\rho} \frac{\partial f}{\partial \varphi} e_\varphi,$$

which we will show in the following. Note that the derivative with respect to the angle includes a scaling $1/\rho$.

Example. Let $g(x, y) = x^2 + y^2$, then $\nabla g(x, y) = (2x, 2y)^T$. Now, defning $\widehat{g}(\rho, \varphi) = \rho^2$, we have with $x = \rho\cos\varphi$, $y = \rho\sin\varphi$ that

$$g(x, y) = x^2 + y^2 = \rho^2((\cos\varphi)^2 + (\sin\varphi)^2) = \rho^2 = \widehat{g}(\rho, \varphi).$$

Using the formula for the gradient $\nabla_{\rho\varphi}$ in polar coordinates, we have

$$\nabla_{\rho\varphi} \widehat{g}(\rho, \varphi) = 2\rho e_\rho + \frac{1}{\rho} 0 e_\varphi = 2\rho \begin{pmatrix} \cos\varphi \\ \sin\varphi \end{pmatrix} = \begin{pmatrix} 2x \\ 2y \end{pmatrix} = \nabla_{xy} g(x, y).$$

■

The previous example shows that we actually want to find operators in polar coordinates that give the same result as in the Cartesian system. To this end, we define the function

$$\phi(\rho, \varphi) = \begin{pmatrix} \rho\cos\varphi \\ \rho\sin\varphi \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix},$$

which maps polar coordinates to Cartesian coordinates. Let $f(x, y)$ be a given function in Cartesian coordinates, then define

$$\widehat{f}(\rho, \varphi) := f(\rho\cos\varphi, \rho\sin\varphi) = f(x, y),$$

which can also be written as $\widehat{f} = f \circ \phi$. Now, the gradient $\nabla_{\rho\varphi}$ in polar coordinates should satisfy

$$\nabla_{\rho\varphi}\widehat{f}(\rho,\varphi) = \nabla f(x,y).$$

With the chain rule, we compute

$$\frac{\partial \widehat{f}(\rho,\varphi)}{\partial \rho} = \frac{\partial (f(\phi(\rho,\varphi))}{\partial \rho} = \frac{\partial f(x,y)}{\partial x}\frac{\partial \phi_1}{\partial \rho} + \frac{\partial f(x,y)}{\partial y}\frac{\partial \phi_2}{\partial \rho} = \nabla f(x,y)\cdot\frac{\partial \phi}{\partial \rho}$$

and doing the same for $\partial_\varphi \widehat{f}$, we get with the Jacobi matrix $D\phi$ of ϕ

$$\begin{pmatrix}\partial_\rho \widehat{f} \\ \partial_\varphi \widehat{f}\end{pmatrix} = \nabla f(x,y)\cdot D\phi^T.$$

Now, we have

$$D\phi = \begin{pmatrix}\cos\varphi & \sin\varphi \\ -\rho\sin\varphi & \rho\cos\varphi\end{pmatrix} \qquad \text{and} \qquad D\phi^{-1} = \frac{1}{\rho}\begin{pmatrix}\rho\cos\varphi & -\sin\varphi \\ \rho\sin\varphi & \cos\varphi\end{pmatrix}.$$

Multiplying from the right with $(D\phi^T)^{-1} = (D\phi^{-1})^T$ gives

$$\begin{pmatrix}\partial_\rho \widehat{f} \\ \partial_\varphi \widehat{f}\end{pmatrix}\cdot(D\phi^T)^{-1} = \nabla f.$$

Evaluating the multiplication gives

$$\begin{pmatrix}\partial_\rho \widehat{f}\cos\varphi - \partial_\varphi \widehat{f}\,\frac{1}{\rho}\sin\varphi \\ \partial_\rho \widehat{f}\sin\varphi + \partial_\varphi \widehat{f}\,\frac{1}{\rho}\cos\varphi\end{pmatrix} = \partial_\rho \widehat{f} e_\rho + \frac{1}{\rho}\partial_\varphi \widehat{f} e_\varphi = \nabla_{\rho\varphi}\widehat{f}.$$

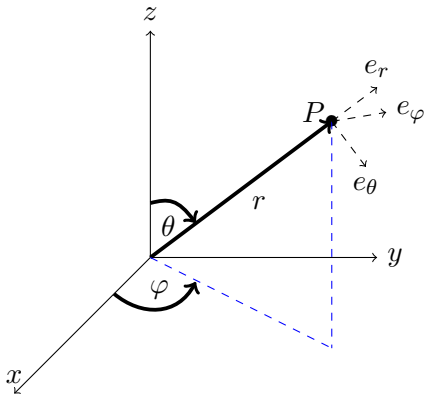
In the same manner, we can also transform the divergence, curl or Laplace operator or any differential operator.

Spherical polar coordinates

We continue with the 3D-coordinate system of spherical polar coordinates, which is commonly used to describe rotationally symmetric objects around a point. In fact, points on earth are specified in the geographical coordinate system (latitude, longitude, elevation), which is a spherical coordinate system (e.g. latitude is measured from the equator (0 degrees) to the poles (± 90 degrees)).

Similarly to the 2D-case, for every point in $\mathbb{R}^3$ there is a unique sphere in $\mathbb{R}^3$ centered at the origin on which the point lies. As a sphere can be represented by a radius r and two angles θ, φ, we write a point P as

$$P = \begin{pmatrix}x \\ y \\ z\end{pmatrix} = \begin{pmatrix}r\sin\theta\cos\varphi \\ r\sin\theta\sin\varphi \\ r\cos\theta\end{pmatrix}.$$



As before, we can define a (non-constant) unit coordinate system

$$\begin{aligned} e_r &= \sin\theta\cos\varphi\ e_1 + \sin\theta\sin\varphi\ e_2 + \cos\theta\ e_3 \\ e_\theta &= \cos\theta\cos\varphi\ e_1 + \cos\theta\sin\varphi\ e_2 - \sin\theta\ e_3 \\ e_\varphi &= -\sin\varphi\ e_1 + \cos\varphi\ e_2. \end{aligned}$$

With the chain rule, one can again compute the transformation of the vector operators with respect to the spherical polar coordinates. E.g., the gradient transforms as

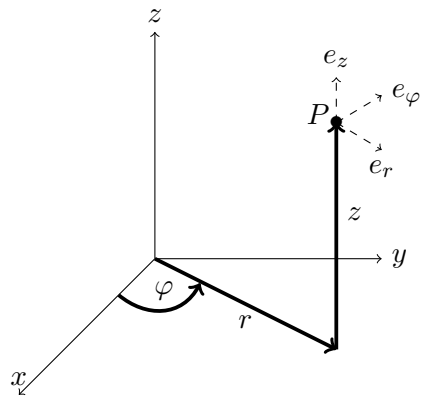
$$\nabla_{r,\theta,\varphi} f = \frac{\partial f}{\partial r} e_r + \frac{1}{r}\frac{\partial f}{\partial \theta} e_\theta + \frac{1}{r\sin\theta}\frac{\partial f}{\partial \varphi} e_\varphi.$$

Up to now, the above transformations (or change of coordinate system) were just motivated by a natural setting for a phyical problem. In the next chapters, we see that these transformations also help to define the surface/volume (of general integrals) of arbitrary (bounded) objects/areas.

Cylindrical coordinates

Another famous coordinate system in $\mathbb{R}^3$ are so called cylindrical coordinates, which are commonly used to describe rotationally symmetric objects around an axis. The main idea hereby is that for every point in $\mathbb{R}^3$, there is a unique cylinder on which the point lies. As a cylinder can be represented by a radius r, an angle φ and an axis z, we can write every point as

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} r\cos\varphi \\ r\sin\varphi \\ z \end{pmatrix}.$$



As before, we can define a (non-constant) unit coordinate system

$$\begin{aligned} e_r &= \cos\varphi\, e_1 + \sin\varphi\, e_2 \\ e_\varphi &= -\sin\varphi\, e_1 + \cos\varphi\, e_2 \\ e_z &= e_3. \end{aligned}$$

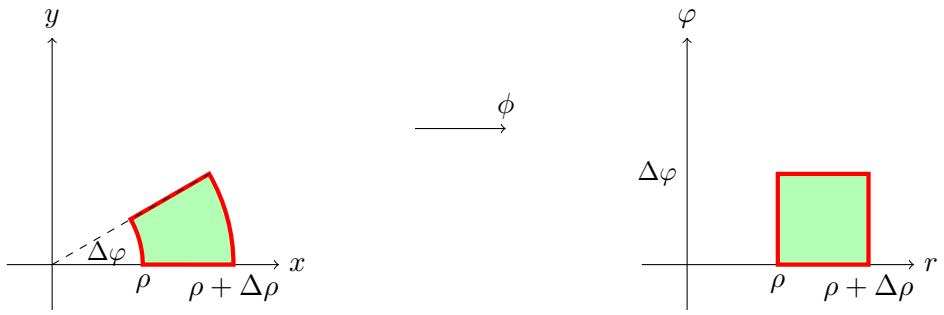
The computation of the gradient in cylindrical coordinates is left to the reader as an exercise.

3.4 The transformation theorem in higher dimensions

In the previous section, we analyzed the transformation of differential operators under coordinate transformation. In this section, we are concerned with the same question for integrals. In fact, we want to generalize the well-known method of substitution for integrals

$$\int_{\phi(a)}^{\phi(b)} f(x)dx = \int_a^b f(\phi(t))\phi'(t)dt \qquad \text{with the substitution } x = \phi(t).$$

In case of multiple variables, this leads to the famous transformation theorem for integrals.



The previous plot shows that in polar coordinates sectors are transformed to rectangles. However, when doing transformations the domains ("objects") may get deformed and change their area/volume, which has to be taken into account. Taking a small circular ring segment of size $\Delta\rho, \Delta\varphi$, we can compute its area by

$$A = \frac{\Delta\varphi}{2}\left((\rho+\Delta\rho)^2 - \rho^2\right) = \frac{\Delta\varphi}{2}(2\rho\Delta\rho + (\Delta\rho)^2) \simeq \rho\Delta\varphi\Delta\rho$$

for small $\Delta\rho$. Comparing that with the rectangle of size $\Delta\varphi\Delta\rho$, we obtain an additional factor r in the area, i.e., this factor describes the deformation of the area. With the chain rule, we could have computed the factor also from the definition of the differential. In fact, this is - as in 1D - linked with the derivatives of the transformation ϕ and comparing this with the Jacobian for the polar coordinates in the previous section shows that this factor is the determinant of the Jacobian. This motivates the following transformation theorem.

Theorem 3.5. *Let $U \subset \mathbb{R}^n$ and $\phi : U \to \mathbb{R}^n$ be an injective function that is additionally differentiable with continuous partial derivatives. Let f be a continuous function that is defined on $\phi(U)$. Then,*

$$\int_{\phi(U)} f(v)dv = \int_U f(\phi(u))\,|\det D\phi(u)|\,du.$$

We finish this section with two examples for applications of the transformation theorem.

Example. We want to compute the area of the unit circle $S = \{(x, y) \in \mathbb{R}^2 \ : \ x^2 + y^2 \leq 1\}$, i.e.,

$$\int_S 1 dx dy.$$

For that, we use the transformation theorem with the polar coordinates of the previous section for the mapping ϕ, i.e.,

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

We compute

$$D\phi = \begin{pmatrix} \cos\varphi & \sin\varphi \\ -r\sin\varphi & r\cos\varphi \end{pmatrix} \quad \longrightarrow \quad |\det D\phi| = r.$$

Then, we have $S = \phi(U)$ with $U = [0, 1] \times [0, 2\pi)$ and the transformation theorem gives

$$\int_S 1 dx dy = \int_U 1 \cdot r \ dr d\varphi = \int_0^{2\pi} \int_0^1 r \ dr d\varphi = \pi.$$

■

Example. We want to evaluate the integral

$$I = \int_{-\infty}^{\infty} e^{-x^2} dx.$$

We note that substitution in this 1D-integral would not lead to a desired form. Therefore, we actually use a different idea by evaluating I^2 as a double integral

$$I^2 = \int_{-\infty}^{\infty} e^{-x^2} dx \cdot \int_{-\infty}^{\infty} e^{-y^2} dy = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-(x^2+y^2)} dx dy.$$

Again, using polar coordinates, we have with the transformation theorem

$$\begin{aligned} I^2 &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-(x^2+y^2)} dx dy = \int_0^{2\pi} \int_0^{\infty} e^{-r^2} r \ dr d\varphi \\ &= \int_0^{2\pi} d\varphi \int_0^{\infty} e^{-r^2} r \ dr = 2\pi \int_0^{\infty} e^{-r^2} r \ dr = 2\pi \left(-\frac{1}{2} e^{-r^2} \right) \Big|_0^{\infty} = \pi. \end{aligned}$$

Taking the square root gives $I = \sqrt{\pi}$. ■

Chapter 4

Line and surface integrals

4.1 Curves

We already introduced the path of a particle by a given vector field in one of the above examples. In general, such a path describes a curve in space.

Definition 4.1. *A curve C in $\mathbb{R}^n$ (with $n = 2, 3$) is a set of points that can be described by a continuous vector valued function $r : \mathbb{R} \to \mathbb{R}^n$, i.e.,*

$$C = \{r(t) : t \in [a, b]\}.$$

The function r is also called a **parametrization** *of the curve C, and the interval $[a, b]$ is called parameter interval. We call a curve* **closed**, *if $r(a) = r(b)$.*

Note that the crucial part of the definition is that we only allow one parameter t to describe the set C. As usual, the parametrization can be written using the unit vectors as

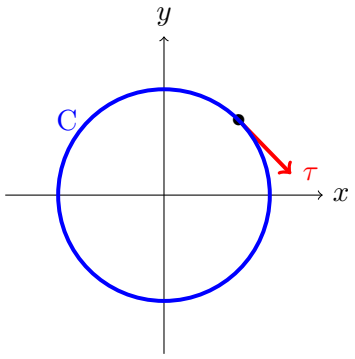
$$r(t) = r_1(t)e_1 + \cdots + r_n(t)e_n.$$

If the parametrization is additionally differentiable, we call C a differentiable curve. In that case, we can introduce the **tangential vector**

$$\tau(t) := \frac{d}{dt}r(t) = (r_1'(t), \ldots, r_n'(t))^T.$$

Example. A simple example of a curve in $\mathbb{R}^2$ is given by the unit-circle described by the set

$$C = \{(x, y) \in \mathbb{R}^2 \ : \ x^2 + y^2 = 1\}.$$



A parametrization of the circle can be given by

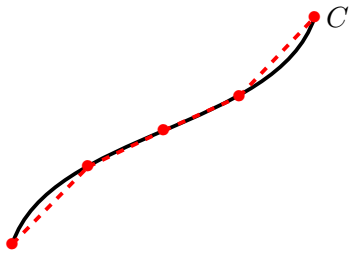
$$r(t) = \begin{pmatrix} \cos(t) \\ \sin(t) \end{pmatrix} \qquad t \in [0, 2\pi]$$

and the tangential vector can be computed as $\tau(t) = \begin{pmatrix} -\sin(t) \\ \cos(t) \end{pmatrix}$.
Another (more inconvenient) way to parametrize the curve C would be putting together $\gamma_1 = \begin{pmatrix} t+1 \\ \sqrt{1-(t+1)^2} \end{pmatrix}$ (upper part) for $t \in [-2, 0]$ and $\gamma_2 = \begin{pmatrix} 1-t \\ -\sqrt{1-(t-1)^2} \end{pmatrix}$ (lower part) for $t \in (0, 2]$ as

$$r(t) = \begin{cases} \gamma_1(t) & t \in [-2, 0] \\ \gamma_2(t) & t \in (0, 2] \end{cases}$$

with parameter interval $[-2, 2]$. Note that this example shows you that parametrizations can also be defined piecewise as long as they are continuous (in our case we have that since $\gamma_1(0) = \gamma_2(0)$ and both parts are continuous). ■

As seen in the previous example, parametrizations are not unique. A curve may also be given in parametric form $r(s)$, where s is the arc-length along the curve measured from a specific point.



For this consider a (uniform) partition of the parameter interval $a = t_0 < t_1 < \cdots < t_{n-1} < t_n = b$ with $h = t_{i+1} - t_i = (b-a)/n$ and approximate the curve C by line segments connecting $r(t_i)$ and $r(t_{i+1})$. This leads to a polygonal approximation of the curve and making the partition more fine (compare this with the definition of the Riemann integral), we actually obtain in the limit the

length of the curve C. Formally, we can write

$$\begin{aligned} L_n &= \sum_{i=1}^{n} |r(t_i) - r(t_{i-1})| = \sum_{i=1}^{n} \left| \frac{r(t_i) - r(t_{i-1})}{t_i - t_{i-1}} \right| h \\ &\simeq \sum_{i=1}^{n} \left| r'(\tau_i) \right| h, \end{aligned}$$

where $\tau_i \in [t_{i-1}, t_i]$. This actually is an approximation like the upper and lower sum in the definition of the Riemann integral (more precisely, the value lies between upper and lower sum, but in the limit if those coincide, we obtain the same value). Taking the limit as in the previous section gives an integral, the so called arc-length of the curve

$$L := \int_a^b \left| r'(t) \right| dt,$$

which motivates the following definition.

Definition 4.2. *Let C be a curve with parametrization $r(t)$, $t \in [a, b]$. Then, the* **arc-length** *of the curve connecting $r(a)$ and $r(\tau)$ for $\tau \in [a, b]$ is given by*

$$s(\tau) := \int_a^\tau \left| r'(t) \right| dt.$$

The **element of arc-length** *is given as $ds = |r'(t)|\, dt$.*

We stress that the arc-length of a curve is independent of the given parametrization.

The function $t \mapsto s(t)$ maps the interval $[a, b]$ onto $[0, L]$ and is strictly monotone and therefore injective, so we can use it as a transformation or reparametrization, i.e., the curve C can also be written as

$$C = \{\widehat{r}(s) : s \in [0, L]\} \qquad \text{where} \qquad \widehat{r}(s(t)) = r(t), \quad t \in [a, b].$$

This is called **arc-length** parametrization.

With the chain rule, we can compute the tangential vector with respect to the arc-length parametrization by

$$\frac{d\widehat{r}(s)}{ds} = \frac{dr(s^{-1}(t))}{ds} = \frac{dr(s^{-1}(t))}{ds^{-1}} \frac{ds^{-1}}{ds} = r'(s^{-1}(t)) \frac{1}{s'(s^{-1}(t))} = r'(s^{-1}(t)) \frac{1}{|r'(s^{-1}(t))|}.$$

Therefore, we have that $t(s) := \frac{d\widehat{r}(s)}{ds}$ is a unit vector, i.e., $|t(s)| = 1$. Since the vector $t(s)$ depends on s, we can also study its rate of change given by the derivative $\frac{dt(s)}{ds}$. The magnitude of this vector, i.e., for a curve with two times differentiable arc-length parametrization

$$\kappa(s) := \left| \frac{dt(s)}{ds} \right| = \left| \frac{d^2\widehat{r}(s)}{ds^2} \right|$$

is called the **curvature** κ. In fact, with the chain rule, we can also compute (exercise!) the curvature in the given parametrization $r(t)$ as

$$\kappa(t) = \frac{|r'(t) \times r''(t)|}{|r'(t)|^3}.$$

Furthermore, we call $n(s) = \frac{1}{\kappa(s)} \frac{dt(s)}{ds}$ the **principal normal** and set $b = t \times n$ (in $\mathbb{R}^3$), which is called the **binormal** to the curve. The vector n is indeed a normal vector in the sense that it is perpendicular to the tangential vector, i.e., we have

$$n(s) \cdot t(s) = \frac{1}{\kappa} \frac{dt(s)}{ds} \cdot t(s) = 0$$

by using differentiation of $1 = t(s) \cdot t(s)$.
Finally, the **torsion** τ measures the local deviation of a curve from a line and is computed as the rate of change of b in direction of the normal vector

$$\tau(s) = -\frac{db(s)}{ds} \cdot n(s).$$

Example. The curvature of a straight line is zero, which can be easily seen from the formula $\kappa(t) = \frac{|r'(t) \times r''(t)|}{|r'(t)|}$ as $r''(t) = 0$.

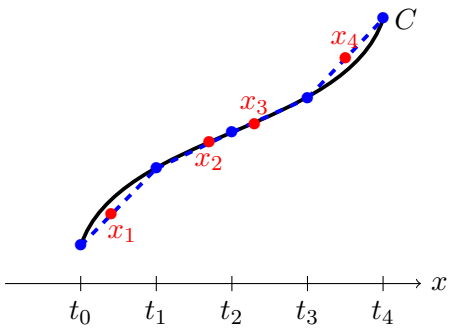
The curvature of a circle of radius a can be computed using the parametrization $r(t) = \begin{pmatrix} a\cos t \\ a \sin t \end{pmatrix}$ as

$$\kappa(t) = \frac{|r'(t) \times r''(t)|}{|r'(t)|^3} = \frac{\left|-a^2 \sin^2 t - a^2 \cos^2 t\right|}{a^3} = \frac{1}{a}.$$

■

4.2 Line Integrals

In Chapter 2 we introduced integration in the 1D-setting. The Riemann-integral was interpreted as the surface area below a function on a given interval $[a, b]$ and the natural generalization to double integrals (as integrals over areas) or triple integrals (as integrals over volumes) was presented.
However, in $\mathbb{R}^2$ or $\mathbb{R}^3$ one could ask whether it is possible to also define integral over lines and surfaces, which is done in the following. We start with the case, where we want to integrate over a curve.
Let C be a given curve joining the points P_1 and P_2. We revisit the idea presented when computing the arc-length of a curve in the previous section.



In the same way as for the Riemann integral and the derivation of the arc-length, we divide C into N small line elements Δr_j with $j = 1, \ldots, N$. Now let ϕ be a given scalar function and let x_j be an arbitrary point on Δr_j. Then, we can write

$$I_N = \sum_{i=1}^{n} \phi(x_j) \left| r(t_i) - r(t_{i-1}) \right| = \sum_{i=1}^{n} \phi(x_j) \left| \Delta r_j \right|,$$

which is a Riemann sum like approximation of the integral of ϕ over C. Taking the limit $N \to \infty$

$$\int_C \phi \, ds = \lim_{N \to \infty} \sum_{j=1}^{N} \phi(x_j) \left| \Delta r_j \right|,$$

where $|\Delta r_j| \to 0$ (as $N \to \infty$), provides a definition of the line integral. Moreover, we note that $|\Delta r_j| = |r'(\tau_i)| \, (t_i - t_{i-1})$ for $\tau_i \in [t_{i-1}, t_i]$, which motivates the following definition.

Definition 4.3 (Line integral of a scalar function). *Let C be a curve with continuously differentiable parametrization $r(t)$ and ϕ a continuous scalar valued function. Then, the* **line integral** *of ϕ over C is defined as the limit*

$$\int_C \phi \, ds = \lim_{N \to \infty} \sum_{j=1}^{N} \phi(x_j) \left| \Delta r_j \right|,$$

where $|\Delta r_j| \to 0$ (as $N \to \infty$) and it can be computed as

$$\int_C \phi \, ds = \int_a^b \phi(r(t)) \left| r'(t) \right| dt.$$

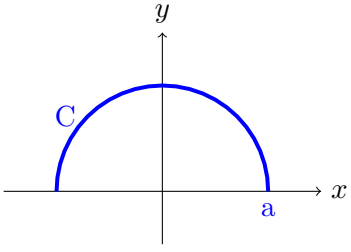
We note that – even though at first glance it looks otherwise – the line integral is independent of the chosen parametrization of the curve C.

Example.

1. We want to evaluate the line integral

$$\int_C (x - y)^2 \, ds,$$

where C is the half circle of radius $a > 0$.



A parametrization of C is given by

$$r(t) = \begin{pmatrix} a\cos t \\ a\sin t \end{pmatrix}$$

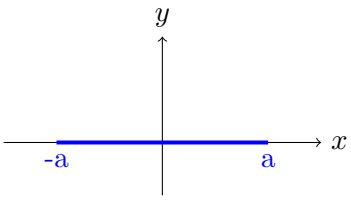
with $t \in [0, \pi]$. We have $r'(t) = \begin{pmatrix} -a\sin t \\ a\cos t \end{pmatrix}$ and therefore $|r'(t)| = \sqrt{a^2\sin^2 t + a^2\cos^2 t} = a$. The previous definition therefore gives

$$\int_C (x-y)^2 \, ds = \int_0^\pi (a\cos t - a\sin t)^2 a \, dt = a^3 \int_0^\pi (1 - \sin(2t))dt = a^3\pi.$$

2. We want to compute

$$\int_C (x-y)^2 \, ds,$$

where C is the line segment connecting $x = -a$ and $x = a$.



This line segment can be parametrized by

$$r(t) = \begin{pmatrix} t \\ 0 \end{pmatrix}$$

for $t \in [-a, a]$. Then, $|r'(t)| = 1$, and we have

$$\int_C (x-y)^2 \, ds = \int_{-a}^a t^2 \, dt = \frac{2}{3}a^3$$

■

We now turn our attention to the case of a vector valued function ψ, for which the line integral can be derived in a similar way. Dividing C into N small line elements Δr_j with $j = 1, \ldots, N$ and evaluating the vector field ψ at an arbitrary point $x_j \in [t_{j-1}, t_j]$ gives the approximation

$$I_N = \sum_{i=1}^n \psi(x_j) \cdot (r(t_i) - r(t_{i-1})) = \sum_{i=1}^n \psi(x_j) \cdot \Delta r_j.$$

Note that here the dot product appears, since for vector valued function not the infinitesimal distances but rather the infinitesimal vector displacements are needed.
Taking the limit $N \to \infty$

$$\int_C \psi \cdot ds = \lim_{N\to\infty} \sum_{j=1}^N \psi(x_j) \cdot \Delta r_j,$$

where $|\Delta r_j| \to 0$ (as $N \to \infty$), provides a definition of the line integral.

Definition 4.4 (Line integral of a vector field). *Let C be a curve with a continuously differentiable parametrization $r(t)$ and ψ a continuous vector valued function. Then, the* **line integral** *of ψ over C is defined as the limit*

$$\int_C \psi \cdot ds = \lim_{N\to\infty} \sum_{j=1}^{N} \psi(x_j) \cdot \Delta r_j,$$

where $|\Delta r_j| \to 0$ (as $N \to \infty$) and it can be computed as

$$\int_C \psi \cdot ds = \int_a^b \psi(r(t)) \cdot r'(t) dt.$$

We previously discussed that a vector field can be written by means of its scalar coordinate functions $\psi = \psi_1 e_1 + \cdots + \psi_n e_n$ ($n = 2, 3$ and e_j are the Cartesian unit vectors). In this sense, we can also, by linearity of the integral, write the line integral over a vector field as

$$\int_C \psi \cdot ds = \int_C \psi_1 e_1 \cdot ds + \cdots + \int_C \psi_n e_n \cdot ds.$$

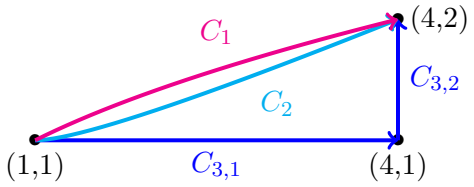
In literature, the summands are oftentimes written using a different notation, which we adopt for the case $n = 2$:

$$\int_C \psi_1 \, dx := \int_C \psi_1 e_1 \cdot ds$$
$$\int_C \psi_2 \, dy := \int_C \psi_2 e_2 \cdot ds.$$

Example.

1. Let $\psi = \begin{pmatrix} x+y \\ y-x \end{pmatrix}$. We want to evaluate $\int_{C_i} \psi \cdot ds$ with

   - C_1 : parabola $y^2 = x$ from $(1,1)$ to $(4,2)$;
   - C_2 : curve $x = 2t^2 + t + 1$, $y = 1 + t^2$ from $(1,1)$ to $(4,2)$;
   - C_3 : the union of the line segments connecting $(1,1)$ to $(4,1)$ and $(4,1)$ to (4,2).



The curve C_1 can be parametrized by $r_1(t) = \begin{pmatrix} t^2 \\ t \end{pmatrix}$ with $t \in [1,2]$. Therefore, we get

$$\begin{aligned}\int_{C_1} \psi \cdot ds &= \int_1^2 \psi(r_1(t)) \cdot r_1'(t) dt = \int_1^2 \begin{pmatrix} t^2+t \\ t-t^2 \end{pmatrix} \cdot \begin{pmatrix} 2t \\ 1 \end{pmatrix} dt \\ &= \int_1^2 2t^3 + t^2 + t \; dt = \frac{34}{3}.\end{aligned}$$

The curve C_2 is given parametrized by $r_2(t) = \begin{pmatrix} 2t^2+t+1 \\ 1+t^2 \end{pmatrix}$ with $t \in [0,1]$. Therefore, we get

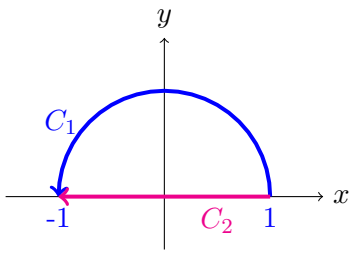
$$\begin{aligned}\int_{C_2} \psi \cdot ds &= \int_0^1 \psi(r_2(t)) \cdot r_2'(t) dt = \int_0^1 \begin{pmatrix} 3t^2+t+2 \\ -t^2-t \end{pmatrix} \cdot \begin{pmatrix} 4t+1 \\ 2t \end{pmatrix} dt \\ &= \int_0^1 10t^3 + 5t^2 + 9t + 2 dt = \frac{32}{3}.\end{aligned}$$

The curve C_3 is composed as the union of the curves $C_{3,1}$ with parametrization $r_{3,1}(t) = \begin{pmatrix} t \\ 1 \end{pmatrix}$ with $t \in [1,4]$ and the curve $C_{3,2}$ with parametrization $r_{3,2}(t) = \begin{pmatrix} 4 \\ t \end{pmatrix}$ with $t \in [1,2]$. By linearity, we have

$$\begin{aligned}\int_{C_3} \psi \cdot ds &= \int_{C_{3,1}} \psi \cdot ds + \int_{C_{3,2}} \psi \cdot ds = \int_1^4 \psi(r_{3,1}(t)) \cdot r_{3,1}'(t) dt + \int_1^2 \psi(r_{3,2}(t)) \cdot r_{3,2}'(t) dt \\ &= \int_1^4 \begin{pmatrix} t+1 \\ 1-t \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} dt \; + \int_1^2 \begin{pmatrix} 4+t \\ t-4 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} dt \\ &= \int_1^4 t+1 \; dt + \int_1^2 t-4 \; dt = \frac{21}{2} - \frac{5}{2} = 8.\end{aligned}$$

2. Let $\psi = \begin{pmatrix} y \\ x \end{pmatrix}$. We want to evaluate $\int_{C_i} \psi \cdot ds$ with

   - C_1 : half-circle connecting $(1,0)$ to $(-1,0)$;
   - C_2 : straight line connecting $(1,0)$ to $(-1,0)$;



The curve C_1 can be parametrized by $r_1(t) = \begin{pmatrix}\cos t \\ \sin t\end{pmatrix}$ with $t \in [0, \pi]$. Therefore, we get

$$\begin{aligned}\int_{C_1} \psi \cdot ds &= \int_0^\pi \psi(r_1(t)) \cdot r_1'(t) dt = \int_0^\pi \begin{pmatrix}\sin t \\ \cos t\end{pmatrix} \cdot \begin{pmatrix}-\sin t \\ \cos t\end{pmatrix} dt \\ &= \int_0^\pi \cos^2 t - \sin^2 t \; dt = 0.\end{aligned}$$

The curve C_2 can be parametrized by $r_2(t) = \begin{pmatrix}1-t \\ 0\end{pmatrix}$ with $t \in [0, 2]$ (note that the orientation is important). Therefore, we get

$$\begin{aligned}\int_{C_2} \psi \cdot ds &= \int_0^2 \psi(r_2(t)) \cdot r_2'(t) dt = \int_0^2 \begin{pmatrix}0 \\ 1-t\end{pmatrix} \cdot \begin{pmatrix}-1 \\ 0\end{pmatrix} dt \\ &= \int_0^2 0 \; dt = 0.\end{aligned}$$

There are several examples in physics, where line integrals need to be employed such as computing the total work done by a force F, when it moves from a point A to a point B or the electrostatic potential energy gained by moving a charge q along a path C in an electric field given by $-q \int_C E \cdot ds$.

Another famous example is a loop of wire C carrying a current I in a magnetic field. Then, the force F is given by $F = I \int_C ds \times B$.

4.3 Potential fields, Green's theorem

The previous examples regarding the line integrals over vector fields provide an interesting insight: In the first example, the path moving from a point A (therein (1,1)) to a point B (therein (4,2)) in $\mathbb{R}^2$ directly impacts the value of the line integral (this is in general always the case) as the line integrals $\int_{C_i} \psi \cdot ds$ have different values for C_1, C_2, C_3.
However, in the second example, the line integrals $\int_{C_1} \psi \cdot ds$ and $\int_{C_2} \psi \cdot ds$ over two different curves connecting the points $A = (1, 0)$ and $B = (-1, 0)$ have the same value. In fact, one can show that for the second example you can choose any curve connecting A to B and get the same value of the line integral, so the value of the line integral is independent of the curve.

Definition 4.5. *We call a line integral $\int_C \psi \cdot ds$ over a vector field ψ, where C connects two points $A, B \in \mathbb{R}^n$* **path independent***, if, for any other curve C_1 connecting the points A, B, we have*

$$\int_C \psi \cdot ds = \int_{C_1} \psi \cdot ds.$$

Clearly, path independence is a property induced by the vector field ψ and vector fields ψ with that property for all (simple) curves in an open set $U \subset \mathbb{R}^n$ are called **conservative fields** *in U.*

In the following, we want to classify a class of functions for which the path independence holds.

Definition 4.6. *A vector field ψ that can be written as $\psi = \nabla\phi$ with a scalar function ϕ is called a* **gradient field**. *The function ϕ is then called a* **scalar potential**.

Example.

1. Every constant vector field $\psi(x,y,z) = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$ is a gradient field with scalar potential $\phi(x,y,z) = c_1x + c_2y + c_3z$.
2. The vector field $\psi(x,y) = \begin{pmatrix} y \\ x \end{pmatrix}$ of the example in the previous subsection is a gradient field with scalar potential $\phi(x,y) = xy$.
3. In physics, examples of gradient fields are given by so called (central) force fields, e.g., given by
$$\psi(x,y,z) = \frac{1}{\sqrt{x^2+y^2+z^2}} \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$
A scalar potential is given by $\phi(x,y,z) = \sqrt{x^2+y^2+z^2}$.

■

We recall the fundamental theorem of calculus stating $\int_a^b f'(t)dt = f(b) - f(a)$, which shows that the given integral can be evaluated using the function f and the points a, b, but <u>not</u> all the values between a and b.
In higher dimensions a similar situation is given, when $\psi = \nabla\phi$ for a scalar function ψ since

$$\int_C \psi \cdot ds = \int_C \nabla\phi \cdot ds = \int_A^B \nabla\phi(r(t))r'(t)dt = \int_a^b \frac{d}{dt}\phi(r(t))dt = \phi(r(b)) - \phi(r(a)),$$

where we used the chain rule. Since the (arbitrary) curve C has to connect the points A and B, we have that $r(b) = B$ and $r(a) = A$, so the right-hand side does only depend on $\phi(B) - \phi(A)$ and we have shown path independence as r does not appear anymore.

Theorem 4.7. *The line integral over a gradient field is path independent.*

In fact, there also holds the converse statement.

Theorem 4.8. *Let ψ be a continuous vector field defined on a region Ω. Then, if ψ is conservative in Ω, we have that ψ is a gradient field.*

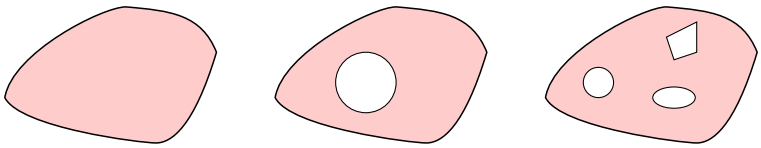
Now, we can ask the question whether we can provide an easy to check characterization of conservative fields?

In order to answer that question, we need to make additional assumption on the region Ω (subset in $\mathbb{R}^n$) enclosed by a <u>closed</u> curve C (i.e. a curve with $r(a) = r(b)$). A crucial quantity of the regions is the so called **connectedness**.

Definition 4.9. *A subset $\Omega \subset \mathbb{R}^n$ is called* **simply connected**, *if every simple closed curve inside Ω can be continuously shrunk to a point inside Ω.*

If Ω is not simply connected but can be decomposed into two simply connected sets, we call Ω **doubly connected**.

Similarly, if Ω can be decomposed into finitely many connected sets, we call Ω **multiply connected**.



By the previous definition, regions containing holes are not simply connected.

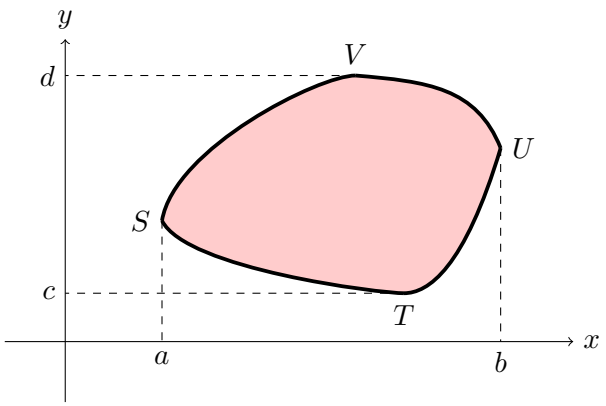
We start with a relation between the line integral over a closed curve C and the integral over the region Ω enclosed by it, which is the statement of Green's theorem in the following.

Theorem 4.10 (Green's theorem in the plane). *Let C be a closed curve that encloses a simply connected region Ω. Let P, Q be functions with continuous partial derivatives inside the region Ω. Then, we have*

$$\int_C P dx + Q dy = \int_C \begin{pmatrix} P \\ Q \end{pmatrix} \cdot ds = \int\int_\Omega \frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y} dx dy.$$

So, the line integral over C can be evaluated using an integral over the region R (double integral) and vice versa.

Proof. We actually 'prove' the theorem for the region Ω given in the following.



Let $y = y_1(x)$ and $y = y_2(x)$ be the curves connecting STU and SVU respectively. We then

compute using the fundamental theorem of calculus

$$\begin{aligned}\int\int_\Omega \frac{\partial P}{\partial y}dxdy &= \int_a^b \int_{y_1(x)}^{y_2(x)} \frac{\partial P}{\partial y}dxdy = \int_a^b P(x,y)\Big|_{y_1(x)}^{y_2(x)}dx = \int_a^b P(x,y_2(x)) - P(x,y_1(x))dx \\ &= -\int_a^b P(x,y_1(x))dx - \int_b^a P(x,y_2(x))dx = -\int_C Pdx\end{aligned}$$

where the last equality follows since y_2 has the opposite direction. In the same way, we can show that

$$\begin{aligned}\int\int_\Omega \frac{\partial Q}{\partial x}dxdy &= \int_c^d \int_{x_1(y)}^{x_2(y)} \frac{\partial Q}{\partial x}dxdy = \int_c^d Q(x,y)\Big|_{x_1(y)}^{x_2(y)}dy = \int_c^d Q(x_2(y),y) - Q(x_1(y),y)dy \\ &= \int_d^c Q(x_1(y),y)dy + \int_c^d Q(x_2(y),y)dx = \int_C Qdy,\end{aligned}$$

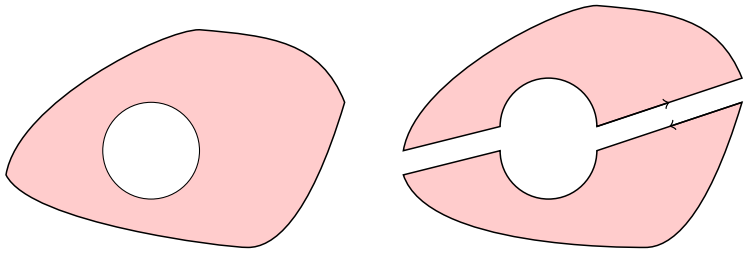
which proves Green's theorem. ■

Example. In the exercise part of the lecture, we computed the area of the ellipse $\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$ by using scaled polar coordinates $x = a\cos\varphi$, $y = b\sin\varphi$ and evaluating $\int\int_\Omega 1dxdy$.
Here, we use Green's theorem to obtain the same result. Taking $P(x,y) = -y$ gives $\frac{\partial P}{\partial y} = -1$ and $Q(x,y) = x$ gives $\frac{\partial Q}{\partial x} = 1$. Therefore, we have

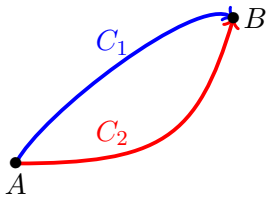
$$\begin{aligned}A = \int\int_\Omega 1dxdy &= \frac{1}{2}\int\int_\Omega 1 + 1dxdy = \frac{1}{2}\int\int_\Omega \frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y}dxdy \\ &\overset{\text{Green}}{=} \frac{1}{2}\int_C Qdx + Pdy = \frac{1}{2}\int_C xdx - ydy = \frac{1}{2}\int_0^{2\pi} ab(\cos^2\varphi + \sin^2\varphi)d\varphi = \pi ab.\end{aligned}$$

■

Green's theorem can also be applied to multiple connected regions by applying Green's theorem on distinct boundaries (curves), whose orientation is such that the region Ω is always on the left (see the following picture). Note that the additional line segments do not appear in the line integrals since they have different orientations.



Green's theorem can now be used to analyze path independence of a line integral. Let C_1 and C_2 be two arbitrary curves connecting the points A and B.



Path independence of the line integral $\int_{C_1} \psi \cdot ds$ with $\psi = (P, Q)^T$ connecting the points A, B means that $\int_{C_i} Pdx + Qdy$ is the same for C_1 and C_2 (and any other curve connecting A and B).
If we consider the closed curve formed by $C := C_1 \cup (-C_2)$, then Green's theorem shows that a sufficient condition for path independence is that

$$\frac{\partial P}{\partial y} = \frac{\partial Q}{\partial x}$$

since

$$\int_{C_1} Pdx + Qdy - \int_{C_2} Pdx + Qdy = \int_C Pdx + Qdy \overset{\text{Green}}{=} \int_\Omega \frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y} dxdy = 0.$$

One can, in fact, also show that this is a necessary condition. In fact, we already know that path independence implies that $\psi = \begin{pmatrix} P \\ Q \end{pmatrix}$ is a gradient field, which means that there exists a function ϕ with $\frac{\partial \phi}{\partial x} = P$ and $\frac{\partial \phi}{\partial y} = Q$. Schwarz theorem then gives

$$\frac{\partial P}{\partial y} = \frac{\partial^2 \phi}{\partial y \partial x} = \frac{\partial^2 \phi}{\partial x \partial y} = \frac{\partial Q}{\partial x},$$

which is the condition stated above.

Theorem 4.11. *Let U be a simply connected region and $\psi : U \to \mathbb{R}^2$ be a vector field with continuous partial derivatives. Then, the following statements are equivalent*

1. *The line integral $\int_C \psi \cdot ds$ connecting two points A, B in U is independent of the chosen path. Consequently, the line integral $\oint_C \psi \cdot ds$ (this is the usual notation for line integrals over closed curves) over closed curves C inside U is zero.*
2. *There exists a scalar potential ϕ with $\nabla \phi = \psi$.*
3. $\frac{\partial \psi_1}{\partial y} = \frac{\partial \psi_2}{\partial x}$.

Example.

- Evaluate $\int_C \psi \cdot ds$ with $\psi = \begin{pmatrix} e^x y + \cos x \sin y \\ e^x + \sin x \cos y + 2y \end{pmatrix}$ over the ellipse $4x^2 + y^2 = 1$.

  Clearly, one can parametrize the ellipse and compute the line integral using the previous formula. However, it is much simpler to check in advance, whether we have a conservative field using the third statement of the above theorem. We compute

$$\frac{\partial \psi_1}{\partial y} = e^x + \cos x \cos y = \frac{\partial \psi_2}{\partial x},$$

so we indeed have a gradient field. Since the ellipse is closed, we directly obtain from the above theorem that

$$\int_C \psi \cdot ds = 0$$

without directly computing the integral.

- Evaluate $\int_C \psi \cdot ds$ for $\psi = \begin{pmatrix} y \\ x \end{pmatrix}$ over the curve starting at the origin, moving along the parabola $y^2 = x$ to the point $(4, 2)$, then moving in a straight line to the point $(4, 0)$, then moving back along a half circle of radius 4 to the point $(-4, 0)$ and finally, moving along a straight line to the point $(-1, -1)$.

  One could of course parametrize the curves described above piece by piece and add the line integrals, or one could apply the previous theorem. The vector field ψ is a gradient field, since $\frac{\partial \psi_1}{\partial y} = 1 = \frac{\partial \psi_2}{\partial x}$ and we know that the line integral is path independent. Therefore, we take the straight line C_1 connecting $(0, 0)$ and $(-1, -1)$ parametrized by $\begin{pmatrix} -t \\ -t \end{pmatrix}$ with $t \in [0, 1]$ and obtain

$$\int_C \psi \cdot ds = \int_{C_1} \psi \cdot ds = \int_0^1 \begin{pmatrix} -t \\ -t \end{pmatrix} \cdot \begin{pmatrix} -1 \\ -1 \end{pmatrix} dt = \int_0^1 2t dt = 1.$$

■

Scalar potentials can be computed by integration in the following way: Let ψ be given and suppose $\dfrac{\partial \psi_1}{\partial y} = \dfrac{\partial \psi_2}{\partial x}$. We want to have a function ϕ with $\nabla \phi = \psi$. Integration with respect to x gives

$$\phi = \int \frac{\partial \phi}{\partial x} dx + g(y) = \int \psi_1 dx + g(y)$$

with an unknown function $g(y)$ that can be determined from differentiation with respect to y:

$$\psi_2 = \frac{\partial \phi}{\partial y} = \partial_y \Big(\int \psi_1 dx \Big) + g'(y).$$

We note that scalar potentials are only unique up to a constant, since $\nabla c = 0$.

Example. We want to compute the scalar potential for $\psi = \begin{pmatrix} e^x y + \cos x \sin y \\ e^x + \sin x \cos y + 2y \end{pmatrix}$. Integration of ψ_1 with respect to x gives

$$\phi = \int e^x y + \cos x \sin y dx + g(y) = e^x y + \sin x \sin y + g(y).$$

Differentiation of this equation with respect to y gives

$$\frac{\partial \phi}{\partial y} = e^x + \sin x \cos y + g'(y) = \psi_2 = e^x + \sin x \cos y + 2y$$

and consequently $g'(y) = 2y$ or $g(y) = y^2$. Therefore, a scalar potential is given by

$$\phi = e^x y + \sin x \sin y + y^2.$$

■

For vector fields $\psi : U \to \mathbb{R}^3$ a similar theorem holds, where the condition in 3. has to be replaced by $\nabla \times \psi = 0$.

Similarly to scalar potentials, one can also find a potential for vector fields ψ with $\operatorname{div} \psi = 0$. Then, there exists a vector field θ with $\nabla \times \theta = \psi$. Whereas ϕ was unique up to a constant (as $\nabla\phi = \nabla(\phi + c)$ for $c \in \mathbb{R}$), we have that θ is uniquely defined up to gradients, since $\nabla \times \nabla g = 0$, we have

$$\nabla \times \theta = \nabla \times (\theta + \nabla g) = \psi.$$

Such vector potentials play an important role in electromagnetics, which we will see in later chapters.

4.4 Surfaces

Similarly to a curve, we can also describe a surface S by a vector valued function in $\mathbb{R}^3$.

Definition 4.12. *A surface S in $\mathbb{R}^3$ is a set of points that can be described by a continuous vector valued function $r(u, v) : \mathbb{R}^2 \to \mathbb{R}^3$, i.e.,*

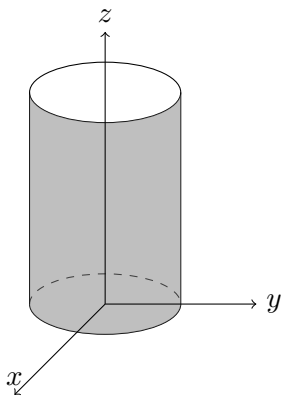
$$S = \{r(u, v) : (u, v) \in G\}.$$

The function r is also called a parametrization of the surface C, and the set $G \subset \mathbb{R}^2$ is is called parameter field.

Note that the crucial part of the definition is that we only allow two parameters u, v to describe the set S. In Cartesian coordinates a surface can be written as

$$r(u, v) = r_1(u, v)e_1 + r_2(u, v)e_2 + r_3(u, v)e_3.$$

Example. The mantle of a cylinder $Z = \{(x, y, z) \in \mathbb{R}^3 \ : \ x^2 + y^2 \leq 1, 0 \leq z \leq 1\}$ is a surface S that can be parametrized using cylindrical coordinates.



The parametrization

$$r(u,v) = \begin{pmatrix} \cos u \\ \sin u \\ v \end{pmatrix} \qquad u \in [0, 2\pi], v \in [0,1]$$

with parameter field $G = [0, 2\pi] \times [0, 1]$ parametrizes the surface S.

In fact, also the top and bottom of the cylinder are surfaces that can be parametrized using polar coordinates as

$$r_1(u,v) = \begin{pmatrix} v\cos u \\ v \sin u \\ 0 \end{pmatrix} \qquad u \in [0, 2\pi], v \in [0,1]$$

$$r_2(u,v) = \begin{pmatrix} v\cos u \\ v \sin u \\ 1 \end{pmatrix} \qquad u \in [0, 2\pi], v \in [0,1].$$

■

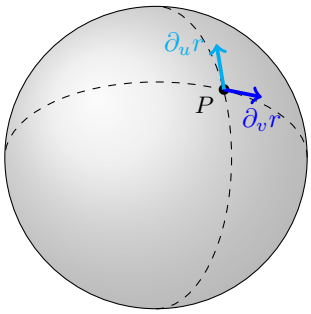
Now, let $c(\lambda)$ be any curve on a surface S. Using the definition of the surface, a parametric representation is given by substitution, i.e,

$$c(\lambda) = r(u(\lambda), v(\lambda)).$$

Here, the chain rule gives

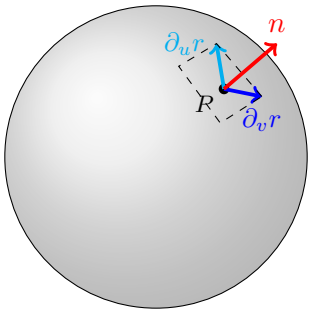
$$\frac{dc}{d\lambda} = \frac{\partial r}{\partial u}\frac{\partial u}{\partial \lambda} + \frac{\partial r}{\partial v}\frac{\partial v}{\partial \lambda}.$$

When either $u(\lambda)$ or $v(\lambda)$ is held constant and pass through a point P (see picture) these are called coordinate curves.



It follows that $\frac{dc}{d\lambda} = \frac{\partial r}{\partial v}\frac{dv}{d\lambda}$ if $u = \text{const}$ or $\frac{dc}{d\lambda} = \frac{\partial r}{\partial u}\frac{du}{d\lambda}$ if $v = \text{const}$. Hence, the tangent vector of c is in the same direction as either $\frac{\partial r}{\partial v}$ or $\frac{\partial r}{\partial u}$. If the surface is smooth, these vectors are linearly independent and span the tangent space at the point P. A vector that is normal to the surface (which corresponds with being normal to the tangent plane at the point P) is given by

$$n = \frac{\partial r}{\partial u} \times \frac{\partial r}{\partial v}.$$



In the neighborhood of P an infinitesimal vector displacement dr is written as

$$dr = \frac{\partial r}{\partial u} du + \frac{\partial r}{\partial v} dv.$$

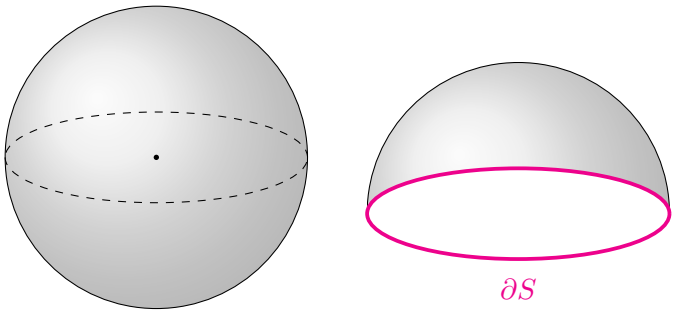
Hence, the element of area given by the infinitesimally small parallelogram can be written as

$$dS = \left| \frac{\partial r}{\partial u} \times \frac{\partial r}{\partial v} \right| dudv = |n| \, dudv.$$

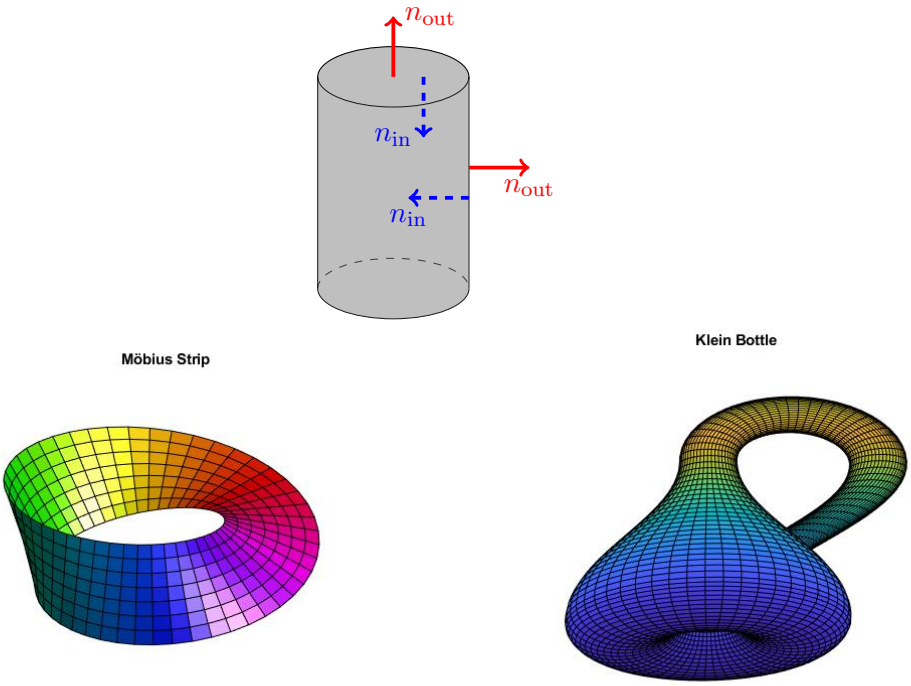
Now, let G be the region in the uv - plane that corresponds to the range of the parameter values of S, then the total area of the surface is given by

$$A = \int_G |n| \, dudv.$$

As in the case of curves, we distinguish between open and closed surfaces. We call a bounded surface **closed**, if it has no boundary, otherwise we denote the boundary of the surface by ∂S. A bounded closed surfaces then encloses a bounded region $\Omega \subset \mathbb{R}^3$ with positive volume.



For curves defining an orientation is straight forward. However, for surfaces the situation becomes unclear. We call a smooth surface **orientable**, if the set of normal vectors depends continuously on the position. In fact, most commonly used surfaces are orientable (such as spheres or cylinders), but there are some examples that are not orientable, most famously the Möbius strip or the Klein bottle.



In the following, we only consider orientable surfaces, such that there is a clear concise choice of a normal vector.

4.5 Surface Integrals

Formally, surface integrals can be defined in the same way as curve integrals by approximating the surface S into small flat areas ΔS_j for $j = 1, \ldots, N$. Let ϕ be a scalar function. With arbitrary points $x_j \in \Delta S_j$, we can define the sum

$$I_N = \sum_{j=1}^{N} \phi(x_j) \, |\Delta S_j|$$

and taking the limit $N \to \infty$ assuming $|\Delta S_j| \to 0$, we can define the surface integral.

Definition 4.13 (Surface integral of a scalar function). *Let S be a surface with continuous partial differentiable parametrization r and ϕ be a continuous scalar function. Then, the* **surface integral** *of ϕ over S is defined as the limit*

$$\int_S \phi \, dS = \lim_{N\to\infty} \sum_{j=1}^{N} \phi(x_j) \, |\Delta S_j| \,,$$

where $|\Delta S_j| \to 0$ (as $N \to \infty$) and it can be computed as

$$\int_S \phi \, dS = \int_G \phi \, |n| \, dA.$$

In the same way, we can define the surface integral over a vector field.

Definition 4.14 (Surface integral of a vector field). *Let S be a surface with continuous partial differentiable parametrization r and ψ be a continuous vector field. Then, the* **surface integral** *of ψ over S is defined as the limit*

$$\int_S \psi \, dS = \lim_{N\to\infty} \sum_{j=1}^{N} \psi(x_j) \cdot n_j \, |\Delta S_j| \,,$$

where n_j is the outer normal vector to S_j and $|\Delta S_j| \to 0$ (as $N \to \infty$). The surface integral can be computed as

$$\int_S \psi \, dS = \int_G \psi \cdot n dA.$$

Note that the orientation of the surface, hence the direction of the normal vector is important and changing the orientation results into a sign change in the surface integral. If the boundary of the surface is given by a curve with a positive orientation (i.e. counter clockwise), the direction of the normal vector is then given by the right hand rule:

If the fingers are curled along the orientation of the boundary curve, then the thumb of the right hand points in the direction of the normal vector.

For closed surfaces, we choose n as the outward normal, i.e., the normal pointing away from the enclosed region of the surface.

Example. We want to evaluate $\int_S \psi \cdot dS$ with $\psi = \begin{pmatrix} x \\ 0 \\ 0 \end{pmatrix}$ and S is the surface of the hemisphere $x^2 + y^2 + z^2 = a^2$, $z \geq 0$.

A parametrization of S can be obtained with polar coordinates as $x = \rho\cos\varphi$, $y = \rho\sin\varphi$. Then the equation $x^2 + y^2 + z^2 = a^2$ transform to $\rho^2 + z^2 = a^2$ or $z = \sqrt{a^2 - \rho^2}$. This gives the

parametrization

$$r(\rho,\varphi) = \begin{pmatrix} \rho\cos\varphi \\ \rho\sin\varphi \\ \sqrt{a^2-\rho^2} \end{pmatrix} \qquad \text{with} \quad \rho \in [0,a], \varphi \in [0,2\pi].$$

We compute the normal vector as

$$n = \frac{\partial r}{\partial \rho} \times \frac{\partial r}{\partial \varphi} = \begin{pmatrix} \cos\varphi \\ \sin\varphi \\ \frac{-\rho}{\sqrt{a^2-\rho^2}} \end{pmatrix} \times \begin{pmatrix} -\rho\sin\varphi \\ \rho\cos\varphi \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{\rho^2\cos\varphi}{\sqrt{a^2-\rho^2}} \\ \frac{\rho^2\sin\varphi}{\sqrt{a^2-\rho^2}} \\ \rho \end{pmatrix}.$$

Inserting this in the formula for the computation of the surface integral gives

$$\begin{aligned} \int_S \psi \, dS = \int_G \psi \cdot n dA &= \int_0^a \int_0^{2\pi} \begin{pmatrix} \rho\cos\varphi \\ 0 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} \frac{\rho^2\cos\varphi}{\sqrt{a^2-\rho^2}} \\ \frac{\rho^2\sin\varphi}{\sqrt{a^2-\rho^2}} \\ \rho \end{pmatrix} d\rho d\varphi \\ &= \int_0^a \int_0^{2\pi} \frac{\rho^3\cos^2\varphi}{\sqrt{a^2-\rho^2}} d\rho d\varphi = \int_0^{2\pi} \cos^2\varphi \, d\varphi \int_0^a \frac{\rho^3}{\sqrt{a^2-\rho^2}} d\rho = \frac{2\pi a^3}{3} \end{aligned}$$

and we have computed the surface integral. ■

Many surfaces are given in **explicit form** $z = f(x,y)$ and can therefore easily be parametrized by $r(x,y) = \begin{pmatrix} x \\ y \\ f(x,y) \end{pmatrix}$ for $(x,y) \in G$. Computing the normal vector gives

$$n = \frac{\partial r}{\partial x} \times \frac{\partial r}{\partial y} = \begin{pmatrix} 1 \\ 0 \\ \partial_x f \end{pmatrix} \times \begin{pmatrix} 0 \\ 1 \\ \partial_y f \end{pmatrix} = \begin{pmatrix} -\partial_x f \\ -\partial_y f \\ 1 \end{pmatrix}$$

and the formulas for the surface integrals reduce to

$$\begin{aligned} \int_S \phi \, dS &= \int_G \phi(x,y,f(x,y)) \sqrt{\partial_x f^2 + \partial_y f^2 + 1} \, dA \\ \int_S \psi \cdot dS &= \int_G \psi(x,y,f(x,y)) \cdot \begin{pmatrix} -\partial_x f \\ -\partial_y f \\ 1 \end{pmatrix} dA. \end{aligned}$$

Example. We use this method to evaluate $\int_S \psi \cdot dS$ with $\psi = \begin{pmatrix} x \\ 0 \\ 0 \end{pmatrix}$ and S is the surface of the hemisphere $x^2 + y^2 + z^2 = a^2$, $z \geq 0$.

In explicit form the surface is given by $z = \sqrt{a^2 - x^2 - y^2}$ and $(x, y) \in G$, where G is the circle of radius a, i.e., $G = \{(x, y) \in \mathbb{R}^2 \ : \ x^2 + y^2 \leq a^2\}$. Using the above formula, we compute using polar coordinates to describe G

$$\int_S \psi \cdot dS = \int_G \begin{pmatrix} x \\ 0 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} \frac{x}{\sqrt{a^2-x^2-y^2}} \\ \frac{y}{\sqrt{a^2-x^2-y^2}} \\ 1 \end{pmatrix} dA = \int_G \frac{x^2}{\sqrt{a^2 - x^2 - y^2}} dA$$

$$= \int_0^a \int_0^{2\pi} \frac{\rho^2 \cos^2 \varphi}{\sqrt{a^2 - \rho^2}} \rho \, d\rho d\varphi = \int_0^{2\pi} \cos^2 \varphi \, d\varphi \int_0^a \frac{\rho^3}{\sqrt{a^2 - \rho^2}} d\rho = \frac{2\pi a^3}{3},$$

and we obtain the same value as in the example above. ■

4.6 The theorems of Gauß and Stokes

In the previous chapter, we defined the vector operators $\nabla, \operatorname{div}, \operatorname{curl}$. As discussed there, the definitions depended on the corresponding coordinate system.
With the surface integrals defined in the previous section, we can provide an equivalent (without proof here) definition that is independent of the coordinate system by

$$\nabla \phi(x) = \lim_{|V| \to 0} \frac{1}{|V|} \int_{S = \partial V} \phi \, dS.$$

Here, V denotes a small set enclosed by the closed curve $S = \partial V$ around the point x and $|V|$ denotes the volume of V. In the same way, one can define

$$\operatorname{div} \psi(x) = \lim_{|V| \to 0} \frac{1}{|V|} \int_{S = \partial V} \psi \cdot dS,$$

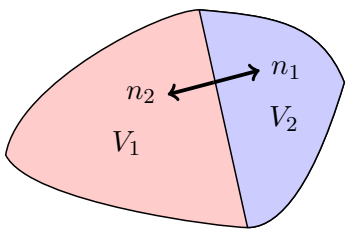
$$\operatorname{curl} \psi(x) \cdot n = \lim_{|A| \to 0} \frac{1}{|A|} \int_C \psi \cdot ds$$

where C is a curve bounding a small area A.

We use these definitions to derive the famous integral theorems of Gauß and Stokes. We start with Gauß' theorem, which is also called the divergence theorem. Decomposing a given volume V into lots of small volumes V_i, we can write using the above definition of the divergence

$$\operatorname{div} \psi \ |V_i| \simeq \int_{\partial V_i} \psi \cdot dS.$$

Now, we sum up over all small volumes V_i. On the right-hand side, this would produce contributions of all boundary parts of the V_i, so also those parts that are inside the volume V. However, such parts appear twice (see the drawing below) with different orientations of the normal vectors, so they add up to zero.



Therefore, taking the limit $|V_i| \to 0$, we arrive at

$$\int_V \operatorname{div} \psi \, dV = \int_{\partial V} \psi \cdot dS,$$

which is the divergence theorem stated in the following.

Theorem 4.15 (Gauß divergence theorem). *Let $V \subset \mathbb{R}^n$ be a bounded region and ∂V its boundary. Let ψ be a continuously differentiable vector field defined on V. Then,*

$$\int_V \operatorname{div} \psi \, dV = \int_{\partial V} \psi \cdot dS.$$

Remark.

- The classical divergence theorem is formulated for regions $V \subset \mathbb{R}^3$, where the above integration over V is a triple integral
$$\int\int\int_V \operatorname{div} \psi \, dV$$
in the volume and the integration over ∂V is a surface integral as introduced in the previous section.

  However, the divergence theorem stated in the previous theorem is also valid for $n = 1, 2$ (or $n > 3$ if a suitable integration over the boundary is defined).

- For $n = 1$, we have that ψ reduces to a scalar function and V is an interval $[a, b]$. Then, we have
$$\int_V \operatorname{div} \psi \, dV = \int_a^b \psi' dx.$$
The boundary of the interval is given by the points a (with outward "normal vector" -1) and b (with outward "normal vector" 1), so the "'surface" integral reduces to
$$\int_{\partial V} \psi \cdot dS = \psi(b) \cdot 1 + \psi(a) \cdot (-1)$$
and the divergence theorem reduces to the fundamental theorem of calculus.

- For $n = 2$, the integral on the left in the divergence theorem is an area integral and the integral on the right is a line integral over a curve parametrized by a function $r(t)$ with parameter interval $[a, b]$. However, the element of surface dS (in 2D) and arc-length ds (in 2D) are not defined in the same way. In fact, the calculation of the line integrals use the tangent vector $\tau(t) = r'(t)$, whereas the calculation of surface integrals takes the normal vector. The normal vector can be computed as $n(t) = \begin{pmatrix} r_2'(t) \\ -r_1'(t) \end{pmatrix}$ and the integral on the right-hand side in the divergence theorem is given by
$$\int_{\partial V} \psi \cdot dS = \int_a^b \psi(r(t)) \cdot \begin{pmatrix} r_2'(t) \\ -r_1'(t) \end{pmatrix} dt = \int_a^b \psi_1(r(t)) r_2'(t) - \psi_2(r(t)) r_1'(t) dt.$$

If we introduce the new vector field $\begin{pmatrix} P \\ Q \end{pmatrix} := \begin{pmatrix} -\psi_2 \\ \psi_1 \end{pmatrix}$, we actually observe that the integral on the right hand side is the classical line integral of $\begin{pmatrix} P \\ Q \end{pmatrix}$, i.e.,

$$\int_a^b \psi_1(r(t))r_2'(t) - \psi_2(r(t))r_1'(t)dt = \int_C \begin{pmatrix} P \\ Q \end{pmatrix} ds.$$

Looking again at the left hand side in the divergence theorem, we have by definition of $\begin{pmatrix} P \\ Q \end{pmatrix}$ that

$$\int_V \operatorname{div} \psi \, dV = \int_V \frac{\partial \psi_1}{\partial x} + \frac{\partial \psi_2}{\partial y} dxdy = \int_V \frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y} dxdy$$

and comparing the two formulas, we have, in fact, reproduced Green's theorem

$$\int_C \begin{pmatrix} P \\ Q \end{pmatrix} ds = \int_V \frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y} dxdy.$$

Thus, the divergence theorem can be seen as a direct generalization of the fundamental theorem of calculus as well as of Green's theorem. ■

The divergence theorem has a very famous interpretation in physics: The sum of all sources (this is given by the divergence of the vector field) in a region is the same as the flux out of the region.

Consequently, an application is given in the derivation of the equation of conservation of mass of a fluid. Conservation of mass is just the statement made above, i.e., for any volume V in the fluid, the increase or decrease of mass M over time in the fluid must equal the rate at which fluid is entering or leaving the volume. Denoting by ρ the density of the fluid and v the velocity field (vector field!), we have

$$\frac{\partial M}{\partial t} = -\int_{\partial V} \rho v \cdot dS.$$

Now, the mass in V can be written as $M = \int_V \rho \, dV$. Interchanging integral and derivative in above equation together with the divergence theorem produces

$$\begin{aligned} 0 = \frac{\partial}{\partial t} \int_V \rho \, dV + \int_{\partial V} \rho v \cdot dS &= \int_V \frac{\partial}{\partial t} \rho \, dV + \int_{\partial V} \rho v \cdot dS \\ \overset{Gauß}{=} \int_V \frac{\partial}{\partial t} \rho \, dV + \int_V \operatorname{div}(\rho v) \, dV &= \int_V \frac{\partial}{\partial t} \rho + \operatorname{div}(\rho v) \, dV. \end{aligned}$$

Since the volume V was arbitrary, the integrand has to vanish, which means

$$\frac{\partial}{\partial t} \rho + \operatorname{div}(\rho v) = 0,$$

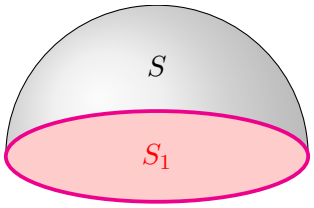
and we have derived the so called equation of **conservation of mass**.

Example. The divergence theorem can be used to compute the volume of a region V by evaluating a surface integral since

$$\int_V \operatorname{div} \begin{pmatrix} x \\ y \\ z \end{pmatrix} dV = 3 \int_V 1 \, dV = 3 \, |V| = \int_{\partial V} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \cdot dS.$$

■

Example. We want to evaluate the surface integral $\int_S \psi \cdot dS$, where $\psi = \begin{pmatrix} y - x \\ x^2 z \\ z + x^2 \end{pmatrix}$ and S is the open surface of the hemisphere $x^2 + y^2 + z^2 = a^2$, $z \geq 0$.
We could directly compute the surface integral by computing the normal vector to the surface. However, it is much easier to use the divergence theorem. Denoting the bottom of the hemisphere by S_1, which is given as $S_1 = \{(x, y, z) \in \mathbb{R}^2 \ : \ x^2 + y^2 \leq a^2, z = 0\}$.



Then, $S_1 \cup S$ encloses the half upper half-ball V and we obtain with the theorem of Gauß that

$$\int_V \operatorname{div} \psi \, dV = \int_{\partial V} \psi \cdot dS = \int_S \psi \cdot dS + \int_{S_1} \psi \cdot dS.$$

The first integral on the left-hand side is what we are looking for, and since $\operatorname{div} \psi = -1 + 0 + 1 = 0$, we obtain

$$\int_S \psi \cdot dS = - \int_{S_1} \psi \cdot dS.$$

S_1 can be parametrized using polar coordinates $r(u, v) = \begin{pmatrix} u \cos v \\ u \sin v \\ 0 \end{pmatrix}$ with $u \in [0, a]$ and $v \in [0, 2\pi]$ and the corresponding outer normal vector is given as $n = \begin{pmatrix} 0 \\ 0 \\ -u \end{pmatrix}$. We compute

$$- \int_{S_1} \psi \cdot dS = \int_0^a \int_0^{2\pi} \begin{pmatrix} u \sin v - u \cos v \\ 0 \\ u^2 \cos^2 v \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 0 \\ -u \end{pmatrix} dv du = \int_0^a \int_0^{2\pi} -u^3 \cos^2 v \, dv du = -\frac{\pi a^4}{4}.$$

■

The divergence theorem implies some very important generalizations to known rules of integration in 1D such as integration by parts.

Corollary 4.16 (Integration by parts formula). *Let V be a bounded region with boundary ∂V. Let ϕ be a scalar function and ψ be a vector field defined on V. Assume that ϕ and ψ have continuous partial derivatives. Then, we have*

$$\int_V \phi \operatorname{div} \psi \, dV = \int_{\partial V} \phi\psi \cdot dS - \int_V \nabla\phi \cdot \psi \, dV.$$

Proof. We apply the divergence theorem to the product $\phi\psi$ to obtain

$$\int_V \operatorname{div}(\phi\psi) \, dV = \int_{\partial V} \phi\psi \cdot dS.$$

On the other hand, we have with the product rule that $\operatorname{div}(\phi\psi) = \phi \operatorname{div}(\psi) + \nabla\phi \cdot \psi$, which gives

$$\int_V \operatorname{div}(\phi\psi) \, dV = \int_V \phi \operatorname{div} \psi \, dV + \int_V \nabla\phi \cdot \psi \, dV$$

and together these two equations imply the integration by parts formula. ■

An application of the integration by parts formula produces the so called Green identities.

Corollary 4.17 (Green's identities). *Let V be a bounded region with boundary ∂V. Let ϕ, f be two times continuously differentiable scalar functions in V. We have*

$$\int_V \phi\Delta f \, dV = \int_{\partial V} \phi\nabla f \cdot dS - \int_V \nabla\phi \cdot \nabla f \, dV,$$

which is known as **Green's first identity**. *Moreover, we have*

$$\int_V \phi\Delta f - \Delta\phi f \, dV = \int_{\partial V} (\phi\nabla f - \nabla\phi f) \cdot dS,$$

which is known as **Green's second identity**.

Proof. We write $\Delta f = \operatorname{div}(\nabla f)$ and apply the integration by parts formula with scalar function ϕ and vector field ∇f. This gives

$$\int_V \phi\Delta f \, dV = \int_V \phi \operatorname{div}(\nabla f) \, dV = \int_{\partial V} \phi\nabla f \cdot dS - \int_V \nabla\phi \cdot \nabla f \, dV,$$

which is the first identity.
Reversing the roles of ϕ, f gives

$$\int_V \Delta\phi f \, dV = \int_{\partial V} \nabla\phi f \cdot dS - \int_V \nabla\phi \cdot \nabla f \, dV.$$

Subtracting both equations leads to a cancellation of the term $\int_V \nabla\phi \cdot \nabla f \, dV$ and shows the second identity. ■

Green's identities will become very useful later on, when we analyze partial differential equations.

Now, we derive another famous integral theorem, Stokes theorem, which can be seen as the "curl analogue" to the divergence theorem. In the same way as for the divergence theorem, we now decompose an open surface S into many small areas S_i with boundaries $C_i = \partial S_i$ and corresponding normals n_i. The equivalent definition of the curl operator implies that

$$\operatorname{curl} \psi \cdot n_i \, |S_i| \simeq \int_{C_i} \psi \cdot ds.$$

In a similar way as in the divergence theorem, we obtain by summing over all S_i and noticing that the interior parts of the boundaries cancel out, we obtain

$$\int_S \operatorname{curl} \psi \cdot dS = \int_{\partial S} \psi \cdot ds,$$

which is Stokes theorem stated in the following.

Theorem 4.18 (Stokes theorem). *Let $S \subset \mathbb{R}^3$ be an open surface with boundary ∂S. Let ψ be a continuously differentiable vector field. Then,*

$$\int_S \operatorname{curl} \psi \cdot dS = \int_{\partial S} \psi \cdot ds.$$

Remark. In contrast to Gauß theorem, we have that Stokes theorem is more closely tied to the case $n = 3$, since it contains the curl-operator, which is defined by using the cross product. However, we also obtained a 2D-curl in the previous chapter as a scalar function $\operatorname{curl} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \frac{\partial \psi_2}{\partial x} - \frac{\partial \psi_1}{\partial y}$ and Stokes theorem in 2D would be the exact statement of Green's theorem. ■

Example. Let $\psi = \begin{pmatrix} y \\ -x \\ z \end{pmatrix}$. We want to verify Stokes theorem on the hemisphere $x^2+y^2+z^2 = a^2$, $z \geq 0$.

We start with the surface integral on the left hand side. Using $\operatorname{curl} \psi = \begin{pmatrix} 0 \\ 0 \\ -2 \end{pmatrix}$ and the normal vector $n = \frac{1}{a} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$. Therefore, we have

$$\begin{aligned} \int_S \operatorname{curl} \psi \cdot dS &= \int_0^{2\pi} \int_0^{\pi/2} \begin{pmatrix} 0 \\ 0 \\ -2 \end{pmatrix} \cdot \begin{pmatrix} \sin\theta \cos\varphi \\ \sin\theta \sin\varphi \\ \cos\theta \end{pmatrix} a^2 \sin\theta \; d\theta d\varphi \\ &= a^2 \int_0^{2\pi} \int_0^{\pi/2} -2 \cos\theta \sin\theta \; d\theta d\varphi = -2\pi a^2. \end{aligned}$$

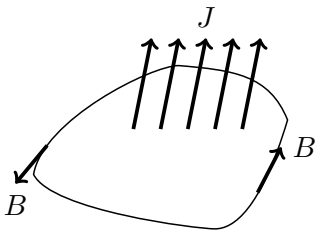
On the other hand, the boundary ∂S is given by the circle in the xy-plane, parametrized by $r(t) = \begin{pmatrix} a\cos t \\ a\sin t \\ 0 \end{pmatrix}$ for $t \in [0, 2\pi]$. Therefore, we obtain

$$\int_{\partial S} \psi \cdot ds = \int_0^{2\pi} \begin{pmatrix} a\sin t \\ -a\cos t \\ 0 \end{pmatrix} \cdot \begin{pmatrix} -a\sin t \\ a\cos t \\ 0 \end{pmatrix} dt = -a^2 \int_0^{2\pi} \sin^2 t + \cos^2 t \, dt = -2\pi a^2.$$

Example. A famous application of Stokes theorem is the derivation of Maxwell's equations in the case of a steady current , i.e.,

$$\operatorname{curl} B - \mu_0 J = 0,$$

where B is the magnetic field density, J is the current density and μ_0 is the magnetic constant.



Ampere's law (relating the magnetic field on the boundary with its inducing current) states that

$$\int_C B \cdot ds = \mu_0 \int_S J \cdot dS.$$

Using Stokes theorem for the integral on the left hand side gives

$$\int_S (\operatorname{curl} B - \mu_0 J) \cdot dS = 0.$$

Since S was arbitrary, this implies the equation $\operatorname{curl} B - \mu_0 J = 0$. Similarly, one can use Stokes theorem on Faraday's law (relating the change of a magnetic field over time to the change of the electric field in space) to derive

$$\operatorname{curl} E = -\frac{\partial B}{\partial t},$$

hence Maxwell's equations. ■

Chapter 5

Integral transformations

In this section, we introduce two widely used integral transformations, the Fourier and Laplace transformation, which can be used to decompose a function into its frequency parts.

5.1 Fourier series

Before we introduce the Fourier transformation, we discuss a similar topic, Fourier series.
The goal hereby is to write a given function f as a series (infinite sum) of certain sine and cosine functions with different frequencies. In the exercise part of the lecture, we introduced a different kind of series expansion, so called Taylor series, where a function was written as a sum of polynomials. In contrast to Taylor expansion, Fourier series use trigonometric functions and therefore can easily be integrated or differentiated.

We call a sum

$$T_N(x) := \frac{a_0}{2} + \sum_{k=1}^{N} [a_k \cos(kx) + b_k \sin(kx)]$$

a **trigonometric polynomial** of degree N and the limit $N \to \infty$ a **trigonometric series**.

In order to be able to expand a function f into a trigonometric series, it has to fulfill some requirements, the so called **Dirichlet conditions for Fourier series**, given by

1. f is periodic,
2. f is single valued and continuous except at a finite number of discontinuities,
3. f has a finite number of maxima and minima in one period,
4. The integral over $|f|$ must be finite.

The trigonometric series representation of a function goes back to the ideas and definition of the Hilbert space $L^2(I)$ in Chapter 2, where $I = [x_0, x_0 + L]$ is an interval of length L and x_0 is an arbitrary starting point. In fact, the previous definition of a trigonometric series is tailored to 2π-periodic functions (by the 2π-periodicity of sine and cosine). However, by making the variable transformation $x \mapsto \frac{2\pi}{L}x$, we can obtain expansions for arbitrary period lengths L.

With the L^2-inner product $(f,g)_{L^2(I)} = \int fg dx$, an orthogonal basis of $L^2(I)$ is given by the sine and cosine functions of different frequencies

$$\int_I \sin\Big(\frac{2\pi j}{L}x\Big)\cos\Big(\frac{2\pi \ell}{L}x\Big)\,dx = 0 \qquad \forall j,\ell$$

$$\int_I \sin\Big(\frac{2\pi j}{L}x\Big)\sin\Big(\frac{2\pi \ell}{L}x\Big)\,dx = \begin{cases} 0 & j=\ell=0 \\ \frac{L}{2} & j=\ell>0 \\ 0 & j\neq\ell \end{cases}$$

$$\int_I \cos\Big(\frac{2\pi j}{L}x\Big)\cos\Big(\frac{2\pi \ell}{L}x\Big)\,dx = \begin{cases} L & j=\ell=0 \\ \frac{L}{2} & j=\ell>0 \\ 0 & j\neq\ell \end{cases}.$$

In Chapter 2, we mentioned that, with an orthonormal basis $\{e_i\}$, a function f can be written as

$$f = \sum_{i=1}^{\infty}(f,e_i)e_i,$$

provided the series on the left-hand side converges. Therefore, the coefficients in the series expansion can be obtained by evaluating the scalar products (f,e_i). Now, taking for $\{e_i\}$ the sine and cosine functions from above (and normalizing those by division of $L/2$ or L respectively), we directly obtain the formulas in the following definition.

Definition 5.1. *Let $I=[x_0,x_0+L]$ and f be a given function defined on I that satisfies the Dirichlet conditions and has a period of length L. We call the expansion into a trigonometric series*

$$f(x) = \frac{a_0}{2} + \sum_{j=1}^{\infty}\left[a_j\cos\Big(\frac{2\pi j}{L}x\Big) + b_j\sin\Big(\frac{2\pi j}{L}x\Big)\right]$$

a Fourier series, if

$$a_0 = \frac{2}{L}\int_I f(x)dx$$
$$a_j = \frac{2}{L}\int_I f(x)\cos\Big(\frac{2\pi j}{L}x\Big)dx$$
$$b_j = \frac{2}{L}\int_I f(x)\sin\Big(\frac{2\pi j}{L}x\Big)dx.$$

The coefficients a_0, a_j, b_j are called the Fourier coefficients of f.

The evaluation of the integrals above usually requires integration by parts and can be lengthy. However, one can shorten some of the calculations for special cases of f. Since the sine functions are odd (i.e. $f(x) = -f(-x)$) and the cosine functions are even (i.e. $f(x) = f(-x)$), this can be exploited if the input function is also either even or odd and I is a symmetric interval around 0. Since the integral over an even function over a symmetric interval is zero, we have that $b_j = 0$ for all j, if f is even. In the same way, we have $a_j = 0$ for all j, if f is odd.

Example. Express the square-wave function given as the periodic extension of

$$f(t) = \begin{cases} -1 & -\frac{\tau}{2} \leq t < 0 \\ 1 & 0 \leq t < \frac{\tau}{2} \end{cases}$$

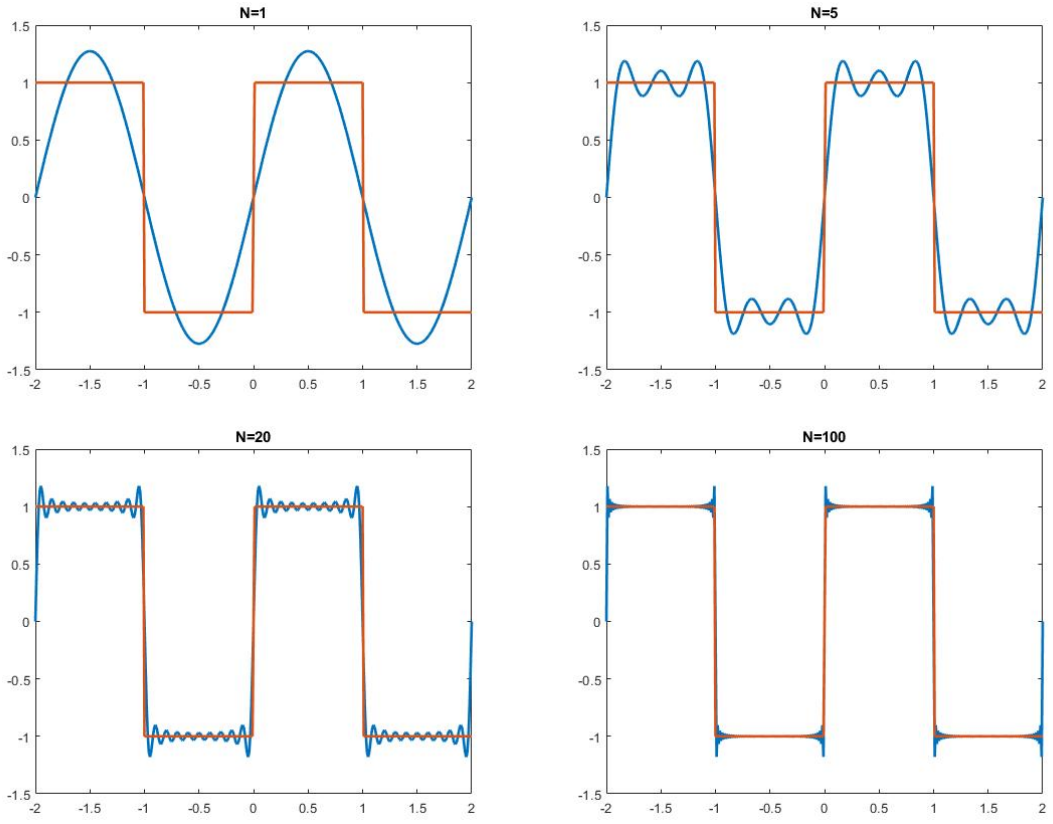
as a Fourier series.
By definition of f, we have that f is an odd function and therefore $a_j = 0$ for all j. It remains to compute the Fourier coefficients b_j. With the interval $I = [-\tau/2, \tau/2]$ and a period of length τ, we have

$$b_j = \frac{2}{\tau} \int_{-\tau/2}^{\tau/2} f(t) \sin\left(\frac{2\pi j}{\tau} t\right) dt = \frac{4}{\tau} \int_0^{\tau/2} \sin\left(\frac{2\pi j}{\tau} t\right) dt = \frac{2}{\pi j} \left(1 - (-1)^j\right),$$

where we used that the product f and the sine function is even (and therefore the integral over the negative part of the interval is the same as the integral over the positive part). Thus, $b_j = 0$ of $j \in \mathbb{N}$ is an even number and $b_j = \frac{4}{\pi j}$ if $j \in \mathbb{N}$ is an odd number. Therefore, we have the Fourier-series

$$f(t) = \frac{4}{\pi} \left(\sin(\omega t) + \frac{1}{3} \sin(3\omega t) + \frac{1}{5} \sin(5\omega t) + \dots \right),$$

where $\omega = \frac{2\pi}{\tau}$. ■



As mentioned previously and confirmed by the previous example, the derivation of a Fourier series works well also for functions with discontinuities, where the value at the discontinuity is an average of the jump values, as stated in the following theorem.

Theorem 5.2 (Dirichlet's theorem). *Let f satisfy the Dirichlet conditions. Then, the Fourier series of f converges to*

- *$f(x)$, if f is continuous at x;*
- *$\frac{f(x^+)+f(x^-)}{2}$, where $f(x^+) = \lim_{h\to 0, h\geq 0} f(x+h)$ and $f(x^-) = \lim_{h\to 0, h\geq 0} f(x-h)$ are the values on the right and left of the discontinuity at x.*

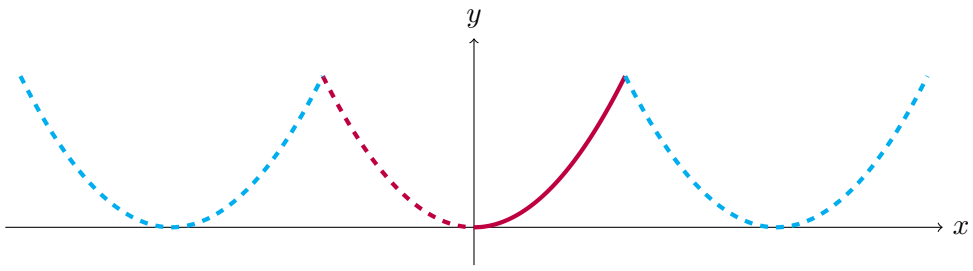
The Fourier series is always a continuous function.

Close to the discontinuity, the trigonometric polynomials with Fourier coefficients will produce an overshoot (compare pictures above), which is known as Gibbs' phenomenon. Increasing the number of terms in the expansion does not reduce the overshoot, it just moves it closer to the discontinuity.

As seen in the previous example, Fourier series can also be computed for non-periodic functions defined on an interval I by periodic extension of the function outside of I. This extension may also be chosen in a clever way, such that one obtained an even or odd function.

Example. We want to find the Fourier series for the function $f(x) = x^2$ in $0 \leq x \leq 2$.

The given function is not periodic, but can be periodically extended. A clever way to do that is to first extend the function to the interval $[-2, 0]$. Then, one has an even function on the interval $[-2, 2]$ that can be periodically extended to $\mathbb{R}$ (see the drawing below) by setting $f(x+4k) = f(x)$ for all $k \in \mathbb{N}$.



Since the extended function is even, we have $b_j = 0$ for all j. For the coefficients a_j, we compute

$$a_j = \frac{2}{4}\int_{-2}^{2} x^2 \cos\Big(\frac{2\pi j}{4}x\Big)dx = \int_{0}^{2} x^2 \cos\Big(\frac{2\pi j}{4}x\Big)dx = \frac{16}{\pi^2 j^2}(-1)^j$$

and for $j = 0$

$$a_j = \frac{2}{4}\int_{-2}^{2} x^2\, dx = \frac{8}{3}.$$

Therefore, we have the Fourier series

$$x^2 = \frac{4}{3} + 16\sum_{j=1}^{\infty} \frac{(-1)^j}{\pi^2 j^2} \cos\Big(\frac{\pi j}{2}x\Big) \qquad \text{for } 0 \le x \le 2.$$

■

We finish this subsection by rewriting the Fourier series by use of complex numbers. Euler's formula gives

$$e^{ikx} = \cos(kx) + i\sin(kx),$$

where i is the imaginary unit. Then, a Fourier series can also be expressed by means of complex exponentials as

$$f(x) = \sum_{k=-\infty}^{\infty} c_k \exp\Big(\frac{2\pi ik}{L}x\Big)$$

with

$$c_k = \frac{1}{L}\int_{x_0}^{x_0+L} f(x)\exp\Big(-\frac{2\pi ik}{L}x\Big)dx.$$

We note that the coefficients c_k are related to the real Fourier coefficients by

$$c_k = \frac{1}{2}(a_k - ib_k)$$
$$c_{-k} = \frac{1}{2}(a_k + ib_k).$$

Example. We want to compute the complex Fourier series of $f(x) = x$ in $I = [-2, 2]$. The above definition gives using integration by parts

$$\begin{aligned} c_k &= \frac{1}{4}\int_{-2}^{2} x\exp\Big(-\frac{\pi ik}{2}x\Big)dx \\ &= -\frac{x}{2\pi ik}\exp\Big(-\frac{\pi ik}{2}x\Big)\Big|_{-2}^{2} + \frac{1}{2\pi ik}\int_{-2}^{2}\exp\Big(-\frac{\pi ik}{2}x\Big)dx \\ &= -\frac{1}{\pi ik}(\exp(-\pi ik) + \exp(\pi ik)) + \frac{1}{\pi^2k^2}\exp\Big(-\frac{\pi ik}{2}x\Big)\Big|_{-2}^{2} = \frac{2i}{\pi k}(-1)^k. \end{aligned}$$

For $k = 0$ above formula is undefined, but setting $k = 0$ in the definition of c_k gives

$$c_0 = \int_{-2}^{2} x\ dx = 0,$$

and we obtain the complex Fourier series

$$x = \sum_{k=-\infty, k\neq 0}^{\infty} \frac{2i(-1)^k}{\pi k}\exp\Big(\frac{\pi ik}{2}x\Big).$$

■

5.2 The Fourier transformation

Roughly speaking, the Fourier transformation can be seen as a generalization of Fourier series for functions that are defined on $\mathbb{R}$ and do not have any particular periodicity.

For the existence of a Fourier transformation of a function $f(t)$ (note that we explicitly use t as a variable, since most applications deal with time dependent signals), we hereby only require $\int_{-\infty}^{\infty} |f(t)|\, dt < \infty$.

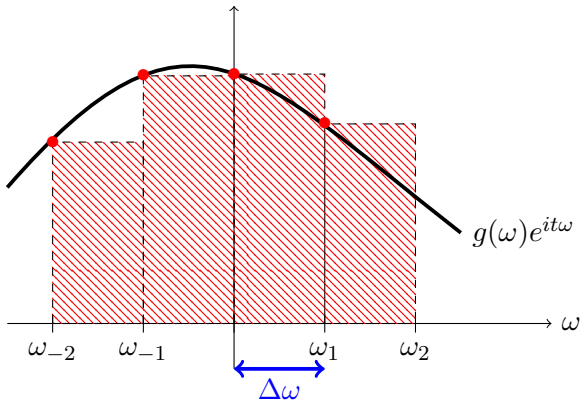
For the derivation of the Fourier transformation, we start with the complex Fourier series on an interval $[-T/2, T/2]$ of length T given by

$$f(t) = \sum_{k=-\infty}^{\infty} c_k \exp\Big(i\omega_k t\Big)$$

with $\omega_k = \frac{2\pi k}{T}$ and the Fourier coefficients

$$c_k = \frac{1}{T}\int_{-T/2}^{T/2} f(y) \exp\Big(-\frac{2\pi i k}{T} y\Big) dy = \frac{\Delta\omega}{2\pi}\int_{-T/2}^{T/2} f(y)\, e^{-i\omega_k y} dy$$

with $\Delta\omega = \frac{2\pi}{T}$.



Now, we can understand $c_k e^{i\omega_k t}$ as an evaluation of the function $\frac{\Delta\omega}{2\pi} g(\omega) e^{it\omega}$ with

$$g(\omega) = \int_{-T/2}^{T/2} f(u) e^{-i\omega u} du$$

at the point ω_k and ω_k is the right endpoint of the interval $[2\pi(k-1)/T, 2\pi kT]$ of length $\Delta\omega$. The union of all this intervals is $\mathbb{R}$ and we, in fact, can understand $\sum_{k=-\infty}^{\infty} \frac{\Delta\omega}{2\pi} g(\omega_k) e^{i\omega_k t}$ as a Riemann-sum and taking the limit $T \to \infty$ (note that T is the length of the period in the Fourier series) gives $\Delta\omega \to 0$ as well as

$$\begin{aligned} f(t) &= \lim_{T\to\infty} \sum_{k=-\infty}^{\infty} \frac{\Delta\omega}{2\pi} g(\omega_k) e^{i\omega_k t} = \frac{1}{2\pi}\int_{-\infty}^{\infty} g(\omega) e^{i\omega t} d\omega \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} f(u) e^{-i\omega u} du\right) e^{i\omega t} d\omega, \end{aligned}$$

which is known as **Fourier's inversion formula** and motivates the following definitions.

Definition 5.3. *Let f be a scalar function satisfying $\int_{-\infty}^{\infty} |f(t)|\,dt < \infty$.*
The **Fourier transformation** *of f is defined as the function*

$$\mathcal{F}[f(t)](\omega) := \widehat{f}(\omega) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{-i\omega t} dt.$$

In the same way, the **inverse Fourier transformation** *is given by*

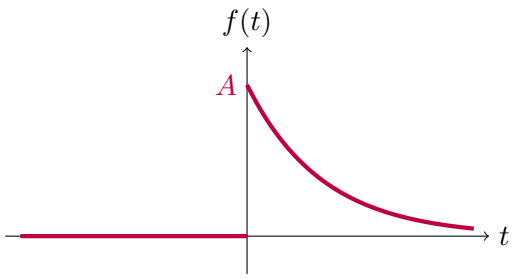
$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widehat{f}(\omega) e^{i\omega t} d\omega.$$

We note that the constants $\frac{1}{\sqrt{2\pi}}$ in front of both integrals was chosen here in the way that both formulas have the same constant. However, different choices are possible as well, as long as the product of both constants is $\frac{1}{2\pi}$ and oftentimes in literature the Fourier transformation is defined with the prefactor $\frac{1}{2\pi}$ and the inverse Fourier transformation with the prefactor 1.

Example. We want to compute the Fourier transformation of the signal

$$f(t) = \begin{cases} 0 & t < 0 \\ Ae^{-\lambda t} & t \geq 0 \end{cases}$$

for $\lambda > 0$.



We have $\int_{-\infty}^{\infty} |f(t)|\,dt < \infty$ and get the Fourier transformation

$$\widehat{f}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{0} 0 e^{-i\omega t} dt + \frac{A}{\sqrt{2\pi}} \int_{0}^{\infty} e^{-\lambda t} e^{-i\omega t} dt = 0 - \frac{A}{\sqrt{2\pi}} \frac{e^{-(\lambda + i\omega)t}}{\lambda + i\omega} \Big|_0^{\infty} = \frac{A}{\sqrt{2\pi}(\lambda + i\omega)}.$$

■

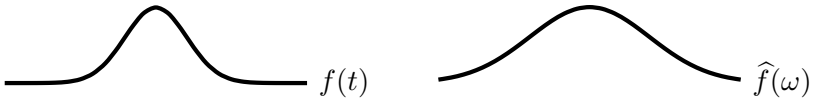
In the following, we consider two important examples from physical applications, the **Gaussian normal distribution** and the Dirac δ-distribution.
Many applications measure random effects, e.g., think about the uncertainty principle in quantum mechanics, that follow a Gaussian distribution given by

$$f(t) = \frac{1}{\sigma\sqrt{2\pi}} e^{-t^2/(2\sigma^2)},$$

where σ^2 is the variance. Then, the Fourier transformation of f is given by

$$\widehat{f}(\omega) = \frac{1}{\sqrt{2\pi}} e^{-\omega^2\sigma^2/2}.$$

Hence, the Fourier transform is again a Gaussian distribution with variance $\widehat{\sigma}^2 = \frac{1}{\sigma^2}$.
In physical terms, this can be stated as: the narrower, e.g., an electrical impulse, in time is, the greater the spread of frequencies it contains is.



The second important application is given by the Dirac δ-distribution, which can be seen as a very sharp narrow pulse (in space, time, density, current, ...). In fact, in physics the Dirac δ appears whenever one models the density of a point mass.

Definition 5.4. *The* **Dirac δ-distribution** *is defined by the properties $\delta(t) = 0$ for all $t \neq 0$ and*

$$f(t) = \int_{-\infty}^{\infty} f(x)\delta(x-t)dx$$

for any function f (that is infinitely times differentiable, only non-zero on a bounded interval).

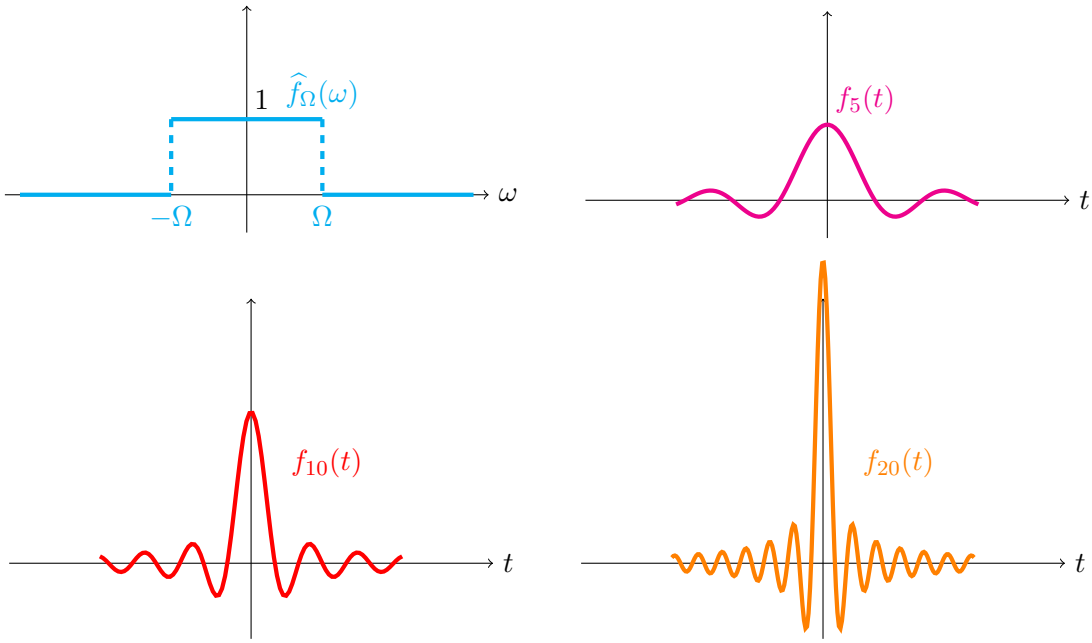
Note that taking $f \equiv 1$ this implies $\int_{-\infty}^{\infty} \delta(x)dx = 1$, so the δ-distribution is zero everywhere but at 0, but has to be infinite there, i.e., it is not a function in the classical sense. Using the Fourier transformation, we may obtain an idea how to interpret it.
The Fourier inversion formula gives

$$\begin{aligned} f(t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty}\left(\int_{-\infty}^{\infty} f(u)e^{-i\omega u}du\right)e^{i\omega t}d\omega \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(u)e^{i\omega(t-u)}d\omega\, du \\ &= \int_{-\infty}^{\infty} f(u)\left(\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega(t-u)}d\omega\right)du. \end{aligned}$$

Comparing this with the equation in the definition of the δ-distribution, we have

$$\delta(t-u) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega(t-u)}d\omega.$$

Therefore, the δ-distribution results from the superposition of a complete spectrum of harmonic waves, where all frequencies have the same amplitude and they are in phase at $t = u$. This suggests that the δ distribution can also be represented as the limit of the transformation of a uniform distribution on $[-\Omega, \Omega]$, i.e., the step function $\widehat{f}_\Omega(\omega) = \begin{cases} 1 & x \in [-\Omega, \Omega] \\ 0 & x \in \mathbb{R}\backslash[-\Omega, \Omega] \end{cases}$.



Applying the inverse Fourier transformation gives

$$f_\Omega(t) = \frac{1}{\sqrt{2\pi}} \int_{-\Omega}^{\Omega} 1 e^{i\omega t} d\omega = \frac{2\Omega}{\sqrt{2\pi}} \frac{\sin(\Omega t)}{\Omega t}$$

Now, as $\Omega \to \infty$, we have that - as expected - the peak at $t = 0$ becomes unbounded, and by the above computed representation with the Fourier inversion Formula, we could also define the δ-distribution by

$$\delta(t) := \lim_{\Omega \to \infty} \left(\frac{\sin(\Omega t)}{\pi t} \right).$$

5.2.1 Properties of the Fourier transformation

The Fourier transformation has the properties:

1. Differentiation turns into multiplication with ω: $\mathcal{F}[f'(t)](\omega) = i\omega \mathcal{F}(f)(\omega)$;
2. Integration turns into division with ω: $\mathcal{F}\left[\int_0^t f(y)dy\right](\omega) = \frac{1}{i\omega}\mathcal{F}[f](\omega) + 2\pi\delta(\omega)$;
3. Scaling: $\mathcal{F}[f(at)](\omega) = \frac{1}{a}\mathcal{F}[f(t)]\left(\frac{\omega}{a}\right)$;
4. Translation turns into multiplication with an exponential: $\mathcal{F}[f(t+a)](\omega) = e^{ia\omega}\mathcal{F}[f(t)](\omega)$.

Exemplary, we prove the first property. The assumption $\int_{-\infty}^{\infty} |f(t)|\, dt < \infty$ implies $\lim_{t \to \pm\infty} f(t) = 0$. Therefore, using integration by parts, we have

$$\begin{aligned}
\mathcal{F}[f'(t)](\omega) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f'(t) e^{-i\omega t} dt \\
&= \frac{1}{\sqrt{2\pi}} f(t) e^{-i\omega t} \Big|_{-\infty}^{\infty} + \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} i\omega f(t) e^{-i\omega t} dt \\
&= i\omega \mathcal{F}(f)(\omega).
\end{aligned}$$

Similarly to Fourier series, the computation of the Fourier transformation can be simplified for even or odd functions f. If f is odd, the Fourier transformation can be reduced to computing the Fourier sine transformation

$$\widehat{f}_s(\omega) = \sqrt{\frac{2}{\pi}} \int_0^\infty f(t) \sin(\omega t) dt.$$

For even functions f one would obtain the Fourier cosine transformation

$$\widehat{f}_c(\omega) = \sqrt{\frac{2}{\pi}} \int_0^\infty f(t) \cos(\omega t) dt.$$

The following theorem, which is called Plancherel identity (or sometimes also called Parseval's identity), links the squared integral of a function to the squared integral of its Fourier transformation and is very useful tool e.g. in error analysis.

Theorem 5.5. *Let f be such that $\int_{-\infty}^{\infty} |f(t)|\, dt < \infty$ and additionally assume $\int_{-\infty}^{\infty} |f(t)|^2\, dt < \infty$. Then,*

$$\int_{-\infty}^{\infty} |f(t)|^2\, dt = \int_{-\infty}^{\infty} \left|\widehat{f}(\omega)\right|^2 d\omega.$$

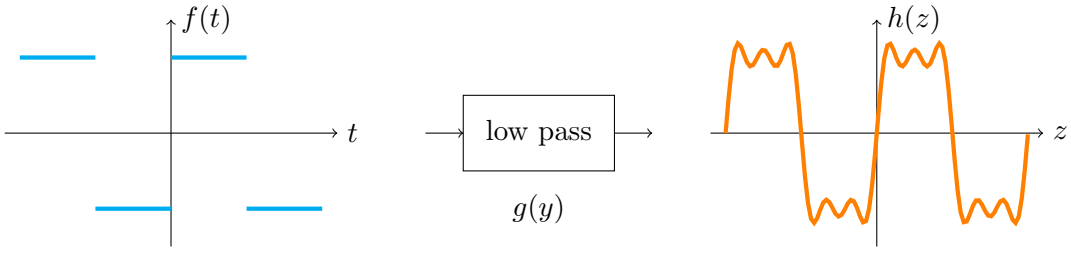
We note that the Fourier transformation is not restricted to the case of functions in one variable as its derivation can be naturally generalized to functions in more variables. E.g., in three dimensions the Fourier transform is given by

$$\widehat{f}(\omega_x, \omega_y, \omega_z) = \frac{1}{(2\pi)^{3/2}} \int\int\int f(x, y, z) e^{-i\omega_x x} e^{-i\omega_y y} e^{-i\omega_z z} dx\, dy\, dz.$$

5.2.2 Convolution and deconvolution

The convolution of signals or functions is a very important tool to describe the output of linear systems, e.g., in electrical engineering.

Going back to the example of the square wave function, we have obtained the Fourier series as a sum of sine functions with different, increasing frequencies. A very useful tool in the analysis of signals is given by filters that allow only certain frequencies to pass through the filter and damp the other frequencies. The most common filters are a low pass filter (that allows low frequencies to pass through) and a high pass filter (that allows high frequencies to pass through).



We assume that we have a low pass filter, that is described by a function $g(y)$. Then, the convolution is the operation that relates the output h with the input f and g and is given by the following definition.

Definition 5.6. *Let f and g be scalar functions. The* **convolution** *of f and g is a scalar function h also written as $f \star g$ defined as*

$$h(z) = f \star g(z) = \int_{-\infty}^{\infty} f(x)g(z-x)dx$$

The convolution has the following properties:

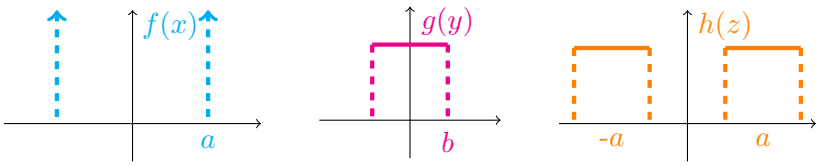
- commutative: $f \star g = g \star f$;
- associative: $f \star (g \star h) = (f \star g) \star h$;
- linear: $(f+g) \star h = f \star h + g \star h$;
- δ-distribution is the "neutral element": $f \star \delta = f$.

Example. We want to compute the convolution of $f(x) = \delta(x+a) + \delta(x-a)$ with $g(y)$, where

$$g(y) = \begin{cases} 1 & |y| \leq b \\ 0 & \text{else.} \end{cases}$$

We compute

$$h(z) = \int_{-\infty}^{\infty} (\delta(x+a) + \delta(x-a))g(z-x)dx = g(z+a) + g(z-a).$$



■

We now compute the Fourier transformation of the convolution $h = f \star g$

$$\begin{aligned} \widehat{h}(\omega) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x)g(z-x)dx\, e^{-i\omega z} dz \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x)g(z-x)e^{-i\omega z} dz\, dx \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \int_{-\infty}^{\infty} g(z-x)e^{-i\omega z} dz\, dx. \end{aligned}$$

Now, making the transformation $u = z - x$, we get

$$\begin{aligned}\widehat{h}(\omega) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \int_{-\infty}^{\infty} g(u) e^{-i\omega(u+x)} du\, dx \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-i\omega x} dx \int_{-\infty}^{\infty} g(u) e^{-i\omega u} du \\ &= \sqrt{2\pi}\, \widehat{f}(\omega)\, \widehat{g}(\omega).\end{aligned}$$

Therefore, up to the prefactor $\sqrt{2\pi}$ the Fourier transformation turns convolution into multiplications and the other way round

$$\begin{aligned}\mathcal{F}[f \star g](\omega) &= \sqrt{2\pi}\mathcal{F}[f](\omega) \cdot \mathcal{F}[g](\omega), \\ \mathcal{F}[f \cdot g](\omega) &= \frac{1}{\sqrt{2\pi}}(\mathcal{F}[f] \star \mathcal{F}[g])(\omega).\end{aligned}$$

The inverse operation to convolution is called deconvolution and allows to reconstruct the function f, when the output h and the filter g are known. In fact, using the Fourier transformation this can be computed as

$$\widehat{h}(\omega) = \sqrt{2\pi}\, \widehat{f}(\omega)\, \widehat{g}(\omega) \quad \Longrightarrow \quad \widehat{f}(\omega) = \frac{1}{\sqrt{2\pi}} \frac{\widehat{h}(\omega)}{\widehat{g}(\omega)} \quad \Longrightarrow \quad f(t) = \frac{1}{\sqrt{2\pi}} \mathcal{F}^{-1}\left(\frac{\widehat{h}(\omega)}{\widehat{g}(\omega)} \right).$$

However, in practice, an exact reconstruction of f is hardly ever possible, since h oftentimes is given by measurements, which always include some kind of measurement error.

5.3 The Laplace transformation

In this section, we present a transformation with similar properties as the Fourier transformation, which can be applied for certain functions that do not meet the requirement $\int_{-\infty}^{\infty} |f(t)|\, dt < \infty$ for the existence of the Fourier transformation such as the function $f(t) = t$. Additionally, we are only interested in functions on $t > 0$, which is motivated by the initial value problems in the next chapter, and we arrive at the so called Laplace transformation.

Definition 5.7. *Let f be a scalar function. Then, the* **Laplace transformation** *of f is defined as the function*

$$\mathcal{L}[f(t)](s) = \overline{f}(s) = \int_0^{\infty} f(t) e^{-st} dt,$$

provided the integral on the right-hand side exists.

Here, we assume that s is real, but an extension to complex numbers is possible.

We note that the integral above is an improper integral (which we defined in the exercise part of the lecture) as the limit

$$\int_0^{\infty} f(t) e^{-st} dt = \lim_{R \to \infty} \int_0^{R} f(t) e^{-st} dt.$$

A sufficient condition for the existence of the limit is that the function f is of **exponential order** $s_0 \in \mathbb{R}$, which means that there are constants $T \geq 0$ and $C > 0$ such that

$$|f(t)| \leq Ce^{s_1 t} \qquad \text{for all } s_1 > s_0 \text{ and } t \geq T.$$

This means that f grows at most exponentially. E.g., the function x^2 is of exponential order with $s_0 = 0$. For functions of exponential order s_0, the integral can be estimated by (for simplicity we set $T = 0$)

$$\int_0^\infty f(t)e^{-st}dt \leq \int_0^\infty |f(t)|\, e^{-st}dt \leq C\int_0^\infty e^{s_1 t}e^{-st}dt = \frac{C}{s - s_1} \qquad s_1 > s_0.$$

As $s_1 > s_0$ was arbitrary, this shows that the integral (only) exists for all s with $s > s_0$. Therefore, the Laplace transformation might only exist from a certain point s_0 onwards (which is determined by the given function).

Example. We compute the Laplace transformation for some simple functions.

1. Let $f(t) = 1$. Then,

$$\mathcal{L}[1](s) = \int_0^\infty e^{-st}dt = \frac{1}{s} \quad s > 0.$$

2. Let $f(t) = e^{at}$ for $a \in \mathbb{R}$. Then,

$$\mathcal{L}[e^{at}](s) = \int_0^\infty e^{at}e^{-st}dt = \int_0^\infty e^{(a-s)t}dt = \frac{1}{s - a} \quad s > a.$$

3. Let $f(t) = t^n$ for $n \in \mathbb{N}$. Then, with integration by parts, we obtain

$$\begin{aligned}\mathcal{L}[t^n](s) &= \int_0^\infty t^n e^{-st}dt = -\frac{t^n e^{-st}}{s}\Big|_0^\infty + \frac{n}{s}\int_0^\infty t^{n-1}e^{-st}dt \\ &= 0 + \frac{n}{s}\mathcal{L}[t^{n-1}](s) \qquad s > 0,\end{aligned}$$

   where the boundary term only disappears for $s > 0$. Thus, we have derived a recursion formula. With $n = 0$ ($t^0 = 1$) being covered by the first example, we can successively insert this in the recursion formula and obtain

$$\begin{aligned}\mathcal{L}[t](s) &= \frac{1}{s}\mathcal{L}[1](s) = \frac{1}{s^2} \\ \mathcal{L}[t^2](s) &= \frac{2}{s}\mathcal{L}[t](s) = \frac{2}{s^3} \\ &\vdots \\ \mathcal{L}[t^n](s) &= \frac{n}{s}\mathcal{L}[t^{n-1}](s) = \frac{n!}{s^{n+1}} \qquad s > 0.\end{aligned}$$

■

One of the main uses of the Laplace transformation - as we will also see in the next chapter - is the solution of differential equations. This is due to the following formula, which is similar to the property of the Fourier transformation applied to derivatives

$$\begin{aligned}\mathcal{L}[f'](s) &= \int_0^\infty f'(t)e^{-st}dt = f(t)e^{-st}\Big|_0^\infty + s\int_0^\infty f(t)e^{-st}dt \\ &= -f(0) + s\mathcal{L}[f](s), \qquad s > 0.\end{aligned}$$

We sum up this together with other important **properties of the Laplace transformation** (which are similar to those of the Fourier transformation):

1. Linearity: Let $a, b \in \mathbb{R}$ and f, g be scalar functions whose Laplace transformations exist. Then,

$$\mathcal{L}[af + bg](s) = a\mathcal{L}[f](s) + b\mathcal{L}[g](s).$$

2. Higher order derivatives: applying the above argument for the first order derivative gives

$$\mathcal{L}\left[\frac{d^n f}{dt^n}\right](s) = s^n\mathcal{L}[f](s) - s^{n-1}f(0) - s^{n-2}f'(0) - \cdots - \frac{d^{n-1}f}{dt^{n-1}}(0)$$

   for $n \in \mathbb{N}$.

3. Conversely, multiplication with a polynomial becomes differentiation

$$\mathcal{L}\left[t^n f(t)\right](s) = (-1)^n \frac{d^n}{ds^n}\mathcal{L}\left[f\right](s).$$

4. Integration becomes division

$$\mathcal{L}\left[\int_0^t f(u)du\right](s) = \frac{1}{s}\mathcal{L}\left[f(t)\right](s).$$

5. Multiplication with an exponential becomes translation

$$\mathcal{L}\left[e^{at}f(t)\right](s) = \int_0^\infty e^{at}e^{-st}dt = \mathcal{L}\left[f(t)\right](s-a).$$

6. Scaling: Let $a \in \mathbb{R}$. Then,

$$\mathcal{L}\left[f(at)\right](s) = \frac{1}{a}\mathcal{L}\left[f(t)\right](s/a)$$

7. Convolution becomes multiplication

$$\mathcal{L}\left[f \star g\right](s) = \mathcal{L}\left[f\right](s) \cdot \mathcal{L}\left[g\right](s).$$

Example. We want to compute the Laplace transformation of $f(t) = t\sin t$. While this can be done directly using integration by parts, a much simpler way is to use the properties stated above. As multiplication with t turns into differentiation, we have

$$\mathcal{L}[t\sin t] = -\frac{d}{ds}\mathcal{L}[\sin(t)](s) = -\frac{d}{ds}\frac{1}{s^2+1} = \frac{2s}{(s^2+1)^2},$$

where the Laplace transformation of the sine function can be directly computed or seen in the table below. ■

While the inverse Fourier transformation is essentially the same operation as the Fourier transformation and is therefore explicitly given, the inverse operation for the Laplace transformation is considerably harder to obtain. A general derivation would require some deeper tools from complex function theory. However, for some simple functions the inverse Laplace transformation is known and we present them in the following table, which can be used for future computations.

$f(t)$	$\mathcal{L}(f)(s)$	$s > s_0$
c	$\frac{c}{s}$	0
t^n	$\frac{n!}{s^{n+1}}$	0
$\sin(bt)$	$\frac{b}{s^2+b^2}$	0
$\cos(bt)$	$\frac{s}{s^2+b^2}$	0
e^{at}	$\frac{1}{s-a}$	a
$t^n e^{at}$	$\frac{n!}{(s-a)^{n+1}}$	a
$e^{at}\sin(bt)$	$\frac{b}{(s-a)^2+b^2}$	a
$e^{at}\cos(bt)$	$\frac{s-a}{(s-a)^2+b^2}$	a
$\sqrt{t}$	$\frac{1}{2}\sqrt{\frac{\pi}{s^3}}$	0
$\frac{1}{\sqrt{t}}$	$\sqrt{\frac{\pi}{s}}$	0
$\delta(t-t_0)$	$e^{-t_0 s}$	0
$H(t-t_0) = \begin{cases} 1 & t \geq t_0 \\ 0 & t < t_0 \end{cases}$	$\frac{e^{-t_0 s}}{s}$	0
$\sinh(bt)$	$\frac{b}{s^2-b^2}$	$\lvert b\rvert$
$\cosh(bt)$	$\frac{s}{s^2-b^2}$	$\lvert b\rvert$

With this dictionary and the linearity of the Laplace transformation (and its inverse), we actually can compute the inverse transformation for a lot of commonly appearing functions.

Example. We want to compute $f(t)$, where the Laplace transformation is given by

$$\mathcal{L}[f](s) = \frac{s+3}{s(s+1)}.$$

With a partial fraction decomposition, we can write

$$\frac{s+3}{s(s+1)} = \frac{3}{s} - \frac{2}{s+1},$$

and the linearity of the inverse Laplace transformation then gives

$$\begin{aligned} f(t) &= \mathcal{L}^{-1}\Big[\mathcal{L}[f]\Big](t) = 3\mathcal{L}^{-1}\Big[\frac{1}{s}\Big](t) - 2\mathcal{L}^{-1}\Big[\frac{1}{s+1}\Big](t) \\ &= 3 - 2e^{-t} \qquad s > 0, \end{aligned}$$

where we used the above table for the inverse transformations of the simple functions. ■

Chapter 6

Differential equations

In this chapter, we are concerned with differential equations, i.e., equations that contain a function and/or derivatives of that function. We distinguish between differential equations of functions in one variable, which we call ordinary differential equations, and differential equations of functions in multiple variables, which we call partial differential equations.
Differential equations have many fields of application, lots of physical laws, chemical processes or population dynamics in biology can be formulated as differential equations.

6.1 Ordinary differential equations

We start with the case of functions in one variable, i.e., $u : \mathbb{R} \to \mathbb{R}$. In the most general form, an **ordinary differential equation** (short: ODE), is given as the equation

$$F(x, u(x), u'(x), \ldots, u^{(n)}(x)) = 0.$$

The **order** of an ODE is given as the largest natural number $n \in \mathbb{N}$, for which the derivative $u^{(n)}$ appears in the equation.
A function u that satisfies the ODE at every point x is called a **solution** of the ODE.

Example.

1. The equation
$$u'(x) + u(x) = 0$$
is an ODE of first order. A solution is given by $u(x) = e^{-x}$, and, in fact, ce^{-x} for every $c \in \mathbb{R}$ also solves the equation.

2. The equation
$$(u''(x))^2 + u(x)^2 = 0$$
is an ODE of second order that has only the solution $u(x) = 0$.

3. The equation
$$(u'(x))^2 = -1$$
is a first order ODE an has no real valued solution.

4. The equation
$$u^{(3)}(x) = x$$
is an ODE of order 3 and can be solved by integrating 3-times. This gives $u(x) = \frac{1}{24}x^4 + ax^2 + bx + c$ as the general solution, where a, b, c are arbitrary constants of integration. ■

The previous examples shows that, in general, solutions to ODEs do not have to exist and do not have to be unique. So, for a general theory about ODEs, some additional assumptions need to be made.

6.1.1 First order ODEs

We start with the case of first order ODE, which in literature are written in either one of two equivalent forms
$$u'(x) = F(x, u) \qquad \text{or } A(x, u)\, dx + B(x, u)\, du = 0,$$
where $F(x, u) = -A(x, u)/B(x, u)$.

Example. Let $T(t)$ be the temperature of an object that is, e.g., surrounded by water with constant temperature T_w. Then, Newton's law of cooling in thermodynamics states that the change of temperature in the object is proportional to the temperature difference to the surrounding, i.e.,
$$T'(t) = -k(T(t) - T_w),$$
where $k > 0$ is a material dependent constant that describes the heat transfer intensity. ■

In the following, we present some special cases of first order ODEs.

Separable first order ODEs

Separable ODEs are a special case of first order ODEs that can be written as
$$u'(x) = f(x)g(u),$$
so the variables x and u on the right-hand side can be multiplicatively separated. Division with $g(u)$, integrating the equation in x and using the transformation theorem, we obtain
$$\int \frac{1}{g(u)} du = \int \frac{1}{g(u(x))} u'(x) dx = \int f(x)\, dx.$$
Now, if both integrals on the left-hand side and right-hand side can be computed, we obtain an equation for the solution u.

Example. The ODE
$$u'(x) = x + xu$$
is separable with $f(x) = x$ and $g(u) = 1 + u$. Using the formula from above, we obtain
$$\int \frac{1}{u+1} du = \int x dx$$
and computing the integrals gives the equation
$$\ln(1 + u) = \frac{x^2}{2} + C \qquad \Longrightarrow \qquad u(x) = e^{x^2/2+c} - 1 = Ce^{x^2/2} - 1,$$
with an arbitrary constant $C \in \mathbb{R}$.

Exact equations

We call an ODE

$$A(x,u)dx + B(x,u)du = 0 \qquad \text{or} \qquad u'(x) = -\frac{A(x,u)}{B(x,u)}$$

exact, if there is a function $H(x,u)$ such that $\frac{\partial H}{\partial x} = A$ and $\frac{\partial H}{\partial u} = B$. In other words, this means that the vectorfield $\begin{pmatrix} A \\ B \end{pmatrix}$ is a gradient field and H is its scalar potential. We recall that one can check whether $\begin{pmatrix} A \\ B \end{pmatrix}$ is a gradient field and correspondingly whether the above ODE is exact, if

$$\frac{\partial A}{\partial u} = \frac{\partial B}{\partial x}.$$

Solving the ODE is then done by computing the scalar potential $H(x,u)$, since

$$\frac{d}{dx}H(x,u(x)) = \frac{\partial H}{\partial x} + \frac{\partial H}{\partial u}u'(x) = A(x,u) + B(x,u)u'(x) = 0$$

gives $H(x,u(x)) = c$ and from that equation, one can express $u(x)$.

Example. We want to solve the ODE

$$xu'(x) + u + 3x = 0.$$

We have $A(x,u) = u + 3x$ and $B(x,u) = x$. Since

$$\frac{\partial A}{\partial u} = 1 = \frac{\partial B}{\partial x}$$

we have an exact ODE and we can compute the scalar potential H as described in the previous section by integration

$$H(x,u) = \int A(x,u)dx + g(u) = \frac{3}{2}x^2 + xu + g(u)$$

and differentiation to fix the function $g(u)$

$$x = B(x,u) = \frac{\partial H}{\partial u} = x + g'(u),$$

which implies that $g'(u) = 0$ and $g(u) = c_1$. Now, from the equation $H(x,u) = c_2$, we see that the solution to the ODE has to satisfy

$$\frac{3}{2}x^2 + xu + c_1 = c_2$$

or $u(x) = \frac{1}{x}(c - \frac{3}{2}x^2)$ with $c = c_2 - c_1$. ■

Inexact equations, integrating factors

As we know from the previous chapter, not all vector fields are gradient fields and consequently, we have that not all ODEs are exact. An inexact first order ODE is characterized by

$$\frac{\partial A}{\partial u} \neq \frac{\partial B}{\partial x}.$$

However, in some cases, it is possible to still solve such equations by introducing so called **integrating factors**. The idea is to multiply the ODE with a function $\mu(x,u)$, i.e., one tries to solve the equation $\mu(x,u)A(x,u)dx + \mu(x,u)B(x,u)du = 0$, where μ is such that

$$\frac{\partial(\mu A)}{\partial u} = \frac{\partial(\mu B)}{\partial x}.$$

Thus, the new ODE is exact. In general, if μ is an arbitrary function of both variables, there is no way to compute it. If, however, μ does only depend on one variable, i.e., $\mu = \mu(x)$ or $\mu = \mu(u)$ (or other cases like $\mu = \mu(x+y)$ or $\mu = \mu(xy)$) one has a chance.
For example, if $\mu = \mu(x)$ the condition for an exact ODE reduces to

$$\mu\frac{\partial A}{\partial u} = \mu\frac{\partial B}{\partial x} + B\frac{\partial \mu}{\partial x},$$

which is a separable ODE in μ that can be solved as explained above and we arrive at the integrating factor

$$\mu = \exp\left(\int f(x)dx\right) \qquad \text{with} \qquad f = \frac{1}{B}\left(\frac{\partial A}{\partial u} - \frac{\partial B}{\partial x}\right).$$

Similarly, if $\mu = \mu(u)$, we have

$$\mu = \exp\left(\int g(u)du\right) \qquad \text{with} \qquad g = \frac{1}{A}\left(\frac{\partial B}{\partial x} - \frac{\partial A}{\partial u}\right).$$

Thus, in order to obtain an integrating factor an ansatz has to be made (by clever guessing) and checked by trying to compute μ.

Example. We want to solve the ODE

$$(4x + 3u^2)\,dx + 2xu\,du = 0 \qquad \text{or} \qquad u'(x) = -\frac{4x+3u^2}{2xu}.$$

We have $A(x,u) = 4x + 3u^2$ and $B(x,u) = 2xu$. The equation is inexact, since

$$\frac{\partial A}{\partial u} = 6u \neq 2u = \frac{\partial B}{\partial x}.$$

But, since

$$f = \frac{1}{B}\left(\frac{\partial A}{\partial u} - \frac{\partial B}{\partial x}\right) = \frac{1}{2xu}(6u - 2u) = \frac{2}{x}$$

is only a function of x, we have that $\mu = \mu(x)$ and by the above formula we obtain

$$\mu(x) = e^{2\int \frac{1}{x}dx} = e^{2\ln x} = x^2.$$

Multiplying the ODE with μ gives the equivalent ODE

$$(4x^3 + 3x^2u^2)dx + 2x^3udu = 0,$$

for which we can compute a scalar potential as $H(x,u) = x^4 + u^2x^3$. Finally, u can be expressed from the equation $H(x,u) = c$.

6.1.2 Higher order ODEs

The solution of higher order ODEs is much harder and solution formulas are only known for very special cases.

In the following, we focus on **linear ODEs**, which means that the function $F(x, u(x), u'(x), \dots)$ depends only linearly on $u(x)$ and all derivatives of u. A linear ODE of order n can be written as

$$a_n(x)u^{(n)}(x) + a_{n-1}(x)u^{(n-1)}(x) + \cdots + a_1(x)u'(x) + a_0(x)u(x) = f(x).$$

If $f(x) = 0$, we call the linear ODE **homogeneous**.

Theorem 6.1. *Let the coefficient functions $a_0, \dots, a_n$ be continuous on an interval $I \subset \mathbb{R}$. Then, we have that the solutions to the corresponding homogeneous linear ODE form an n-dimensional vector space.*

This theorem implies that the **general solution** to the ODE can be written by linear combination of n functions b_i that are linearly independent and all solve the ODE, i.e.,

$$u(x) = \sum_{i=1}^{n} c_i b_i(x).$$

In order to fix the constants c_i and obtain a unique solution, n values of u (or derivatives of u) have to be prescribed. If only values at 0 (or in general a starting point t_0) are prescribed, i.e.,

$$\begin{aligned} u(0) &= u_0 \\ u'(0) &= u_1 \\ &\vdots \\ u^{(n-1)}(0) &= u_{n-1} \end{aligned}$$

we speak of so called **initial value problems**. If one is interested on the solution on a bounded interval $I = [0, T]$, another way to determine the constants c_i would be to prescribe both values of u (or derivatives of u) at $x = 0$ and $x = T$. In that case, we have a so called **boundary value problem**.

Equations with constant coefficients

In the following, we assume that all coefficients $a_0, \dots, a_n \in \mathbb{R}$ are constant, i.e., they do not depend on the variable x. Then, the homogeneous ODE

$$a_n u^{(n)}(x) + a_{n-1}u^{(n-1)}(x) + \cdots + a_1 u'(x) + a_0 u(x) = 0$$

can be solved by making the ansatz $u(x) = ce^{\lambda x}$. Plugging this into the equation gives

$$\left(a_n\lambda^n + a_{n-1}\lambda^{n-1} + \cdots + a_1\lambda + a_0\right) ce^{\lambda x} = 0,$$

which is fulfilled (in a non trivial way) if and only if the equation

$$a_n\lambda^n + a_{n-1}\lambda^{n-1} + \cdots + a_1\lambda + a_0 = 0$$

holds. This equation is also called the **characteristic equation** for the ODE.
As we now have a polynomial of degree n in λ, we know by the fundamental theorem of algebra that there exists n solutions $\lambda_1, \dots, \lambda_n$ to this equation. Here, the following cases can occur:

1. All solutions are real and distinct. Then, we have n linearly independent functions $e^{\lambda_j x}$, which by the previous theorem, span the whole solution space, i.e., we can write

$$u(x) = \sum_{j=1}^{n} c_j e^{\lambda_j x}$$

with coefficients $c_j \in \mathbb{R}$ for all $j = 1, \ldots, n$.

2. All solutions are distinct but some are complex. Then, again, by the fundamental theorem of algebra, we know that if $\lambda_j = \alpha + i\beta$ solves the equation, we also have that $\overline{\lambda_j} = \alpha - i\beta$ solves the equation. In this case, we would obtain complex valued solutions $e^{\lambda_j x}$ and $e^{\overline{\lambda_j} x}$. However, using Euler's formula, they can be linearly combined as

$$c_1 e^{(\alpha+i\beta)x} + c_2 e^{(\alpha-i\beta)x} = e^{\alpha x}(d_1 \cos(\beta x) + d_2 \sin(\beta x))$$

and replacing $e^{\lambda_j x}$ and $e^{\overline{\lambda_j} x}$ in the basis by the linearly independent functions $e^{\alpha x}\cos(\beta x)$ and $e^{\alpha x}\sin(\beta x)$ gives a real valued basis.

3. Not all solution are distinct (e.g. $(\lambda - 1)^2 = 0$ gives a double root 1). If λ_j is a root of order $k > 1$, then we obtain k linearly independent solutions as

$$e^{\lambda_j x}, xe^{\lambda_j x}, \ldots, x^{k-1}e^{\lambda_j x}$$

(this can be checked by factorizing the polynomial in the characteristic equation, which provides a factorization of the ODE and then inserting the functions). Doing this for every root that appears multiple times, then gives n-linearly independent functions that span the basis of the solution vector space.

Example.

1. The ODE

$$u^{(3)}(x) + 2u''(x) + u'(x) + 2u(x) = 0$$

has the characteristic equation $\lambda^3 + 2\lambda^2 + \lambda + 2 = 0$ with roots $\lambda_1 = -2, \lambda_2 = i, \lambda_3 = -i$. As all roots are different, the solution space is spanned by e^{-2x}, e^{ix} and e^{-ix} or - as described above - spanned by the real functions e^{-2x}, $\sin(x)$ and $\cos(x)$ and the general solution is given as

$$u(x) = c_1 e^{-2x} + c_2 \sin(x) + c_3 \cos(x).$$

2. The ODE

$$u''(x) - 2u'(x) + u(x) = 0$$

has the characteristic equation $\lambda^2 - 2\lambda + \lambda = 0$ with roots $\lambda_1 = \lambda_2 = 1$. Therefore, the solution space is spanned by the basis functions e^x and xe^x and the general solution has the form

$$u(x) = c_1 e^x + c_2 x e^x.$$

■

Now, we turn our attention to inhomogeneous linear ODEs with constant coefficients

$$a_n u^{(n)}(x) + a_{n-1} u^{(n-1)}(x) + \cdots + a_1 u'(x) + a_0 u(x) = f(x).$$

For all linear ODEs (also for those with non constant coefficients), we have the so called **superposition principle**, which states that a solution to the inhomogeneous ODE can be written as

$$u(x) = u_h(x) + u_p(x),$$

where $u_h(x)$ is the general solution of the homogeneous system (i.e. with $f = 0$), which can be computed as explained above, and $u_p(x)$ is one particular solution to the inhomogeneous equation.

Now, the question remains how to determine this particular solution. A general formula for that (that also holds for systems with non-constant coefficients) is given at the end of this section, but evaluating that formula can be tedious. Most of the times it s better to make a clever ansatz for the particular solution. The idea hereby is that, if f consists of polynomials, trigonometric functions or exponentials, the particular solution u_p may have the same structure:

1. If $f(x) = \sum_{\ell=0}^{N} \alpha_\ell x^\ell$, then a possible ansatz is

   $$u_p(x) = \sum_{\ell=0}^{N} \beta_\ell x^\ell$$

   and plugging that into the equation and comparing coefficients may give the particular solution.

2. If $f(x) = \alpha e^{rx}$, then a possible ansatz is

   $$u_p(x) = \beta e^{rx}$$

   and plugging that into the equation one may be able to compute the coefficient β.

3. If $f(x) = \alpha_1 \sin(rx) + \alpha_2 \cos(rx)$ (note that one of the coefficients α_1, α_2 can be zero, but still in this case the full ansatz below has to be made), then a possible ansatz is

   $$u_p(x) = \beta_1 \sin(rx) + \beta_2 \cos(rx)$$

   and plugging that into the equation one may be able to compute the coefficients β_1, β_2 by comparing coefficients.

4. If f is a sum of some of the functions above, one can split $f = f_1 + \cdots + f_m$, where all f_j are of one of the cases above, one can compute particular solutions $u_{p,j}$ for the right-hand side f_j and then sum them up to

   $$u_p = u_{p,1} + \cdots + u_{p,m}.$$

We note that the previous statements are formulated in a way that the ansatz might work. In fact, all the presented formulas only fail, if the ansatz made is a function that is already in the homogeneous solution vector space. In that case, one has to multiply the ansatz with x^k, where

k is the smallest integer such that the ansatz function is not in the solution vector space of the homogeneous problem.

Example. We want to solve the ODE

$$u''(x) - 2u'(x) + u(x) = e^x.$$

We have previously already solved the homogeneous equation and obtained the general solution

$$u_h(x) = c_1 e^x + c_2 x e^x.$$

By the above statement on the structure of the particular solution, we would want to make the ansatz $u_p(x) = \beta e^x$. However, this function is already in the solution space of the homogeneous problem and the same holds for $\beta x e^x$. The correct ansatz for the particular solution is therefore

$$u_p(x) = \beta x^2 e^x$$

and inserting that ansatz in the equation using

$$u_p' = \beta(2xe^x + x^2 e^x), \qquad u_p'' = \beta(2e^x + 4xe^x + x^2 e^x)$$

gives

$$\beta(2e^x + 4xe^x + x^2 e^x) - \beta(4xe^x + 2x^2 e^x) + \beta x^2 e^x = e^x$$

or $\beta 2e^x = e^x$, which implies $\beta = \frac{1}{2}$ and

$$u_p(x) = \frac{1}{2} x^2 e^x.$$

Therefore, we have the general solution

$$u(x) = u_h(x) + u_p(x) = c_1 e^x + c_2 x e^x + \frac{1}{2} x^2 e^x.$$

If one would prescribe the initial conditions $u(0) = 1$ and $u'(0) = 0$, the constants c_1, c_2 can be computed from

$$\begin{aligned} u(0) &= c_1 = 1 \\ u'(0) &= c_1 + c_2 = 0 \end{aligned}$$

as $c_1 = 1$ and $c_2 = -1$ and we have the unique solution that satisfies the initial value problem. ■

Systems of ordinary differential equations

We note that the results of this section also apply to **systems of ODEs**, which are given as

$$u'(x) = f(x, u(x)),$$

where $u : \mathbb{R} \to \mathbb{R}^n$ and $f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ are vector valued functions.
In fact, ODEs of higher order $u^{(n)}(x) = F(x, u(x), \ldots, u^{(n-1)}(x))$ can be expressed as first order systems by setting

$$v_1 := u, \quad v_2 := u', \quad \ldots, \quad v_n := u^{(n-1)},$$

which leads to the system of ODEs

$$\begin{aligned} v_1' &= v_2 \\ v_2' &= v_3 \\ &\vdots \\ v_{n-1}' &= v_n \\ v_n' &= F(x, v_1, \ldots, v_n). \end{aligned}$$

In general, **linear systems** can be written in matrix notation

$$u'(x) = A(x)u(x)$$

with a matrix-valued function $A : \mathbb{R} \to \mathbb{R}^{n\times n}$. If A is a continuous function, Theorem 6.1 holds verbatim.

If the matrix valued function $A(x)$ does not depend on x, we have a linear system with constant coefficients. For such systems (with A constant!!) a basis of the solution space can be computed by $e^{\lambda_j} w_j$, where λ_j are the eigenvalues and w_j are the corresponding eigenvectors. If there are multiple eigenvalues to the same eigenvector, one has to compute eigenvectors of second order (which coincides with the computation of the Jordan normal form in linear algebra).

We finish this section with a general formula for the computation of particular solutions for systems

$$u'(x) = a(x)u(x) + g(x),$$

the so called **variation of constants formula** introduced in the following.

Let $U(x)$ be the matrix valued function $U : \mathbb{R} \to \mathbb{R}^{n\times n}$, where the columns consist of (vector valued!) basis functions of the solution space for the homogeneous problem. We note that for an ODE of order n reformulated as a system, the columns are $(b_j, b_j', \ldots, b_j^{(n-1)})^T$, where the b_j are scalar basis functions of the solution space. U is also called **fundamental matrix**. Then, the general solution can be written as

$$u(x) = U(x) \cdot c,$$

where $c \in \mathbb{R}^n$ and the product is a matrix vector product.

The general idea behind the variation of constant formula is that a particular solution should have a similar structure, i.e., look like

$$u_p(x) = U(x) \cdot c(x),$$

now with a vector valued function $c(x)$ instead of the constant vector. Plugging this formula into the equation then gives the variation of constants formula

$$u_p(x) = U(x) \int U^{-1}(y)g(y)dy.$$

For first order linear equations (i.e. u, a, g are scalar functions), this formula reduces to

$$u_p(x) = e^{A(x)} \int e^{-A(y)} g(y) dy,$$

where $A(x) = \int a(x)dx$.

Example. We want to solve the inhomogeneous ODE

$$u''(x) + u'(x) = e^{-x}$$

with the variation of constants formula. Using the characteristic equation $\lambda^2 + \lambda = 0$, we obtain the general solution $c_1 + c_2 e^{-x}$ of the homogeneous equation. Now, we rewrite the ODE into a first order system by introducing $v_1 := u$ and $v_2 := u'$. Then,

$$\begin{aligned} v_1' &= v_2 \\ v_2' &= -v_2 + e^{-x} \end{aligned}$$

or in matrix notation

$$\begin{pmatrix} v_1 \\ v_2 \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} + \begin{pmatrix} 0 \\ e^{-x} \end{pmatrix}.$$

Now, the matrix $U(x)$ is given by

$$U(x) = \begin{pmatrix} 1 & e^{-x} \\ 0 & -e^{-x} \end{pmatrix} \qquad \Longrightarrow U(x)^{-1} = \frac{1}{-e^{-x}} \begin{pmatrix} -e^{-x} & -e^{-x} \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 0 & -e^{x} \end{pmatrix}$$

and employing the variation of constant formula leads to

$$\begin{aligned} v_p(x) &= U(x) \int U^{-1}(y) g(y) dy = \begin{pmatrix} 1 & e^{-x} \\ 0 & -e^{-x} \end{pmatrix} \cdot \int \begin{pmatrix} 1 & 1 \\ 0 & -e^{y} \end{pmatrix} \cdot \begin{pmatrix} 0 \\ e^{-y} \end{pmatrix} dy \\ &= \begin{pmatrix} 1 & e^{-x} \\ 0 & -e^{-x} \end{pmatrix} \cdot \int \begin{pmatrix} e^{-y} \\ -1 \end{pmatrix} dy = \begin{pmatrix} 1 & e^{-x} \\ 0 & -e^{-x} \end{pmatrix} \cdot \begin{pmatrix} -e^{-x} \\ -x \end{pmatrix} = \begin{pmatrix} -e^{-x} - xe^{-x} \\ xe^{-x} \end{pmatrix}. \end{aligned}$$

So, the general solution to the system is given by

$$\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = c_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + c_2 \begin{pmatrix} e^{-x} \\ -e^{-x} \end{pmatrix} + \begin{pmatrix} -e^{-x} - xe^{-x} \\ xe^{-x} \end{pmatrix}$$

and with $v_1 = u$, we obtain the solution of the ODE as

$$u(x) = c_1 + c_2 e^{-x} - e^{-x} - xe^{-x}.$$

■

6.1.3 Existence and uniqueness of solutions

We have seen in the previous subsection that some ODEs have unique solutions, but others do not have solutions. In the following, we present two theorems that show existence (and uniqueness) of a large class of ODEs.

The following theorem, known as Peano's theorem, shows that continuity of the right-hand side of a system of ODEs guarantees existence of solutions.

Theorem 6.2 (Peano). *Let $f = f(x, u)$ be a continuous (vector valued) function. Then, the initial value problem*

$$\begin{aligned} u'(x) &= f(x, u) \\ u(0) &= u_0 \end{aligned}$$

has a solution defined on an interval I and u is continuously differentiable.

Example. The initial value problem

$$\begin{aligned} u'(x) &= \sqrt{u(x)} \\ u(0) &= 0 \end{aligned}$$

has a solution by the previous theorem, since $\sqrt{u}$ is a continuous function in u. Clearly, the trivial solution $u = 0$ solves the initial value problem. However, the function $u(x) = \frac{x^2}{4}$ solves the initial value problem too. ■

The previous example shows that in order to obtain uniqueness of the solution, additional assumptions need to be made.

Definition 6.3 (Local Lipschitz condition). *A (possibly vector valued) function $f(x, u)$ satisfies a (local)* **Lipschitz condition** *on a region R, if we have*

$$|f(x, u(x)) - f(x, v(x))| \leq L_R \, |u(x) - v(x)|$$

for all $(x, u), (x, v) \in R$. Here, the constant L_R is called the **Lipschitz constant**.

If for every point $(x, u) \in \mathbb{R} \times \mathbb{R}^n$ there exists a region R with $(x, u) \in R$ and the continuous function f satisfies a Lipschitz condition on R, we call f **locally Lipschitz continuous**.

Example.

1. The function $f(x, u) = \sqrt{u}$ from the previous example is not Lipschitz continuous, since we observe
$$|f(x, u) - f(x, v)| = \left|\sqrt{u} - \sqrt{v}\right| = \left|\frac{u - v}{\sqrt{u} + \sqrt{v}}\right| = \frac{1}{\sqrt{u} + \sqrt{v}} \, |u - v| \, .$$
For $u = 0$, there is no region containing $(x, 0)$ such that $\frac{1}{\sqrt{v}}$ is bounded for all $(x, v) \in R$.

2. Let $f(x,u) = a(x)u(x)$ with a continuous matrix valued function a. Then, we have

$$|f(x,u) - f(x,v)| = |a(x)u(x) - a(x)v(x)| = |a(x)|\,|u(x) - v(x)|\,.$$

   Now, every continuous function on a bounded region is bounded, i.e., for every (x,u) there is a region R such that $|a(x)| \leq L_R$, and we have shown Lipschitz continuity for linear ODEs.

3. Every continuously differentiable function is Lipschitz continuous. ■

The following theorem is called the theorem of Picard-Lindelöf and provides existence and uniqueness under mild assumptions on the ODE.

Theorem 6.4 (Picard-Lindelöf). *Let $f = f(x,u)$ be continuous and let f be locally Lipschitz continuous. Then, the initial value problem*

$$\begin{aligned} u'(x) &= f(x,u) \\ u(0) &= u_0 \end{aligned}$$

has a unique solution defined on an interval I and u is continuously differentiable.

A consequence of the previous theorem and the preceding example is that initial value problems for linear ODEs with continuous right-hand side always have a unique solution.

6.1.4 Laplace transformation method

The Laplace transformation $\mathcal{L}$, introduced in the previous chapter, can also be used to solve ODEs. We have already established the property that the Laplace transform turns derivatives into multiplications, i.e.,

$$\mathcal{L}\left[\frac{d^n u}{dt^n}\right](s) = s^n \mathcal{L}[u](s) - s^{n-1}u(0) - s^{n-2}u'(0) - \cdots - u^{(n-1)}(0)$$

for $n \in \mathbb{N}$.
Therefore, applying the Laplace transformation onto an ODE with constant coefficients turns the ODE into an algebraic equation to determine the Laplace transformation of the solution. As algebraic equations are oftentimes simpler to solve, we can obtain a solution of the ODE by computing the inverse Laplace transformation of the solution of the algebraic equation.

Example. We want to solve the initial value problem

$$\begin{aligned} u''(x) - 3u'(x) + 2u(x) &= 2e^{-x} \\ u(0) &= 2 \\ u'(0) &= 1. \end{aligned}$$

Applying the Laplace transformation to the equation gives

$$s^2\mathcal{L}[u](s) - s\underbrace{u(0)}_{2} - \underbrace{u'(0)}_{1} - 3(s\mathcal{L}[u](s) - \underbrace{u(0)}_{2}) + 2\mathcal{L}[u](s) = \mathcal{L}[2e^{-x}](s) = \frac{2}{s+1}$$

or the equation

$$(s^2 - 3s + 2)\mathcal{L}[u](s) - 2s + 5 = \frac{2}{s+1}$$

which can be solved to obtain the Laplace transformation of u as

$$\begin{aligned}\mathcal{L}[u](s) &= \frac{1}{s^2 - 3s + 2}\left(\frac{2}{s+1} + 2s - 5\right) = \frac{2s^2 - 3s - 3}{(s+1)(s-1)(s-2)} \\ &= \frac{1}{3(s+1)} + \frac{2}{s-1} - \frac{1}{3(s-2)}.\end{aligned}$$

Now, using linearity and the table of Laplace transforms to determine the inverse transformation, we arrive at

$$u(x) = \mathcal{L}^{-1}\left[\frac{1}{3(s+1)} + \frac{2}{s-1} - \frac{1}{3(s-2)}\right](x) = \frac{1}{3}e^{-x} + 2e^{x} - \frac{1}{3}e^{-2x}.$$

■

6.2 Partial differential equations

Partial differential equations (PDEs) are a generalization of ordinary differential equations (ODEs) in the sense that a PDE is an equation describing the relation between a function and its derivatives, but several input arguments are allowed. Therefore, a PDE includes also partial derivatives (which explains the name PDE).
In general, we are looking at equations

$$F(u, \nabla u, \nabla^2 u, \dots) = f(x).$$

In the same way as for ODEs, we call a PDE **linear**, if the function F only depends linearly on u and all partial derivatives of u. If $f = 0$ the PDE is called **homogeneous**, and the highest appearing derivative defines the **order** of the equation.

Example. In Chapter 4, we already mentioned a PDE, when using the divergence theorem to derive the equation for conservation of mass, which was given as

$$\partial_t \rho + \operatorname{div}(\rho v) = 0,$$

where ρ was the density of the fluid and v the velocity field for the fluid. This is a linear, homogeneous PDE of first order. For constant velocity fields v and in one space dimension, the equation simplifies to

$$\partial_t \rho + v\partial_x \rho = 0,$$

which is also called the **transport equation**. ■

Studying general PDEs is very hard, but lots of physical problems are described with PDEs of second order, which means that only derivatives up to second order appear. For those, some classifications and results are known and presented in the following.

6.2.1 Elliptic, hyperbolic and parabolic PDEs

In this section, we consider only **linear PDEs of second order**, i.e., the highest appearing partial derivatives are of order 2, and F depends only linearly on u and its derivatives. To that end, let $u : \mathbb{R}^n \to \mathbb{R}$ and define

$$\sum_{i,j}^{n} a_{ij}(x) \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^{n} b_i(x) \frac{\partial u}{\partial x_i} + c(x)u(x) = f(x).$$

Here, the right-hand side f, the (symmetric) matrix valued function $A(x) = (a_{ij}(x))_{i,j=1}^n$, the vector valued function $b(x) = (b_i)_{i=1}^n$ and the (scalar) coefficient function $c(x)$ are given.

The classification of the PDE will only depend on the symmetric matrix $A(x) = (a_{ij}(x))_{ij}$, or more precisely on the eigenvalues of A. We call the PDE

- **elliptic** at the point x, if all eigenvalues of $A(x)$ fulfill $\lambda_i > 0$ for all $i = 1, \dots, n$ or all eigenvalues fulfill $\lambda_i < 0$ for all $i = 1, \dots, n$, i.e., all eigenvalues should have the same sign.
- **parabolic** at x, if there exists a zero eigenvalue $\lambda_j = 0$ of $A(x)$ and all other eigenvalues have the same sign.
- **hyperbolic** at x, if one eigenvalue of $A(x)$ has a different sign than the others. I.e., there is a $\lambda_j > 0$ and all other eigenvalues satisfy $\lambda_k < 0$ for $k \neq j$ (or the other way round).

For simplicity, we assume in the following that $A(x) = A$ is a constant, symmetric matrix and we consider the case $n = 2$. Then, we have

$$\sum_{i,j}^{2} a_{ij} \frac{\partial u^2}{\partial x_i \partial x_j} = a_{11}u_{xx} + 2a_{12}u_{xy} + a_{22}u_{yy},$$

where we used the short notations $u_{xx} = \partial_x^2 u$, $u_{xy} = \partial_x \partial_y u$, $u_{yy} = \partial_y^2 u$. Then, the above classification of the PDE can be simplified to

- **elliptic**, if $a_{12}^2 - a_{11}a_{22} < 0$;
- **parabolic**, if $a_{12}^2 - a_{11}a_{22} = 0$;
- **hyperbolic**, if $a_{12}^2 - a_{11}a_{22} > 0$.

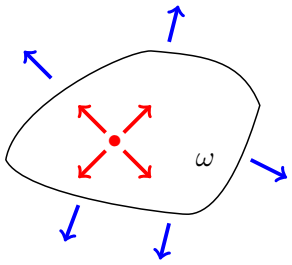
The classification of the second order PDEs is useful since, for each category separately, a general solution theory and numerical approximation techniques can be made. In the following, we introduce the most famous PDEs of each category.

6.2.2 The heat equation (parabolic)

Let $\Omega \subset \mathbb{R}^d$ be a given region. We seek the temperature distribution $T(x, t)$ for each point $x \in \Omega$ and time $t > 0$.

For the derivation of the equations consider a small (arbitrary) "control" volume $\omega \subset \Omega$. The conservation of energy implies the conservation of temperature, so we get the balance equation

Change of temperature in ω = produced temperature in ω - temperature loss through $\partial\omega$



The total thermal energy in ω is given by

$$\int_\omega C(x)T(x,t)\,dx,$$

where the function C is called the specific heat. The left side in the balance equation above then becomes

$$\frac{d}{dt}\int_\omega C(x)T(x,t)\,dx = \int_\omega C(x)\frac{\partial}{\partial t}T(x,t)\,dx.$$

Let $f(x,t)$ be a given external heat source, then the produced heat in ω is

$$\int_\omega f(x,t)\,dx.$$

Finally, the heat flow through $\partial\omega$ is proportional to the normal gradient of T (including some material parameters) and given by the surface integral

$$-\int_{\partial\omega} \kappa\nabla T(x,t)\cdot dS,$$

where κ is the thermal conductivity. With the divergence theorem, we get

$$-\int_{\partial\omega} \kappa\nabla T(x,t)\cdot dS = \int_\omega \operatorname{div}(\kappa\nabla T(x,t))dx,$$

and the balance equation reads as

$$\int_\omega C\partial_t T(x,t)dx = \int_\omega f(x,t) + \operatorname{div}(\kappa\nabla T(x,t))dx.$$

As this equation is valid for all ω, the equation without the integrals has to hold, i.e.,

$$C\partial_t T = \operatorname{div}(\kappa\nabla T) + f.$$

For homogeneous materials, the material parameters C, κ are constants and with the thermal diffusivity $\alpha = \frac{\kappa}{C}$ and $g = \frac{f}{C}$, we arrive at

$$\partial_t T = \alpha \Delta T + g \qquad \forall x \in \Omega, t > 0,$$

which is the so called **heat equation**.

Since the matrix $A = (a_{ij})_{ij}$ is constant and given by $a_{11} = 0$, $a_{jj} = 1$ for all $j = 2, \dots, n$ and $a_{ij} = 0$ if $i \neq j$, we have that one eigenvalue is 0 and all other eigenvalues are positive. Therefore, the above classification shows that we are dealing with a **parabolic equation**.

In the same way as for ODEs, solutions to PDEs are in general not unique and additional conditions (initial or boundary conditions) need to be applied. The initial condition at $t = 0$ looks like

$$T(x, 0) = T_0(x) \qquad \forall x \in \Omega.$$

Moreover, the interaction with the surrounding media of Ω is usually defined with boundary conditions on $\partial\Omega$. The specific choice of the boundary condition depends on the physical model. Common types of boundary conditions are

1. **Dirichlet-conditions:** Prescribe the values at the boundary, e.g.,

   $$T(x, t) = T_D(x) \qquad x \in \partial\Omega,$$

   with a given function T_D. Oftentimes, T_D is a constant, e.g., $T_D = 0$.

2. **Neumann-conditions:** Prescribe the normal flux at the boundary, e.g.,

   $$-\kappa \nabla T \cdot n = T_N \qquad x \in \partial\Omega,$$

   with a given function T_N. Oftentimes, T_N is a constant, e.g., $T_N = 0$.

3. **Robin-conditions:** Mix the conditions from above, e.g.,

   $$-\kappa \nabla T \cdot n - \alpha T = T_R \qquad x \in \partial\Omega,$$

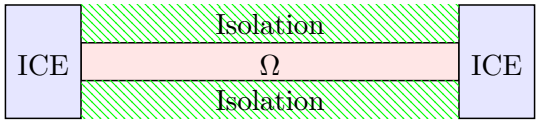
   with a given function T_R. A more intuitive interpretation is given by setting $T_R = \alpha T_1$, where T_1 is a given outside temperature. Then, we have

   $$-\kappa \nabla T \cdot n = \alpha (T - T_1)$$

   and the normal flux is proportional to the temperature difference (compare that to Newton's law of cooling).

Separation of variables

We consider the following one dimensional setting on $\Omega = [0, L]$.



Then, the heat equation initial/boundary value problem reads as

$$\begin{aligned} T_t &= \alpha T_{xx} && \text{in } \Omega \\ T(x,t) &= 0 && \text{on } \partial\Omega \\ T(x,0) &= T_0(x). \end{aligned}$$

In the following, we want to solve this problem by making the ansatz (also called Fourier's guess) that the solution can be separated into a function depending only on x and a function depending only on t, i.e.,

$$T(x,t) = u(x)v(t).$$

Plugging this into the equation gives $u(x)v_t(t) = \alpha u_{xx}(x)v(t)$ and after division with αuv, we arrive at

$$\frac{u_{xx}(x)}{u(x)} = \frac{v_t(t)}{\alpha v(t)} = \text{const} =: -\lambda,$$

where the last equality holds since functions in different variables can only be equal, if they are constant. From this equation, we deduce the ODEs

$$v'(t) = -\alpha\lambda v(t) \qquad \Longrightarrow \qquad v(t) = c_1 e^{-\alpha\lambda t}$$

and

$$u''(x) = -\lambda u(x),$$

which is a second order ODE whose solution depends on the sign of λ and the given boundary conditions. Imposing the conditions

$$u(0) = u(L) = 0$$

implies the boundary conditions for T. We note that problems of this form are called **eigenvalue problems**. Since the characteristic equation has the zeros $\sqrt{-\lambda}$ and $-\sqrt{-\lambda}$ (which are complex, if λ is positive), we have three cases for the solutions

1. $\lambda = 0$: Then, the equation becomes $u''(x) = 0$ with the general solution $u(x) = c_2 x + c_3$ and inserting the boundary conditions leads to $c_2 = c_3 = 0$, i.e., the trivial solution $u = 0$.
2. $\lambda < 0$: Then, we have real roots and the general solution $u(x) = c_2 e^{\sqrt{-\lambda}x} + c_3 e^{-\sqrt{-\lambda}x}$ and, again, inserting the boundary conditions show that the only possible solution is the trivial solution $u = 0$.

3. $\lambda > 0$: In this case, we have that $i\sqrt{\lambda}$ and $-i\sqrt{\lambda}$ are the conjugate complex roots and the general (real valued) solution is given by

$$u(x) = c_2 \sin(\sqrt{\lambda}x) + c_3 \cos(\sqrt{\lambda}x)$$

Inserting the boundary condition $u(0) = 0$ implies $c_3 = 0$. However, inserting the condition $u(L) = 0$ then gives

$$u(L) = c_2 \sin(\sqrt{\lambda}L) = 0,$$

which either is fulfilled, if u is the trivial solution $u \equiv 0$ or

$$\sin(\sqrt{\lambda}L) = 0 \qquad \Longrightarrow \qquad \sqrt{\lambda} = \frac{n\pi}{L}.$$

In this case, the general solution is given by $u(x) = c_2 \sin\left(\frac{n\pi}{L}x\right)$.

We note that inserting the trivial solution $u(x) = 0$ into the ansatz gives $T(t, x) = 0$, which can only be a solution provided $T_0(x) = 0$. Otherwise, we are not interested in the trivial solution, and therefore only the solution of case 3. remains. Inserting this into the ansatz gives

$$T_n(x,t) = e^{-\alpha\left(\frac{n\pi}{L}\right)^2 t} \sin\left(\frac{n\pi}{L}x\right) \qquad n \in \mathbb{N}.$$

Since the heat equation is linear, we obtain the general solution by taking a (infinite) linear combination of the solutions T_n as

$$T(x,t) = \sum_{n=1}^{\infty} b_n e^{-\alpha\left(\frac{n\pi}{L}\right)^2 t} \sin\left(\frac{n\pi}{L}x\right).$$

Finally, the coefficients b_n can be computed using the initial condition $T(x, 0) = T_0$, which gives

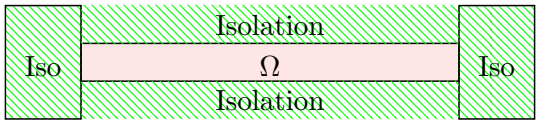
$$T(x,0) = \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi}{L}x\right) = T_0(x).$$

Comparing this with the Fourier series of the previous chapter shows that the coefficients b_n are just the Fourier coefficients (noting that $T(x, 0)$ is periodic and odd on $[-L, L]$)

$$b_n = \frac{2}{L} \int_0^L T_0(x) \sin\left(\frac{n\pi}{L}x\right) dx.$$

We note that from the solution formula, we deduce $T(x, t) \to 0$ for $t \to \infty$, as no external heat source is employed. Moreover, we see that for $t \to -\infty$ the solution blows up, i.e., going backwards in time is unstable.

Now, we change the setting by changing the boundary conditions.



The drawn setting corresponds to the case of Neumann boundary conditions, which gives the problem

$$\begin{aligned} T_t &= \alpha T_{xx} && \text{in } \Omega \\ \nabla T(x,t) \cdot n &= 0 && \text{on } \partial\Omega \\ T(x,0) &= T_0(x). \end{aligned}$$

Here, the same ansatz $T(x,t) = u(x)v(t)$ can be made, which leads to the same ODEs

$$\frac{u_{xx}(x)}{u(x)} = \frac{v_t(t)}{v(t)} = \text{const} =: -\lambda,$$

just with the boundary conditions

$$u'(0) = u'(L) = 0.$$

The function $v(t) = c_1 e^{-\alpha\lambda t}$ is therefore unchanged, and it remains to solve the ODE $u''(x) = -\lambda u(x)$ with the different boundary conditions. We check the three cases for the eigenvalue problem:

1. $\lambda = 0$: Then, the equation becomes $u''(x) = 0$ with the general solution $u(x) = c_2 x + c_3$ and inserting the boundary conditions leads to $u'(0) = c_2 = u'(L)$, i.e., the general solution $u = c_3$.

2. $\lambda < 0$: Then, we have real roots and the general solution $u(x) = c_2 e^{\sqrt{-\lambda}x} + c_3 e^{-\sqrt{-\lambda}x}$ and, again, inserting the boundary conditions show that the only possible solution is the trivial solution $u = 0$.

3. $\lambda > 0$: In this case, we have that $i\sqrt{\lambda}$ and $-i\sqrt{\lambda}$ are the conjugate complex roots and the general (real valued) solution is given by

   $$u(x) = c_2 \sin(\sqrt{\lambda}x) + c_3 \cos(\sqrt{\lambda}x)$$

   Inserting the boundary condition $u'(0) = 0$ implies $c_2 = 0$. However, inserting the condition $u'(L) = 0$ then gives

   $$u'(L) = -\sqrt{\lambda} c_3 \sin(\sqrt{\lambda}L) = 0,$$

   which either is fulfilled, if u is the trivial solution $u \equiv 0$ or

   $$\sin(\sqrt{\lambda}L) = 0 \qquad \Longrightarrow \qquad \sqrt{\lambda} = \frac{n\pi}{L}.$$

   In this case, the general solution is given by $u(x) = c_3 \cos\left(\frac{n\pi}{L}x\right)$.

Therefore, we obtain non-trivial cases for $\lambda = 0$ and $\lambda = \frac{n^2\pi^2}{L^2}$ and summation over all solutions gives

$$T(x,t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n e^{-\alpha \frac{n^2\pi^2}{L^2} t} \cos\left(\frac{n\pi}{L}x\right).$$

with constants a_0, a_n that are the Fourier coefficients of the initial condition T_0 and given by

$$a_n = \frac{2}{L}\int_0^L T_0(x)\cos\left(\frac{n\pi}{L}x\right) dx.$$

We note that from the solution formula, we deduce $T(x,t) \to \frac{a_0}{2}$ for $t \to \infty$, i.e., the temperature converges to the mean value of the initial function T_0. This is concise with the physical intuition, since there is isolation around Ω, so no heat is lost.

A similar technique can also be employed for Robin boundary conditions.

Non homogeneous boundary conditions

Previously, we only considered homogeneous boundary conditions, which was essential for the representation of the solution by a sum of particular solutions.
In the following, we consider inhomogeneous boundary conditions for the heat equation

$$\begin{aligned} T_t &= \alpha T_{xx} \\ T(0,t) &= A \qquad T(L,t) = B \\ T(x,0) &= T_0(x), \end{aligned}$$

which we solve with the following technique that is called homogenization.

1. We solve the stationary (i.e. not dependent on time) heat equation with the given boundary conditions to obtain the equilibrium temperature T_E

   $$\begin{aligned} T_{Exx} &= 0 \\ T_E(0) &= A \\ T_E(L) &= B. \end{aligned}$$

   This is an ODE of second order, which has the unique solution $T_E(x) = A + \frac{B-A}{L}x$.

2. Denoting the difference between the solution $T(x,t)$ and the equilibrium temperature by

   $$U(x,t) = T(x,t) - T_E(x),$$

   plugging this into the PDE and using the linearity of the PDE shows that $U(x,t)$ solves the PDE

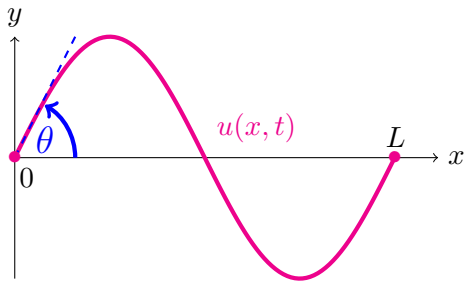
   $$\begin{aligned} U_t &= \alpha U_{xx} \\ U(0,t) &= 0 \qquad U(L,t) = 0 \\ U(x,0) &= T_0(x) - T_E(x). \end{aligned}$$

   Thus, we have a heat equation with homogeneous boundary conditions, which can be solved with separation of variables as above. With the computed solutions $U(x,t)$ and $T_E(x)$, we get the sought solution $T(x,t) = U(x,t) + T_E(x)$.

6.2.3 The wave equation

Let $\Omega = [0, L]$. In the following, we derive an equation for the displacement of a vibrating string that is fixed at 0 and L.
We assume the following simplifications:

- The wave is plane and transversal (i.e., horizontal to the clamped string).
- The material of the string is homogeneous, i.e., it has constant density.
- The displacement (or deformation) $u(x, t)$ is small.



If the string is moved, it creates a resistance. This force is called tension and denoted by $T(x, t)$. Now, we take a sub-part of the string $[a, b]$. The components of T that appear on $[a, b]$ are $T(b, t)\sin(\theta(b, t))$ and $-T(a, t)\sin(\theta(a, t))$, where $\theta(x, t)$ denotes the angle between the string and the x-axis. The force is minimal if $\theta = 0$ and maximal if $\theta = \pi/2$. The sum of the forces at a and b now give

$$\text{tension force} = T(b, t)\sin(\theta(b, t)) - T(a, t)\sin(\theta(a, t)) = \int_a^b \frac{\partial}{\partial x}(T\sin\theta)dx.$$

Newton's law provides that the force is equal to the product of mass $\rho(b-a)$ (where ρ is the density) with the acceleration (second derivative), hence,

$$\text{mass} \times \text{acceleration} = \rho(b-a)\frac{1}{b-a}\int_a^b \frac{\partial^2 u(x, t)}{\partial t^2}dx.$$

Here, the acceleration is actually taken as the mean value of the acceleration on $[a, b]$, which can be motivated by looking at the movement of the center of mass of $[a, b]$. Consequently, Newton's law now gives

$$\int_a^b \rho\, u_{tt} - (T\sin\theta)_x dx = 0$$

and since a, b are arbitrary, this implies $\rho u_{tt} = (T\sin\theta)_x$ for $x \in (0, L)$ and $t > 0$.
Since $\tan\theta = u_x$, we can write using $\sin^2\theta + \cos^2\theta = 1$

$$\sin\theta = \frac{\sin\theta}{\sqrt{\sin^2\theta + \cos^2\theta}} = \frac{\sin\theta}{\cos\theta\sqrt{1 + \tan^2\theta}} = \frac{\tan\theta}{\sqrt{1 + \tan^2\theta}} = \frac{u_x}{\sqrt{1 + u_x^2}}.$$

Plugging this into the equation derived above gives

$$\rho u_{tt} = \left(\frac{T u_x}{\sqrt{1+u_x^2}} \right)_x .$$

Now, we use the assumption that the displacement is small to simplify the equation. If $u = 0$m we have the initial tension $T = T_0$, hence if u and u_x are small, i.e., $|u| << 1$, $|u_x| << 1$, we can replace T by T_0 and $1 + u_x^2$ by 1.
This leads to the classical form of the **wave equation**

$$u_{tt} = c^2 u_{xx} \qquad x \in (0, L), t > 0,$$

where $c^2 = T_0/\rho$ is called the **wave speed**.

For a unique solution, as for the heat equation, initial and boundary conditions need to be specified. As we have an equation with second order derivatives both in time and space, we actually need two boundary conditions and two initial conditions. Taking homogeneous Dirichlet conditions (as we are modeling a clamped string), this reads as

$$\begin{aligned} u(0,t) &= 0, & u(L,t) &= 0 \\ u(x,0) &= u_0(x) & u_t(x,0) &= u_1(x). \end{aligned}$$

As we have $a_{11} = 1$ and $a_{22} = -1$ (or in higher dimensions $a_{jj} = -1$ for all $j > 1$) and $a_{ij} = 0$ for all $i \neq j$, the classification at the beginning of this section shows that we are dealing with a **hyperbolic** equation.

D'Alembert's solution

In the exercise part, we already have found solutions to the wave equation $u_{tt} = u_{xx}$ by using a variable transformation. For the case of general wave speeds c, with the transformations

$$r = x + ct \qquad s = x - ct,$$

we compute using the chain rule

$$\begin{aligned} \frac{\partial}{\partial r} &= \frac{\partial}{\partial x}\frac{\partial x}{\partial r} + \frac{\partial}{\partial t}\frac{\partial t}{\partial r} = \frac{1}{2c}\left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x} \right) \\ \frac{\partial}{\partial s} &= \frac{\partial}{\partial x}\frac{\partial x}{\partial s} + \frac{\partial}{\partial t}\frac{\partial t}{\partial s} = -\frac{1}{2c}\left(\frac{\partial}{\partial t} - c\frac{\partial}{\partial x} \right). \end{aligned}$$

This directly implies that

$$0 = u_{tt} - c^2 u_{xx} = \left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x} \right)\left(\frac{\partial}{\partial t} - c\frac{\partial}{\partial x} \right) u = -4c^2 \frac{\partial^2 u}{\partial r \partial s}(r,s).$$

Consequently, we see that (by integration in r and s) that the solution has to have the form

$$u(r,s) = F(s) + G(r) \qquad \Longrightarrow \qquad u(x,t) = F(x-ct) + G(x+ct)$$

with arbitrary functions F and G that can be determined by the initial and boundary conditions. The initial conditions $u(x,0) = u_0(x)$ and $u_t(x,0) = u_1(x)$ then lead to

$$\begin{aligned} F(x) + G(x) &= u_0(x) \\ -cF'(x) + cG'(x) &= u_1(x) \end{aligned} \qquad \Longrightarrow \qquad -cF(x) + cG(x) = \int_0^x u_1(\zeta)d\zeta + A.$$

Therefore, we have two linear equations for the two unknowns F, G and solving these gives

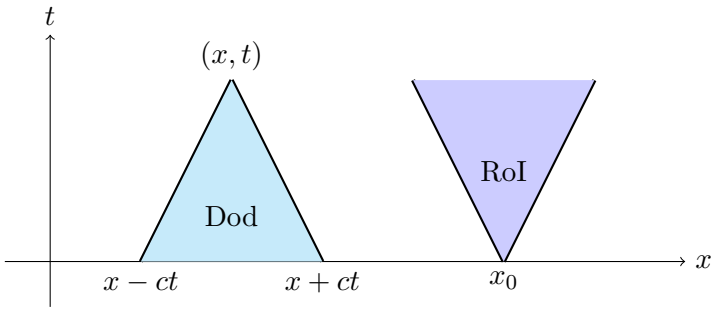
$$\begin{aligned} F(x) &= \frac{1}{2c}\left(cu_0(x) - \int_0^x u_1(\zeta)d\zeta - A\right) \\ G(x) &= \frac{1}{2c}\left(cu_0(x) + \int_0^x u_1(\zeta)d\zeta + A\right). \end{aligned}$$

Consequently, the solution to the wave equation reads as

$$u(x,t) = \frac{1}{2}\left(u_0(x-ct) + u_0(x+ct)\right) + \frac{1}{2c}\int_{x-ct}^{x+ct} u_1(\zeta)d\zeta.$$

If $u_1 = 0$, then the solution reduces to a wave $u_0(x-ct)$ that travels with speed c and a wave $u_0(x+ct)$ that travels with speed $-c$.

The lines $x - ct = x_0$ and $x + ct = x_0$ are called the characteristics of the equation that start at the point $(x_0, 0)$ and along these lines the information is propagated by the equation. In fact, we see that the solution $u(x,t)$ only depends on the initial data that is moved along the characteristics. The function value $u(x_0, 0)$ influences the values $u(x,t)$ in a region bounded by the characteristics that emanate from $(x_0, 0)$, which is called the **region of influence** (blue below). Conversely, the function value $u(x,t)$ only depends on initial values in $[x-ct, x+ct]$, which is bounds the **domain of dependence** (cyan below).

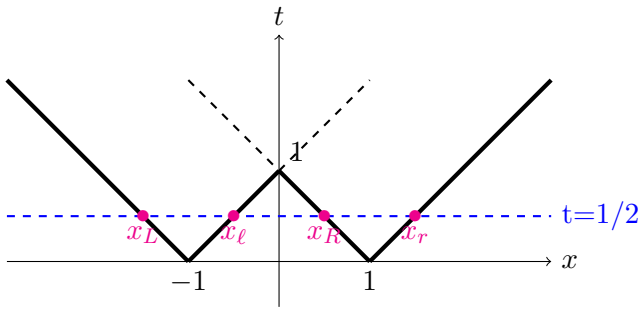


We note that the solution of the wave equation exists for all points in time (also negative times) in contrast to parabolic equations.

Example. Let $u_0(x) = \begin{cases} 1 & |x| < 1 \\ 0 & |x| > 1 \end{cases}$, $u_1 = 0$ and $c = 1$.
Then, the solution is given by

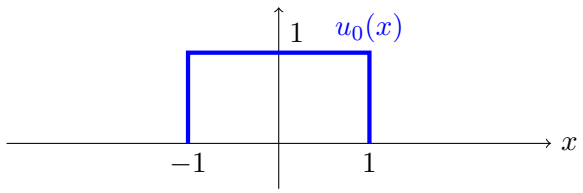
$$u(x,t) = \frac{1}{2}\left(u_0(x-t) + u_0(x+t)\right)$$

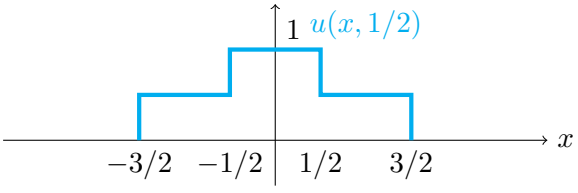
We want to find the solution at $t = 1/2, 1, 2$.
For $t = 1/2$, we first look at the characteristics $x_r - 1/2 = 1$ (here 1 is taken since it is the right point, where u_0 jumps) and $x_R + 1/2 = 1$, which give $x_r = 3/2$ and $x_R = 1/2$. Doing the same for the characteristics $x_\ell - 1/2 = -1$ (here -1 is taken since it is the left point, where u_0 jumps) and $x_L + 1/2 = -1$ gives $x_\ell = -1/2$ and $x_L = -3/2$.



This shows that

$$\begin{aligned} u(x,1/2) &= \frac{1}{2} \qquad x \in [x_L, x_\ell] \\ u(x,1/2) &= 1 \qquad x \in [x_\ell, x_R] \\ u(x,1/2) &= \frac{1}{2} \qquad x \in [x_R, x_r] \end{aligned}$$



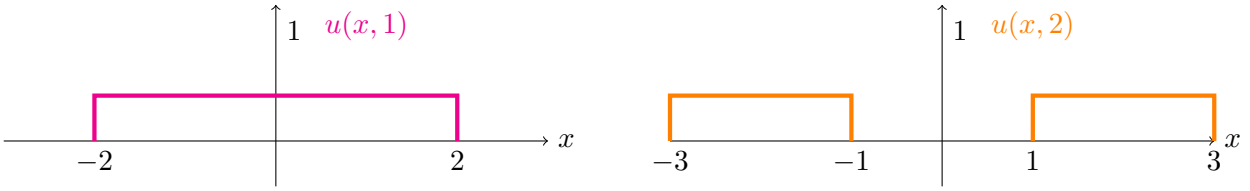


For $t = 1$ the same can be done and we compute $x_r = 2$, $x_R = 0$ as well as $x_\ell = 0$ and $x_L = -2$ and the solution is

$$u(x,1) = \frac{1}{2} \qquad x \in [x_L, x_r]$$

Finally, for $t = 2$, we have $x_r = 3$, $x_R = -1$ as well as $x_\ell = 1$ and $x_L = -3$ and the solution is

$$\begin{aligned} u(x,1/2) &= \frac{1}{2} \qquad x \in [x_L, x_R] \\ u(x,1/2) &= 0 \qquad x \in [x_R, x_\ell] \\ u(x,1/2) &= \frac{1}{2} \qquad x \in [x_\ell, x_r]. \end{aligned}$$



From these plots, one can clearly see the nature of d'Alembert's solution as traveling waves. ■

Separation of variables

In the same way as for the heat equation, we can also employ the technique of separation of variables to the heat equation. Writing $u(x,t) = X(x)T(t)$ and inserting that into the PDE

$$\begin{aligned} u_{tt} &= c^2 u_{xx} && \text{in } \Omega, t > 0 \\ u(x,t) &= 0 && \text{on } \partial\Omega \\ u(x,0) &= u_0(x) \\ u_t(x,0) &= u_1(x) \end{aligned}$$

gives

$$\frac{T_{tt}(t)}{c^2 T(t)} = \frac{X_{xx}(x)}{X(x)} = -\lambda.$$

Thus, we have two second order ODEs, and the eigenvalue problem (in x) can be solved as for the heat equation by distinguishing the cases $\lambda > 0$, $\lambda = 0$ and $\lambda < 0$ (exercise!). This gives the non trivial solutions

$$X_n(x) = c_n \sin\left(\frac{n\pi x}{L}\right)$$

and

$$T_n(t) = a_n \sin\left(\frac{n\pi ct}{L}\right) + b_n \cos\left(\frac{n\pi ct}{L}\right)$$

and the solution to the wave equation has the series expansion

$$u(x,t) = \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi ct}{L}\right) \sin\left(\frac{n\pi x}{L}\right) + B_n \cos\left(\frac{n\pi ct}{L}\right) \sin\left(\frac{n\pi x}{L}\right)$$

Inserting the initial conditions then allows the computation of A_n and B_n (exercise!).

Remark. It can be shown that separation of variables and d'Alembert's procedure produce the same solution.

6.2.4 The Poisson equation

We consider the steady state (i.e. $u_t = u_{tt} = 0$) of the heat and the wave equation. In n-space dimensions, this gives

$$\Delta u = \frac{\partial^2 u}{\partial x_1^2} + \cdots + \frac{\partial^2 u}{\partial x_n^2} = f,$$

where f is a given external force. If $f = 0$, the above equation is called **Laplace equation**, otherwise it is called the **Poisson equation**. Studying the Poisson equation in $\mathbb{R}^n$ shows that we have $a_{ii} = 1$ for all $i = 1, \ldots, n$ and $a_{ij} = 0$, if $i \neq j$, so by the above classification, we are dealing with an **elliptic PDE**.
In order to obtain a unique solution, here, only boundary conditions on $\partial\Omega$ (like Dirichlet, Neumann or Robin boundary conditions) need to be employed.

We stress that the method of separation of variables can also be applied to solve the Laplace equation, which again leads to solving eigenvalue problems as in the previous subsections.
In the following, we are more interested in solving the inhomogeneous equation. Before we formulate the uniqueness theorem, we state an interesting result for solutions of Laplace's equation, the so called maximum/minimum principle.

Theorem 6.5. *Let u solve $\Delta u = 0$ in Ω. Then, the maximum and minimum of the solution is obtained on $\partial\Omega$.*

Now, we take two solutions u_1, u_2 of the Poisson equation with inhomogeneous boundary conditions

$$\begin{aligned} \Delta u_i &= f \qquad \text{in } \Omega \\ u_i &= g \qquad \text{on } \partial\Omega. \end{aligned}$$

Then, the difference $u := u_1 - u_2$ solves the homogeneous problem

$$\begin{aligned} \Delta u &= 0 \qquad \text{in } \Omega \\ u &= 0 \qquad \text{on } \partial\Omega \end{aligned}$$

and by the previous theorem, we know that u has its maximum and minimum at $\partial\Omega$. As $u = 0$ on $\partial\Omega$, we obtain

$$0 \leq u = u_1 - u_2 \leq 0 \qquad \Longrightarrow \qquad u_1 = u_2.$$

Therefore, we have shown the uniqueness of solutions to the Poisson equation with Dirichlet boundary conditions (but not the existence of solutions!).
Now, the question remains how to solve the inhomogeneous problem, which is discussed in the following.

Method of Green's functions

Previously, we introduced the Dirac δ-distribution in one dimension. Similarly, one can define the δ-distribution in higher dimension, e.g., in $n = 2$ by $\delta(x, y) = 0$, if $(x, y) \neq 0$ and

$$f(a, b) = \int_{\mathbb{R}^2} f(x, y)\delta(x - a, y - b)dA$$

for arbitrary (smooth) functions f.

We consider the Poisson equation on a region $\Omega \subset \mathbb{R}^2$ in two dimensions with inhomogeneous Dirichlet boundary conditions

$$\begin{aligned} \Delta u &= f \qquad \text{in } \Omega \\ u &= u_D \qquad \text{on } \partial\Omega. \end{aligned}$$

The idea of the following procedure is to find a function G that satisfies the Poisson equation with homogeneous boundary conditions and right-hand side $f = \delta$. More precisely, we fix a point $(x, y) \in \Omega$ and another point $(\zeta, \eta) \in \mathbb{R}^2$. Then, the function G solves

$$\begin{aligned} \Delta G(\zeta, \eta) &= \delta(\zeta - x, \eta - y) \qquad \text{in } \Omega \\ G &= 0 \qquad \text{on } \partial\Omega. \end{aligned}$$

Now, the definition of the δ-distribution gives

$$u(x, y) = \int_{\mathbb{R}^2} u(\zeta, \eta)\delta(\zeta - x, \eta - y)d\zeta d\eta = \int_\Omega u(\zeta, \eta)\Delta G(\zeta, \eta)d\zeta d\eta,$$

where we used the equation for G on Ω and $\delta = 0$ on $\mathbb{R}^d \backslash \Omega$. Recall Green's identity

$$\int_\Omega u\Delta G - G\Delta u dA = \int_{\partial\Omega} (u\nabla G - G\nabla u) \cdot dS.$$

Now, applying this together with the fact that $G = 0$ on $\partial\Omega$ to the above formula gives

$$\begin{aligned} u(x, y) &= \int_\Omega u(\zeta, \eta)\Delta G(\zeta, \eta)d\zeta d\eta \\ &= \int_\Omega \Delta u(\zeta, \eta)G(\zeta, \eta)d\zeta d\eta + \int_{\partial\Omega} u\nabla G \cdot dS \\ &= \int_\Omega fG \, dA + \int_{\partial\Omega} u_D \nabla G \cdot dS. \end{aligned}$$

Thus, we have found a solution formula for u that only includes G and the given functions f and u_D. At first glance, finding G seems equally hard to finding u. However, G does only depend on Ω, but not on f, u_D (in contrast to u), and in the following, we actually compute the Green's function.

Computing the Green's function

We start with the simple case, where we suppose that we have a solution to the Laplace equation that is rotational symmetric, i.e., $\Phi = \Phi(r)$. With $r = \sqrt{(x - \zeta)^2 + (y - \eta)^2}$, we can write the 2D-$\delta$-distribution as $\delta(\zeta - x, \eta - y) = \delta(r)$. Thus, we want to solve (where we use the Laplace operator in polar coordinates)

$$\Delta\Phi = \Phi_{rr} + \frac{1}{r}\Phi_r = \delta(r).$$

For $r > 0$, we have $\delta(r) = 0$, and therefore the equation $\Phi_{rr} + \frac{1}{r}\Phi_r = 0$, which can be solved by integration and separation as

$$\Phi(r) = A \ln(r) + B.$$

For simplicity, we set $B = 0$ and in order to fix the constant A, we integrate over the ball $B_\varepsilon(x, y)$ centered at (x, y) of radius ε

$$\begin{aligned} 1 &= \int_{\mathbb{R}^2 \setminus B_\varepsilon(x,y)} \delta(r) dA + \int_{B_\varepsilon(x,y)} \delta(r) dA = \int_{B_\varepsilon(x,y)} \Delta\Phi \, dA = \int_{\partial B_\varepsilon(x,y)} \nabla\Phi \cdot dS \\ &= \int_{\partial B_\varepsilon(x,y)} \frac{A}{r} \cdot dS = \int_{\partial B_\varepsilon(x,y)} \frac{A}{\varepsilon} \cdot dS = A 2\pi. \end{aligned}$$

Therefore, we obtained the function

$$\Phi(r) = \frac{1}{2\pi} \ln(r),$$

which is called the **fundamental solution** of the Poisson equation in 2D. However, up until now, we did not take the region Ω and associated boundary conditions (at $\partial\Omega$) into account. The Green's function is now given as

$$G(x, y; \zeta, \eta) = \frac{1}{2\pi} \ln(r) + h,$$

where h solves

$$\begin{aligned} \Delta h &= 0 && \text{in } \Omega \\ h &= -\frac{1}{2\pi} \ln(r) && \text{on } \partial\Omega. \end{aligned}$$

Moreover, h should be two times continuously differentiable, and we have reduced the problem of finding the Green's function to computing h (which depends only on Ω).
We provide some examples for the Green's function

1. For $\Omega = \mathbb{R}^2$ there are no boundary conditions, and therefore, we have $h = 0$, and consequently

$$G(r) = \frac{1}{2\pi} \ln(r).$$

2. We consider the half space $\Omega = \{(x, y) \ : \ y \geq 0\}$. We compute the Green's function by a technique called mirroring. For that, we introduce for the point (x, y) the mirror point $(x, -y)$. Let r be the distance from (ζ, η) to (x, y) and r' be the distance from (ζ, η) to $(x, -y)$. Then, we add $h(x, y) = -\frac{1}{2\pi} \ln(r')$ to G. As at the boundary $y = 0$, we have $G = h$, we obtained a function that vanishes at the boundary. Moreover, h is regular, since $(x, -y)$ is not in Ω and by the preceding discussion, we have $\Delta h = 0$. Therefore, we have

$$G = \frac{1}{4\pi} \ln\left(\frac{(\zeta - x)^2 + (\eta - y)^2}{(\zeta - x)^2 + (\eta + y)^2} \right).$$

   Note that $G \to -\infty$ as $(\zeta, \eta) \to (x, y)$ and $G < 0$. These are general properties of the Green's function.

3. For $\Omega = \mathbb{R}^3$, a similar discussion as above gives the Green's function

$$G(r) = -\frac{1}{4\pi} \frac{1}{r}.$$

6.2.5 More fundamental solutions

Heat equation

We go back to the 1D-heat equation, i.e., we seek $u(x,t)$ that solves

$$\begin{aligned} u_t &= u_{xx} \\ u(x,0) &= u_0(x) \end{aligned}$$

on the whole space $\Omega = \mathbb{R}$ (thus, no boundary conditions need to be employed). In this case, we can use the Fourier-transformation (in x) on the equation and by the computational rules of the Fourier transformation, we turn the x-derivatives into multiplications

$$0 = \mathcal{F}[u_t - u_{xx}](\omega) = \partial_t \mathcal{F}[u](\omega) + |\omega|^2 \mathcal{F}[u](\omega).$$

Thus, we have derived the ODE $v'(\omega) = |\omega|^2 v(\omega)$ for the Fourier transformation $\mathcal{F}[u](\omega)$ that has the solution

$$\mathcal{F}[u](\omega, t) = C(\omega) e^{-|\omega|^2 t},$$

and the constant $C(\omega)$ can be computed as the Fourier transformation of the given initial data $C(\omega) = \mathcal{F}[u_0](\omega)$. Now, using the Fourier inversion formula, we get

$$u(x,t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathcal{F}[u_0](\omega) e^{-|\omega|^2 t} e^{i\omega x} d\omega.$$

We want to simplify this formula by using the Fourier convolution formula. For that, we define $w = \mathcal{F}^{-1}[e^{-|\omega|^2 t}]$. Then, since the Fourier transform turns convolutions into multiplications (and the inverse transform does the opposite), we obtain

$$\begin{aligned} u(x,t) &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathcal{F}[u_0](\omega) \mathcal{F}[w](\omega) e^{i\omega x} d\omega = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathcal{F}[u_0 \star w](\omega) e^{i\omega x} d\omega \\ &= \mathcal{F}^{-1}[\mathcal{F}[u_0 \star w]](x,t) = u_0 \star w(x,t). \end{aligned}$$

Now, we compute w by making the variable transformation $y = \sqrt{2t}\omega$

$$\begin{aligned} w(x,t) &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-|\omega|^2 t} e^{i\omega x} d\omega = \frac{1}{\sqrt{2\pi}\sqrt{2t}} \int_{\mathbb{R}} e^{-y^2/2} e^{iyx/\sqrt{2t}} dy \\ &= \frac{1}{\sqrt{4\pi t}} e^{-x^2/4t}, \end{aligned}$$

where the last equality follows from $\mathcal{F}[e^{-x^2/2}] = e^{-\omega^2/2}$. The function w is the **fundamental solution of the heat equation**. Plugging the formula of w into the above identity gives the solution formula for the heat equation on $\mathbb{R}$ in 1D

$$u(x,t) = \frac{1}{\sqrt{4\pi t}} \int_{\mathbb{R}} e^{-(x-y)^2/4t} u_0(y) dy.$$

Wave equation

We go back to the 1D-wave equation, i.e., we seek $u(x,t)$ that solves

$$\begin{aligned} u_{tt} &= c^2 u_{xx} \\ u(x,0) &= u_0(x) \\ u_t(x,0) &= u_1(x). \end{aligned}$$

Similarly as in the derivation of d'Alembert's solution, one can show that the **fundamental solution of the wave equation** is given by

$$\Phi(x,t) = \frac{H(ct-|x|)}{2c},$$

where H is the so called Heaviside-function given as $H(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x \leq 0 \end{cases}$.

We note that, in general, if a fundamental solution Φ is available for the differential equation $Lu = 0$ (here L is a differential operator, e.g., $L = \Delta$), then the inhomogeneous problem $Lu = f$ has the solution

$$u = \Phi \star f = \int_{\mathbb{R}^n} \Phi(x-y) f(y) dy.$$

6.2.6 Notion of solution

For PDEs there are different ideas and definitions of solutions. We previously were only looking at functions u that solve the differential equation at every point and are m-times continuously differentiable (where m is the order of the PDE). Such solutions are called **classical solutions**. For example, a classical solution to Poisson's equation

$$\begin{aligned} -\Delta u &= f \qquad \text{in } \Omega \\ u &= 0 \qquad \text{on } \partial\Omega \end{aligned}$$

is a function that satisfies $\Delta u(x) = f(x)$ for every point $x \in \Omega$ and is two times continuously differentiable.

Thus, we require a lot of differentiability (also called smoothness) of solutions. This may be problematic, if the right-hand side is not a continuous function, since by the equation, we have $\Delta u = f$, so, there is a second derivative of u that is not continuous, and no classical solution exists.

In order to still be able to solve the equation, the notion of solution has to be weakened. A way to do this is presented as follows: We multiply the equation with a function v that also satisfies $v = 0$ on $\partial\Omega$ and integrate over Ω

$$-\Delta u = f \qquad \Longrightarrow \qquad -\Delta uv = fv \qquad \Longrightarrow \qquad \int_\Omega -\Delta uv \, dV = \int_\Omega fv \, dV.$$

Now, integrating by parts using the divergence theorem gives

$$\begin{aligned} -\int_\Omega \Delta u v \, dV &= -\int_\Omega \operatorname{div}(\nabla u) v \, dV = -\int_{\partial\Omega} \nabla u v \cdot dS + \int_\Omega \nabla u \cdot \nabla v \, dV \\ &= \int_\Omega \nabla u \cdot \nabla v \, dV, \end{aligned}$$

where the last equality follows from $v \equiv 0$ on $\partial\Omega$. Now inserting this into the equation above gives

$$\int_\Omega \nabla u \cdot \nabla v \, dV = \int_\Omega f v \, dV.$$

Now, we call functions u that satisfy the equation for all v that are differentiable once and satisfy $v = 0$ on $\partial\Omega$ **weak solutions** to the Poisson equation, and above equation is called the **weak formulation of the PDE**.

The advantage of the weak formulation is that, for it to be well-defined, one only needs that u is one time differentiable. Weak formulations are also called variational formulation, which is motivated in the following section.

6.2.7 Other famous PDEs

In this subsection, we give a short description of three famous PDEs in physics.

The Schrödinger equation

The complex-valued **Schrödinger equation** describes the time evolution of the state function of a quantum mechanical system and is one of the basic equations of quantum mechanics. It reads as

$$i\hbar u_t = -H(u).$$

Here, $\hbar$ is the reduced Planck constant and H is the Hamilton operator for the system. The most famous example for H leads to the non-relativistic Schrödinger equation for the wave function of a single point particle in a potential V

$$i\hbar u_t = -\frac{\hbar}{2m}\Delta u + V(x,t)u,$$

where m is the particle mass.
Although it looks very similar to the heat equation, it is not a parabolic equation (due to the complex prefactor). In fact, its solutions can behave like waves (although it is not a hyperbolic equation either).

The Navier-Stokes equations

The Navier-Stokes equations are used to model the dynamics of a viscous fluid. Let u be the velocity of the fluid and ν the kinematic viscosity (constant). Assume that the fluid is homogeneous (constant density) and incompressible. Then, the equations

$$\begin{aligned} u_t + (u \cdot \nabla)u - \nu\Delta u &= f \\ \operatorname{div} u &= 0, \end{aligned}$$

where u is vector-valued, are called the **incompressible Navier-Stokes equations**. Here, we are dealing with a non-linear PDE of second order.
Solution theory for the Navier-Stokes equations in 3D is one of the most famous open problems in mathematics (in 2D one can fairly easily show that the equations have a unique solution).

The Navier-Stokes equations are used in many application, such as modeling the flow in a pipe, blood in a vessel or ocean currents. Additionally, they are right now the state of the art in weather simulations, used to simulate the air flow around an object (like a wing in planes or race cars) or even used in video games to realistically simulate water flow.

Maxwell's equations

In Chapter 4, we have already derived two equations linking the magnetic field intensity B to the current density J as

$$\operatorname{curl} B = J$$

(scaling such that $\mu_0 = 1$) as well as linking the electric field intensity E to the magnetic field intensity by

$$\operatorname{curl} E = -\partial_t B.$$

Gauß' law for magnetic and electric fields additionally implies

$$\begin{aligned} \operatorname{div} B &= 0 \\ \operatorname{div} E &= \rho/\varepsilon, \end{aligned}$$

where ε is called the permittivity and ρ is the charge density. Finally, the material laws

$$B = \mu H, \qquad J = \sigma E,$$

with the parameters μ being the permeability and σ being the electric conductivity and H being the magnetic field intensity, allow the reduction of variables to the system of PDEs

$$\begin{aligned} \operatorname{curl} E &= -\mu \partial_t H \\ \operatorname{curl} H &= \sigma E \end{aligned}$$

Taking the $\operatorname{curl} \mu^{-1}$ of the first equation and the partial derivative ∂_t of the second equation and combining both gives a linear second order PDE

$$\operatorname{curl} \mu^{-1} \operatorname{curl} E = -\sigma \partial_t E,$$

where the only unknown is the electric field intensity E (a 3D-vectorfield), and which is oftentimes referred to as **Maxwell's equations**.

Oftentimes, one models time harmonic problems, i.e., the dependence in time is of the form $E(x,t) = e^{i\omega t}E(x)$ and plugging that into the equation gives the **time harmonic Maxwell equations**

$$\operatorname{curl} \mu^{-1} \operatorname{curl} E + \kappa E = 0,$$

with $\kappa = i\omega\sigma$.

Chapter 7

Calculus of variations

7.1 Calculus of Variations

Variational problems are optimization problems, thus, the task is to find maxima and minima, but in contrast to the previous cases of functions, we are now interested in minimizing/maximizing so called functionals. In general, functionals are mappings that act on functions and map into $\mathbb{R}$ (or $\mathbb{C}$).

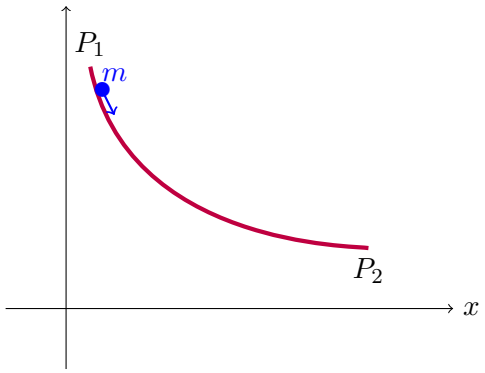
Example.

1. Let a surface $\begin{pmatrix} x \\ y \\ u(x,y) \end{pmatrix}$ in $\mathbb{R}^3$ with $(x,y) \in \Omega \subset \mathbb{R}^2$ be given. Then, by the discussion of Chapter 4.4, we have that the surface area is given by

$$A(u) = \int_\Omega |n| \; dxdy = \int_\Omega \sqrt{1 + |\nabla u|^2} \, dxdy.$$

   Thus, $A(u)$ takes a function and mapps it onto a number (the corresponding surface area). Now, one could ask the question, which surfaces minimize the surface area under the constraint that $u = g$ on $\partial\Omega$. This is a variational problem and solutions to it are called **minimal surfaces**.

2. A very famous problem is the so called **Brachistochrone-problem**: The goal is to find a curve $u(x)$ describing the movement of a mass m without friction in a constant gravitational force field between two points P_1 and P_2. Hereby, the curve $u(x)$ should be such that the time getting from the P_1 to P_2 is minimal (which explains the name brachystos = shortest, chronos = time).



For simplicity, we assume that P_1 is the origin write $P_2 = (x_0, u_0)$. Let s be the traveled distance along the path u (arclength!!) and $v = \frac{ds}{dt}$ the velocity of the mass. Conservation of energy (potential energy and kinetic energy) then gives

$$\frac{1}{2}mv^2 = mgu \qquad \Longrightarrow \qquad v = \sqrt{2gu}$$

We recall that the element of arclength is given by $ds = \sqrt{1 + u'(x)^2}dx$ and denote the traveled total arclength by L.

Using $v(t) = \frac{ds}{dt}$ and consequently $\frac{1}{v(s)} = \frac{ds}{dt}$, the total time traveled T is given as

$$T = \int_0^T dt = \int_0^L \frac{1}{v(s)}\, ds = \int_0^{x_0} \frac{1}{\sqrt{2gu(x)}} \sqrt{1 + u'(x)^2}\, dx.$$

Therefore, the corresponding variational problem is finding the minimum of the functional

$$\mathcal{F}(u) := \int_0^{x_0} \sqrt{\frac{1 + u'(x)^2}{2gu(x)}}\, dx$$

for functions u satisfying the constraints $u(0) = 0$ and $u(x_0) = u_0$. We will solve this problem later on. ■

7.2 The Euler-Lagrange equations

From now on, we only consider functionals in integral form, i.e., given as

$$I(u) = \int_a^b F(x, u, u')\, dx.$$

Here, the function F and the interval $[a, b]$ are fixed by the considered application, e.g., by physical laws.

The question is now finding the stationary points of $I(\cdot)$. In order to do that, we assume that the function $u(x)$ is this stationary point and we consider a small perturbation of u, i.e.,

$$u(x) \simeq u(x) + \alpha\eta(x),$$

where α is a small parameter and η a (smooth) function that reproduces some properties of u (such as boundary conditions). Fixing $\eta(x)$ (and having already fixed $u(x)$), we can reduce the functional to a function of α by defining

$$\widetilde{I}(\alpha) = I(u + \alpha\eta).$$

Now, a stationary point of $\widetilde{I}$ is easily computed by differentiation with respect to α. Consequently, for $u(x)$ to be a stationary point of I, we need to have

$$\begin{aligned} 0 = \frac{d\widetilde{I}}{d\alpha}\Big|_{\alpha=0} &= \frac{d}{d\alpha} I(u+\alpha\eta)\Big|_{\alpha=0} \\ &= \frac{d}{d\alpha}\int_a^b F(u+\alpha\eta, u'+\alpha\eta', x)\, dx\Big|_{\alpha=0} \\ &= \int_a^b \partial_u F(x,u,u')\eta + \partial_{u'} F(x,u,u')\eta'\, dx \qquad \forall \eta. \end{aligned}$$

The quantity

$$\delta I(u,\eta) = \int_a^b \frac{\partial}{\partial u} F(x,u,u')\eta + \frac{\partial}{\partial u'} F(x,u,u')\eta'\, dx$$

is called the **first-order variation** of I (as it measures the change done by the perturbation/variation of u in direction η). By the calculation above, we see that stationary points of I are characterized by the equation

$$\delta I(u,\eta) = 0 \qquad \forall \eta.$$

Integration by parts in the second term of the first-order variation gives

$$0 = \delta I(u,\eta) = \int_a^b \left(\frac{\partial}{\partial u} F(x,u,u') - \frac{d}{dx}\frac{\partial}{\partial u'} F(x,u,u')\right)\eta\, dx - \eta \frac{\partial F}{\partial u'}\Big|_a^b.$$

For simplicity, we now assume that the perturbations η vanish at the endpoints, i.e., $\eta(a) = \eta(b) = 0$, then the last term is zero, and stationary points satisfy

$$0 = \delta I(u,\eta) = \int_a^b \left(\frac{\partial}{\partial u} F(x,u,u') - \frac{d}{dx}\frac{\partial}{\partial u'} F(x,u,u')\right)\eta\, dx \qquad \forall \eta.$$

As this equation holds for all η (that vanish at the boundaries), the integrand has to be zero, which gives rise to the following definition.

Definition 7.1. *The second order partial differential equation*

$$\frac{\partial F}{\partial u} = \frac{d}{dx}\frac{\partial F}{\partial u'},$$

is called the **Euler-Lagrange equation** *corresponding to the functional* $I(u) = \int F(x,u,u')\, dx$.

Remark. Solving the Euler-Lagrange equations gives stationary points of the functional $I(u)$. In the same way as when finding minima or maxima, this method does not provide any information

about whether the computed stationary point maximizes or minimizes the functional or does neither. For that, one can either insert the stationary point into the functional and check whether a neighborhood of the stationary point contains bigger/smaller values or one can compute second-order variations similarly to above (which we won't do here). ■

Additionally, solving the Euler-Lagrange equations can be hard, as they are PDEs. In the following, we present some special cases.

7.2.1 F does not contain u explicitly

This means that

$$\frac{\partial F}{\partial u} = 0$$

and hence, the Euler-Lagrange equations give together with integration with respect to x

$$0 = \frac{d}{dx}\frac{\partial F}{\partial u'} \qquad \Longrightarrow \qquad \frac{\partial F}{\partial u'} = \text{const.}$$

Example. The minimal surface problem from the beginning of the section is of this form (albeit in higher dimensions).
Here, we consider the slightly simpler problem of a minimal path, i.e., we seek a curve $(x, u(x))$ connecting the points $A = (a, u(a))$ and $B = (b, u(b))$ with minimal arclength. Therefore, we want to minimize the functional

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

The Euler-Lagrange equation gives

$$\text{const} =: \kappa = \frac{\partial F}{\partial u'} = \frac{u'}{\sqrt{1 + u'(x)^2}}.$$

Rearranging this equation gives the ODE

$$u' = \frac{\kappa}{\sqrt{1 - \kappa^2}}$$

with the solution

$$u(x) = \frac{\kappa}{\sqrt{1 - \kappa^2}} x + c,$$

which is – as it should be – a straight line, and the constants κ and c can be computed using the conditions on the endpoints A, B, which gives the function $u(x) = \frac{u(b)-u(a)}{b-a}(x-a)+u(a)$. Inserting this into the functional L gives

$$L(u) := \int_a^b \sqrt{1 + \left(\frac{u(b) - u(a)}{b - a}\right)^2}\, dx = \sqrt{(u(b) - u(a))^2 + (b - a)^2},$$

which one would also obtain from Pythagoras law. ■

7.2.2 F does not contain x explicitly

We start with the product rule that implies

$$\frac{d}{dx}\left(u'\frac{\partial F}{\partial u'}\right) - u''\frac{\partial F}{\partial u'} = u'\frac{d}{dx}\frac{\partial F}{\partial u'}.$$

Consequently, multiplying the Euler-Lagrange equations with u' gives

$$u'\frac{\partial F}{\partial u} = u'\frac{d}{dx}\frac{\partial F}{\partial u'} = \frac{d}{dx}\left(u'\frac{\partial F}{\partial u'}\right) - u''\frac{\partial F}{\partial u'}$$

or

$$\frac{d}{dx}\left(u'\frac{\partial F}{\partial u'}\right) = u'\frac{\partial F}{\partial u} + u''\frac{\partial F}{\partial u'}.$$

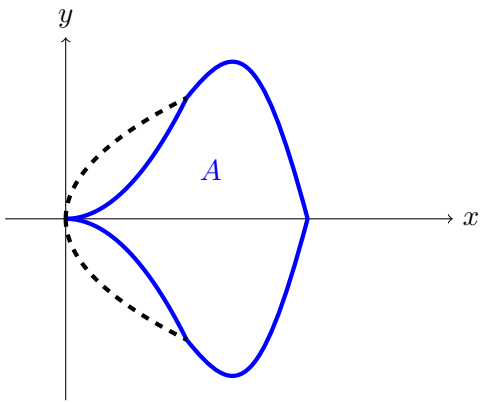
Now, by assumption F does not depend on x explicitly, which means $\frac{\partial F}{\partial x} = 0$, and therefore, the right-hand side in the equation above is the total derivative $\frac{dF}{dx}$. Consequently, integration gives

$$u'\frac{\partial F}{\partial u'} + \kappa = F,$$

where κ is the integration constant. Therefore, again, the Euler-Lagrange equation reduces to a first-order ODE.

Example. The task is to find the closed curve of fixed length ℓ that encloses the largest possible area.

We can assume (without loss of generality) that the sought curve passes through the origin and is convex (otherwise one can easily enlarge the area as visualized by the dotted lines below) and symmetric with respect to the x-axis.



We denote the arclength along the curve measured from the origin by s. Our additional assumptions lead to the conditions $u(0) = u(\ell/2) = 0$. The total area below the curve u is just the integral of u. In terms of the arclength parametrization this turns into

$$A(u) = 2\int_0^{\ell/2} u(s)\sqrt{1-u'(s)^2}\,ds.$$

Here, the integrand does not explicitly depend on s, so we can use the derived Euler-Lagrange equation from above, which reads

$$\kappa = F - u' \frac{\partial F}{\partial u'} = u\sqrt{1-u'^2} - \frac{uu'^2}{\sqrt{1-u'^2}}.$$

Expressing u' from this equation gives

$$\kappa u' = \pm\sqrt{\kappa^2 - u^2},$$

which, together with $u(0) = 0$ has the solution

$$u(s) = \kappa \sin\left(\frac{s}{\kappa}\right).$$

The second condition $u(\ell/2) = 0$ now gives $\kappa = \ell/(2\pi)$, which leads to

$$u(s) = \frac{\ell}{2\pi}\sin\left(\frac{2\pi s}{\ell}\right) \qquad \text{and} \qquad du = \cos\left(\frac{2\pi s}{\ell}\right) ds.$$

It remains to go back to Cartesian coordinates. Together with $ds^2 = dx^2 + du^2$ and $x(0) = 0$ we get $dx = \pm\sin\left(\frac{2\pi s}{\ell}\right) ds$ and integration now gives an expression of x in terms of s as

$$x - \frac{\ell}{2\pi} = -\frac{\ell}{2\pi}\cos\left(\frac{2\pi s}{\ell}\right).$$

Finally, we observe that this is indeed the expected result since x, u lie on the circle with radius $\frac{\ell}{2\pi}$ given by

$$\left(x - \frac{\ell}{2\pi}\right)^2 + u^2 = \frac{\ell^2}{4\pi^2}.$$

■

7.3 Some extensions

The theory of Euler-Lagrange equations is not limited to the case of one variable and scalar functions. Possible extensions are:

7.3.1 Functions in several variables

Here, we seek a function $u(x_1, \ldots, x_n)$ that minimizes a functional in integral form

$$I(u) = \int \cdots \int F\left(x_1, \ldots, x_n, u, \frac{\partial u}{\partial x_1}, \ldots, \frac{\partial u}{\partial x_n}\right) dx_1 \ldots dx_n$$

with the integrand $F\left(x_1, \ldots, x_n, u, \frac{\partial u}{\partial x_1}, \ldots, \frac{\partial u}{\partial x_n}\right)$ depending on all variables and partial derivatives. Here, the Euler-Lagrange equation takes the form

$$\frac{\partial F}{\partial u} = \sum_{i=1}^{n} \frac{d}{dx_i}\frac{\partial F}{\partial u_{x_i}},$$

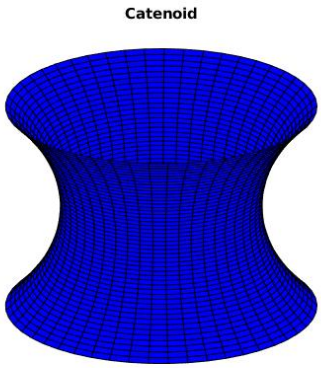
where u_{x_i} abbreviates $\frac{\partial u}{\partial x_i}$.

Example.

1. For the minimal surface problem stated at the beginning of this chapter, the Euler-Lagrange equation is given by

$$\begin{aligned} \operatorname{div} \frac{\nabla u}{\sqrt{1+|\nabla u|^2}} &= 0 \qquad \text{in } \Omega \\ u &= g \qquad \text{on } \partial\Omega. \end{aligned}$$

   A three dimensional example of a minimal surface (the first non trivial one discovered by Leonhard Euler in 1744) is the so called catenoid, which minimizes the surface area between two circular rings.



2. The potential energy of the (small) displacement $u(x, y)$ of a membrane above the region Ω can be expressed by the Dirichlet integral

$$I(u) = \int \int_{\Omega} |\nabla u|^2 + f(x, y)u \, dxdy,$$

   where f is an external force and boundary values $u = g$ at $\partial\Omega$ are prescribed. Then, by the previous discussion, we can compute the Euler-Lagrange equations as

$$-\Delta u + f = 0 \qquad \text{in } \Omega,$$

   i.e., the Euler-Lagrange equation is the Poisson equation. ■

7.3.2 Vector valued functions

Here, we seek a function $u : \mathbb{R} \to \mathbb{R}^n$ with coordinate functions $u_i(x)$ that minimizes the functional

$$I(u) = \int_a^b F\left(x, u_1, u_1', \ldots, u_n, u_n'\right) \, dx$$

with the integrand $F\left(x, u_1, u_1', \ldots, u_n, u_n'\right)$ on the component functions and their first order derivative.
Here, the Euler-Lagrange equations are a system of PDEs given by

$$\frac{\partial F}{\partial u_i} = \frac{d}{dx}\frac{\partial F}{\partial u_i'} \qquad i = 1, \ldots, n.$$

7.3.3 Higher order derivatives

Here, we seek a function $u(x)$ that minimizes the functional in integral form

$$I(u) = \int_a^b F\left(x, u, u', \ldots, u^{(n)}\right)\, dx$$

with the integrand $F\left(x, u, u', \ldots, u^{(n)}\right)$ depending also on higher derivatives of u.
Here, the Euler-Lagrange equations can be derived in the same way as for the first-order case by repeated integration by parts. Assuming that $u = u' = \ldots u^{(n-1)} = 0$ at both endpoints (otherwise additional constraints appear), this gives the Euler-Lagrange equations

$$\frac{\partial F}{\partial u} = \frac{d}{dx}\left(\frac{\partial F}{\partial u'}\right) - \frac{d^2}{dx^2}\left(\frac{\partial F}{\partial u''}\right) + \cdots - (-1)^n \frac{d^n}{dx^n}\left(\frac{\partial F}{\partial u^{(n)}}\right).$$

7.3.4 Variable endpoints

Here, we again we consider the functional

$$I(u) = \int_a^b F(x, u, u')\, dx,$$

but we only fix the value at a and let $u(b)$ be arbitrary. As in the derivation of the Euler-Lagrange equations, we obtain

$$0 = \delta I(u, \eta) = \int_a^b \left(\frac{\partial}{\partial u}F(x, u, u') - \frac{d}{dx}\frac{\partial}{\partial u'}F(x, u, u')\right)\eta\, dx - \eta\frac{\partial F}{\partial u'}\Big|_a^b \qquad \forall \eta.$$

Since we fixed the value at the starting point, we require $\eta(a) = 0$. The above equation holds for all such η. If we additionally require $\eta(b) = 0$, we obtain the same Euler-Lagrange equation as before. Therefore, for η that do not vanish at b, the above equation reduces to

$$0 = \eta(b)\frac{\partial F}{\partial u'}\Big|_b \qquad \Longrightarrow \qquad 0 = \frac{\partial F}{\partial u'}\Big|_b,$$

and we have derived an additional condition.

We note that, if we allow both endpoints to vary, $\frac{\partial F}{\partial u'}$ has to vanish on both endpoints.

Example. We consider a variant of the Brachistochrone example, where we allow the endpoint P_2 to vary anywhere on the vertical line $x = x_0$. We recall that the problem is to minimize the functional

$$\mathcal{F}(u) := \int_0^{x_0} \sqrt{\frac{1 + u'(x)^2}{2gu(x)}}dx.$$

Since $F = \sqrt{\frac{1+u'(x)^2}{2gu(x)}}$ does not depend on x explicitly, the previous discussion shows that the Euler-Lagrange equation is given by

$$u'\frac{\partial F}{\partial u'} + \kappa = F,$$

which is the equation

$$\sqrt{u(1+u'^2)} = \kappa.$$

Solving for u' gives the ODE

$$u'(x) = \sqrt{\frac{\kappa^2 - u(x)}{u(x)}}$$

Using separation of variables and the variable transformation $u = \kappa^2 \sin^2 t$, we obtain

$$x + C = \int \sqrt{\frac{u}{\kappa^2 - u}} du = 2\kappa^2 \int \sin^2 t \, dt.$$

Now, with the formula $2\sin^2 t = 1 - \cos(2t)$, we compute

$$x + C = \kappa^2 \int 1 - \cos(2t) \, dt = \kappa^2 (t - \frac{1}{2}\sin(2t)).$$

Consequently, we have the parametrization of the solution curve as

$$\begin{aligned} x(t) &= \kappa^2 \left(t - \frac{1}{2}\sin(2t) \right) + C \\ u(t) &= \frac{\kappa^2}{2} \left(1 - \cos(2t) \right). \end{aligned}$$

It remains to fix the constants C and κ. Using that the curve passes through $(0, 0)$ (at $t = 0$), we obtain $C = 0$. From the discussion on the Euler-Lagrange equation with variable endpoints, we obtain the constraint

$$0 = \frac{\partial F}{\partial u'}\Big|_{x=x_0} = \frac{u'}{\sqrt{u(1+u')^2}}\Big|_{x=x_0} \qquad \Longrightarrow \qquad u'(x_0) = 0.$$

Therefore, the tangent to the curve at P_2 must be parallel to the x-axis, which implies that $\frac{\pi}{2}\kappa^2 = x_0$. ■

7.4 Constrained variations

For optimization problems for functions with constraints, we introduced the technique of Lagrange multipliers in the exercise part. Here, we employ a similar technique to optimize functionals under side constraints. We again look at the functional

$$I(u) = \int_a^b F(x, u, u') \, dx$$

subject to the additional constraint

$$J(u) = \int_a^b G(x, u, u') \, dx = \text{const.}$$

As in the method of Lagrange multipliers, let $\lambda \in \mathbb{R}$ and define the new functional

$$\mathcal{L}(u) := I(u) + \lambda J(u) = \int_a^b F(x, u, u') + \lambda G(x, u, u') dx.$$

Stationary points of this functional can again be computed by solving the Euler-Lagrange equation. Here, we just replace the function F by $F + \lambda G$, which gives the Euler-Lagrange equations

$$\frac{\partial F}{\partial u} - \frac{d}{dx}\frac{\partial F}{\partial u'} + \lambda \left(\frac{\partial G}{\partial u} - \frac{d}{dx}\frac{\partial G}{\partial u'} \right) = 0.$$

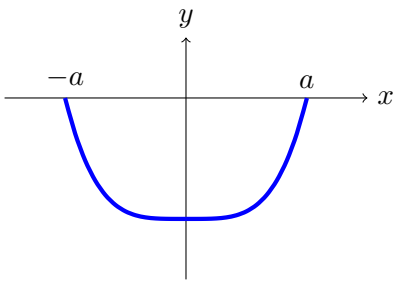
From this equation and the constraint $J = \text{const}$ one can compute the solution u.

We note that this method can easily be generalized to more constraints by setting

$$\mathcal{L}(u) := I(u) + \sum_{j=1}^{n} \lambda_i J_i(u),$$

where $J_i = \text{const}$ denote the constraints.

Example. The goal is to compute the shape of a uniform rope that is suspended by its ends from two points at equal heights.



Let $2L > 0$ be the length of the rope and the rope be suspended at $x = \pm a$ and $y = 0$. Denote by ρ the uniform density of the rope. In order to solve the problem, we have to find a stationary point to the gravitational potential energy of the rope given by

$$I(u) = -\rho g \int u \, ds = -\rho g \int_{-a}^{a} u(x)\sqrt{1 + u'(x)^2} dx$$

under the constraint that

$$J(u) = \int ds = \int_{-a}^{a} \sqrt{1 + u'(x)^2} \, dx = 2L.$$

For simplicity, change the negative sign in $I(u)$ (which is allowed since we can take $-\lambda$ instead of λ in the following) and compute a stationary point of the functional

$$\mathcal{L}(u) = -(I(u) - \lambda J(u)) = \int_{-a}^{a} (\rho g u(x) + \lambda)\sqrt{1 + u'(x)^2} \, dx.$$

Now, the integrand does not contain x explicitly, and consequently, we obtain the Euler-Lagrange equation

$$(\rho g u + \lambda)(1 + u'^2)^{1/2} - (\rho g u + \lambda)(1 + u'^2)^{-1/2} u'^2 = \kappa.$$

Rearranging terms, we arrive at the nonlinear ODE

$$u'(x)^2 = \left(\frac{\rho g u(x) + \lambda}{\kappa} \right)^2 - 1.$$

With separation of variables and the substitution $\rho g u + \lambda = \kappa \cosh(z)$ (which gives $du = \frac{\kappa}{\rho g} \sinh(z)$), we get

$$x + C = \int \frac{1}{\left(\frac{\rho g u + \lambda}{\kappa} \right)^2 - 1} du = \int \frac{1}{\sqrt{\cosh^2(z) - 1}} \frac{\kappa}{\rho g} \sinh(z)\, dz = \int \frac{\kappa}{\rho g}\, dz = z \frac{\kappa}{\rho g}.$$

Reverting the substitution gives the formula for the solution

$$\frac{\kappa}{\rho g} \cosh^{-1} \left(\frac{\rho g u + \lambda}{\kappa} \right) = x + C,$$

and we now have three unknowns, λ, κ, C and three constraints $u(\pm a) = 0$ and $J = 2L$. From the first two constraints, we get

$$\cosh \left(\frac{\rho g (a + C)}{\kappa} \right) = \frac{\lambda}{\kappa} = \cosh \left(\frac{\rho g (-a + C)}{\kappa} \right).$$

Since $a \neq 0$, the symmetry of the hyperbolic cosine implies $C = 0$, and we have $\lambda = \kappa \cosh\left(\frac{\rho g a}{\kappa}\right)$. Inserting that together with $u' = \sinh\left(\frac{\rho g x}{\kappa}\right)$ into the side constraint gives

$$\begin{aligned} 2L &= \int_{-a}^{a} \sqrt{1 + u'(x)^2}\, dx = \int_{-a}^{a} \sqrt{1 + \sinh\left(\frac{\rho g x}{\kappa} \right)^2}\, dx = \int_{-a}^{a} \cosh\left(\frac{\rho g x}{\kappa} \right)\, dx \\ &= \frac{2\kappa}{\rho g} \sinh\left(\frac{\rho g a}{\kappa} \right), \end{aligned}$$

which is an equation that can be solved for κ and the stationary point is given by

$$u(x) = \frac{\kappa}{\rho g} \left[\cosh\left(\frac{\rho g x}{\kappa} \right) - \cosh\left(\frac{\rho g a}{\kappa} \right) \right].$$

■

Chapter 8

Complex analysis

8.1 Complex analysis

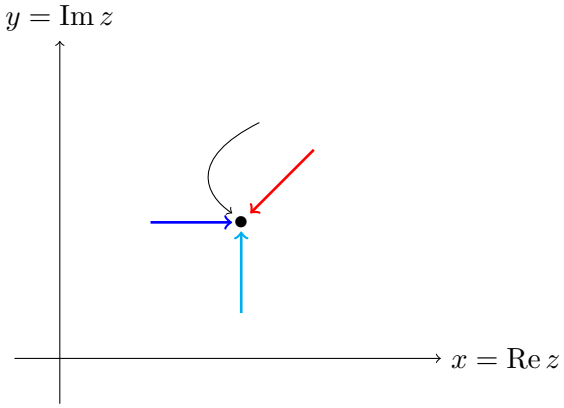
In this chapter, we are concerned with complex valued functions $f : \mathbb{C} \to \mathbb{C}$.
With the imaginary unit i satisfying $i^2 = -1$, a complex number can be written as

$$z = x + iy,$$

where x is called the real part and y is called the imaginary part. Therefore, each complex number can also be interpreted as a vector $(x, y) \in \mathbb{R}^2$. In the same way, we can write a complex valued function f as

$$f(z) = u(x, y) + iv(x, y),$$

where the real and the imaginary part $u, v : \mathbb{R}^2 \to \mathbb{R}^2$ are real-valued functions and sometimes denoted by $u = \operatorname{Re} f$ and $v = \operatorname{Im} f$.
In the following, we want to introduce the meaning of complex differentiation. In order to do so, we stress that limits $z \to z_0$ are understood as in the case of $\mathbb{R}^2$ in Chapter 2, i.e., any direction has to be taken into account.



Definition 8.1. *A complex function $f : \mathbb{C} \to \mathbb{C}$ is called* **complex differentiable** *at the point z_0, if the limit*

$$f'(z_0) = \lim_{\Delta z \to 0} \frac{f(z_0 + \Delta z) - f(z_0)}{\Delta z}$$

exists and is unique, regardless of the direction from which Δz approaches 0.

If a function is complex differentiable in every point of a region D, it is called **analytic** *or* **holomorphic**.

If a function is complex differentiable in a region D except at a finite number of points, we call these points **singularities** *and the function* **analytic except on the singularities**.

Example.

1. The function $f(z) = z^n$ is analytic in $\mathbb{C}$, since

$$\lim_{\Delta z \to 0} \frac{(z_0 + \Delta z)^n - z_0^n}{\Delta z} = \lim_{\Delta z \to 0} \left(n z_0^{n-1} + \frac{n(n-1)}{2} z_0^{n-2} \Delta z + \cdots + (\Delta z)^{n-1} \right) = n z_0^{n-1},$$

   which shows that the limit exists and is unique at every point $z_0 \in \mathbb{C}$. Consequently, all complex polynomials are complex differentiable everywhere.

2. The function $f(z) = \overline{z}$ (which denotes the complex conjugation) is not differentiable, since we get

$$\lim_{\Delta z \to 0} \frac{\overline{(z_0 + \Delta z)} - \overline{z_0}}{\Delta z} = \lim_{\Delta z \to 0} \frac{\overline{\Delta z}}{\Delta z}.$$

   Now if $\Delta z \to 0$ parallel to the real axis, we have $\overline{\Delta z} = \Delta z$ and the value of the limit is 1. On the other hand, if $\Delta z \to 0$ parallel to the imaginary axis, we have that $\overline{\Delta z} = -\Delta z$, and the limit is -1. Consequently, the function is not complex differentiable.

8.1.1 The Cauchy-Riemann equations

In the following, we provide a criterion that is fairly easy to check to determine whether a function is complex differentiable or not.
We start by writing $f(z) = u(x, y) + iv(x, y)$ and abbreviate $\Delta u = u(x_0 + \Delta x, y_0 + \Delta y) - u(x_0, y_0)$. If f is differentiable at z_0, the limit

$$f'(z_0) = \lim_{\Delta z \to 0} \frac{\Delta u + i \Delta v}{\Delta z} = \lim_{\Delta z \to 0} \left(\frac{\Delta u}{\Delta z} + i \frac{\Delta v}{\Delta z} \right)$$

has to exist and be independent of $\Delta z \to 0$. Now, taking $\Delta z \to 0$ parallel to the real axis, we have $\Delta z = \Delta x$, $\Delta y = 0$ and consequently

$$f'(z_0) = \lim_{\Delta z \to 0} \left(\frac{\Delta u}{\Delta x} + i \frac{\Delta v}{\Delta x} \right) = \frac{\partial u}{\partial x} + i \frac{\partial v}{\partial x}.$$

On the other hand, taking $\Delta z \to 0$ parallel to the imaginary axis, we have $\Delta x = 0$, and $\Delta z = i\Delta y$ and consequently

$$f'(z_0) = \lim_{\Delta z \to 0} \left(\frac{\Delta v}{\Delta y} - i \frac{\Delta u}{\Delta y} \right) = \frac{\partial v}{\partial y} - i \frac{\partial u}{\partial y}.$$

Now, for f to be differentiable, both relations need to be the same and comparing real and imaginary parts, we motivate the following definition.

Definition 8.2. *The partial differential equations*

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}$$
$$\frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}$$

are called the **Cauchy-Riemann equations** *corresponding to the complex function* $f(x+iy) = u(x,y) + iv(x,y)$.

Due to the previous discussion, the Cauchy-Riemann equations are a necessary condition for complex differentiation. By themselves they cannot be a sufficient condition, as only two directions are taken into account. However, the following theorem also states a sufficient condition.

Theorem 8.3. *A function f is complex differentiable at z_0, if and only if*

1. *The functions u, v are continuously partially differentiable at z_0, and*
2. *the partial derivatives satisfy the Cauchy-Riemann equations at z_0.*

Example.

1. We go back to the example of the function $f(z) = \overline{z} = x - iy$. Here, we have that $u(x,y) = x$ and $v(x,y) = -y$. Thus, the Cauchy-Riemann equations are violated, since
$$\frac{\partial u}{\partial x} = 1 \neq -1 = \frac{\partial v}{\partial y}.$$

2. We consider the function $f(z) = \frac{1}{z}$. Writing $z = x + iy$, we compute
$$f(z) = \frac{1}{z} = \frac{x - iy}{x^2 + y^2} \qquad \Longrightarrow \qquad u(x,y) = \frac{x}{x^2+y^2}, v(x,y) = -\frac{y}{x^2+y^2}.$$
Checking the Cauchy-Riemann equations gives
$$\frac{\partial u}{\partial x} = \frac{y^2 - x^2}{(x^2+y^2)^2} = \frac{\partial v}{\partial y}$$
$$\frac{\partial u}{\partial y} = \frac{-2xy}{x^2+y^2} = -\frac{\partial v}{\partial x}.$$
However, at $z = 0$ the function is not continuous (and consequently the functions u, v can not be continuously partially differentiable there). Thus, the function is analytic everywhere but at $z = 0$.

8.1.2 Complex integration and Cauchy's integral formula

We have essentially already introduced everything necessary for the integration of complex functions. In fact, the integral

$$\int_\alpha^\beta f(z)dz$$

between two points $\alpha, \beta \in \mathbb{C}$ should be understood as a path integral (as $\mathbb{C}$ corresponds with $\mathbb{R}^2$), i.e., as there are infinitely many possibilities to connect α, β in the complex plane, one needs to to specify the path C connecting the points. Consequently, with a parametrization $\gamma : [a, b] \to \mathbb{C}$ we write

$$\int_C f(z)dz := \int_a^b f(\gamma(t))\gamma'(t)\, dt$$

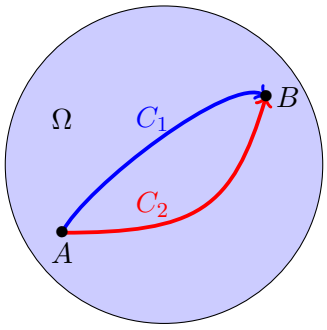
for the path integral and use the notation $\oint_C f(z)\, dz$ for closed curves. In the following, we always assume that the closed curve C only circles once around each point inside of the curve C.

The following theorem is the most important result regarding integration of complex functions and is called **Cauchy's integral theorem**. In fact, the theorem is closely connected to the discussion of path independence of line integrals of Chapter 4 and provides a condition on this for complex functions.

Theorem 8.4 (Cauchy's integral theorem). *Let C be a closed curve and let f be analytic on C and in the region bounded by C. Then,*

$$\oint_C f(z)\, dz = 0.$$

Indeed, a direct consequence of the theorem is path independence of all line integrals inside a region Ω, on which the function f is analytic. Let C_1 and C_2 be two curves with the same endpoints completely contained in Ω.



Then, $C_1 \cup -C_2$ is a closed curve inside Ω and f is therefore analytic inside the region bounded by $C_1 \cup -C_2$. Thus, Cauchy's theorem gives

$$0 = \oint_{C_1 \cup -C_2} f(z)\, dz = \int_{C_1} f(z)\, dz - \int_{C_2} f(z)\, dz$$

and consequently

$$\int_{C_1} f(z)\,dz = \int_{C_2} f(z)\,dz.$$

Another very useful result, e.g., in physics, is the so called **Cauchy integral formula**. It states, that the value of an analytic function at z_0 can be computed by a path integral of the function $\frac{f(z)}{z-z_0}$.

Theorem 8.5 (Cauchy's integral formula). *Let C be a closed curve and let f be analytic on C and in the region bounded by C. Let z_0 be an arbitrary point inside the region bounded by C. Then,*

$$f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z - z_0}\,dz.$$

Remark. We note that, if the point z_0 lies outside the region bounded by C, we have that the function $\frac{1}{z-z_0}$ is analytic (compare the previous example) and consequently $\frac{f(z)}{z-z_0}$ is analytic inside C. Consequently, Cauchy's integral theorem gives that the value of the integral on the left-hand side in the equation above is zero. ■

Cauchy's integral formula can also be applied to the derivative of f or more general to the n-th order derivative, which gives the formula

$$f^{(n)}(z_0) = \frac{d^n}{dz_0^n}\left(\frac{1}{2\pi i}\oint_C \frac{f(z)}{z - z_0}\,dz\right) = \frac{n!}{2\pi i}\oint_C \frac{f(z)}{(z - z_0)^{n+1}}\,dz.$$

An amazing consequence of this formula is that any analytical function is **infinitely many times complex differentiable**!

8.1.3 Complex power series

In the following, we are concerned with expressing a complex function in a complex power series around a point z_0, i.e., we want to write

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n$$

with some coefficients $a_n \in C$ for all $n \in \mathbb{N}$.

For real valued functions, we introduced Taylor series in the exercise part, where an infinitely times differentiable function at a point x_0 can be written as the sum

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

Using Cauchy's integral formula, we can easily extend the theory of Taylor series to complex valued functions. We start with expressing the function $\frac{1}{\zeta - z}$ as a geometric series, i.e.,

$$\frac{1}{\zeta - z} = \frac{1}{\zeta - z_0} \sum_{n=0}^{\infty} \left(\frac{z - z_0}{\zeta - z_0}\right)^n.$$

Inserting this into the Cauchy integral formula gives

$$f(z) = \frac{1}{2\pi i}\oint_C \frac{f(\zeta)}{\zeta - z}\,d\zeta = \frac{1}{2\pi i}\oint_C \frac{f(\zeta)}{\zeta - z_0}\sum_{n=0}^{\infty}\left(\frac{z-z_0}{\zeta - z_0}\right)^n d\zeta$$
$$= \frac{1}{2\pi i}\sum_{n=0}^{\infty}(z-z_0)^n \oint \frac{f(\zeta)}{(\zeta - z_0)^{n+1}} = \sum_{n=0}^{\infty}(z-z_0)^n \frac{f^{(n)}(z_0)}{n!},$$

which is exactly the Taylor series.

As we used the Cauchy integral formula, we have to assume that f is analytic on and inside the curve C. If that is not the case, we cannot express f by its Taylor series. However, it is oftentimes possible to derive a power series representation

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z-z_0)^n,$$

which includes also negative powers. This is called a **Laurent series**.

Theorem 8.6. *Let $f : \mathbb{C} \to \mathbb{C}$ be analytic inside and on a closed curve C except at a point z_0, which lies inside of C. Then, f can be written as*

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z-z_0)^n \qquad a_n = \frac{1}{2\pi i}\oint_C \frac{f(\zeta)}{(\zeta - z_0)^{n+1}}\,d\zeta \qquad n \in \mathbb{Z}.$$

A Laurent series can be written as

$$f(z) = \sum_{n=0}^{\infty} a_n (z-z_0)^n + \sum_{n=1}^{\infty} a_{-n}(z-z_0)^n,$$

where the first sum (containing the positive powers) is called the **regular part** and the second sum (negative powers) is called the **principal part**.

Example.

1. The function $f(z) = \frac{1}{1-z}$ can for all $z \in \mathbb{C}$ with $|z| < 1$ be expressed as a Taylor series by use of a geometric series, i.e.,

   $$f(z) = \frac{1}{1-z} = \sum_{n=0} z^n.$$

   This is actually the Taylor expansion around $z_0 = 0$. However, the function is not analytic at $z = 1$. For $|z| > 1$, we can write

   $$f(z) = \frac{1}{1-z} = \frac{1}{z}\frac{1}{1/z - 1} = -\frac{1}{z}\sum_{n=0} z^{-n} = \sum_{n=0} z^{-n-1},$$

   and we obtained a Laurent series expansion.

2. We want to compute the Taylor/Laurent series of $f(z) = \frac{1}{(z-1)^2}$ around $z_0 = 0$. Here, we use a trick involving differentiation, since $\frac{d}{dz}\frac{1}{1-z} = \frac{1}{(z-1)^2}$. Now, for $|z| < 1$, we have computed $\frac{1}{1-z} = \sum_{n=0} z^n$, which leads to

$$\frac{1}{(z-1)^2} = \frac{d}{dz}\frac{1}{1-z} = \frac{d}{dz}\sum_{n=0}^{\infty} z^n = \sum_{n=0}^{\infty}(n+1)z^n.$$

In the same way, we compute for $|z| > 1$ that

$$\frac{1}{(z-1)^2} = \frac{d}{dz}\frac{1}{1-z} = \frac{d}{dz}\sum_{n=0}^{\infty} z^{-n-1} = -\sum_{n=0}^{\infty}(n+1)z^{-(n+2)},$$

which is the Laurent series expansion. ■

The previous example shows that a power series may not represent the function on the whole space $\mathbb{C}$, but only on a region (in the example this would be the unit circle $|z| < 1$). This is related to the so called **circle of convergence** of a power series, which is the circle $B_R := \{z \in \mathbb{C} \,:\, |z| < R\}$ of maximal radius R around zero, such that the power series

$$\sum_{n=0}^{\infty} |a_n|\, z^n$$

converges for all $z \in B_R$. In fact, this is called **absolute convergence**. The radius of the circle can be computed directly from the coefficients a_n by either

$$R = \lim_{n\to\infty} \left|\frac{a_n}{a_{n+1}}\right| \qquad \text{or}$$
$$R = \lim_{n\to\infty} \frac{1}{\lim_{n\to\infty} \sqrt[n]{|a_n|}}$$

if the limits exist. Hereby, the radius can be 0, finite or ∞ (which means the power series converges on $\mathbb{C}$).

The previous example suggests that somewhere at the boundary of the circle of convergence, analyticity does not hold, which is precisely the statement of the following theorem.

Theorem 8.7. *Let the power series $\sum_{n=0}^{\infty} a_n z^n$ converge on the circle B_R. Then, there lies at least on singularity on the line $|z| = R$.*

As previously defined, a singularity of a complex function f is a point z_0, where the function is not analytic. In the following, we are only concerned with so called **isolated singularities**, which means that there is a circle around z_0 on which f is analytic everywhere except at z_0.

Isolated singularities at z_0 can be classified as:

1. **Removable singularities:** Here, f is bounded in a (small) ball around z_0 except possibly at z_0.
2. **Poles of order n:** Here, for $n \in \mathbb{N}$, f has the form
$$f(z) = \frac{g(z)}{(z - z_0)^n},$$
where g is analytic (in a region around z_0).
3. **Essential singularities:** Here, the Laurent series of f around z_0 has an infinite amount of non-zero terms that involve negative powers of $(z - z_0)$.

In general, one could define the value at a removable singularity in a way that one obtains an analytic function (which explains the name removable singularity). Moreover, removable singularities can be characterized by having no principal part in the Laurent series expansion.

Poles can also be characterized by having a finite principal part in the Laurent series.

Example.

1. The function $f(z) = \frac{\sin(z)}{z}$ has an undefined value at $z = 0$. However, using the Taylor series of $\sin(z) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} z^{2n+1}$, one can compute
$$\lim_{z \to 0} \frac{\sin(z)}{z} = \lim_{z \to 0} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} z^{2n} = 1.$$
Therefore, $f(z)$ is bounded around $z = 0$, and we have a removable singularity.
2. The function $f(z) = \frac{1}{z}$ has a pole of order 1 at $z = 0$ and is already given in its Laurent-expansion around zero.
3. The function $f(z) = \frac{1}{(1-z)^2} - \frac{1}{1+z} = \frac{z(3-z)}{(1-z)(1+z)}$ has two poles at $z = 1$ (order 2) and $z = -1$ (order 1).
4. The function $f(z) = e^{1/z}$ has the Laurent series
$$e^{1/z} = \sum_{n=0}^{\infty} \frac{1}{n!} z^{-n},$$
which is valid for all $|z| > 0$. Hence, the principal part is infinite, and we have an essential singularity at $z = 0$. ■

The following theorem is very useful for determining types of singularities. Hereby, a **rational function** is defined as a function $f(z) = \frac{p(z)}{q(z)}$, where p, q are complex polynomials, and $n(q, z_0)$ denotes the order of the zero point z_0 of a polynomial q.

Theorem 8.8. *For rational functions $f(z) = p(z)/q(z)$ only the following singularities can occur:*

- *If p, q do have no common zeros, then f has only poles at the zeros of q of order $n(q, z_0)$.*
- *For common zeros z_0 of p, q with the orders $n(q, z_0) > n(p, z_0)$, we have that f has a pole of order $n(q, z_0) - n(p, z_0) > 0$.*
- *For common zeros z_0 of p, q with the orders $n(q, z_0) \leq n(p, z_0)$, we have a removable singularity.*

Conversely, an analytic function that has only singularities that are poles has to be a rational function.

8.1.4 Calculus of Residues

In the following, we are interested in the computation of complex line integrals. As the Cauchy theorem states that for an analytic integrand we obtain the value zero for integration over a closed curve, we are interested in the case of functions with singularities inside a closed curve C. In fact, we will obtain a rather easy and very useful formula for the evaluation provided by the so called residue theorem.

Definition 8.9. *Let f be a complex function and z_0 an isolated singularity of f. Then, the* **residue** $\mathrm{Res}(f, z_0)$ *of f at z_0 is defined by*

$$\mathrm{Res}(f, z_0) := a_{-1},$$

where a_{-1} is the coefficient corresponding to the power -1 in the Laurent expansion $f(z) = \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n$ around z_0.

The following theorem allows for a fairly simple computation of residues, if the singularity is a pole.

Theorem 8.10. *Let f be a complex function and z_0 be a pole of order m of f. Then,*

$$\mathrm{Res}(f, z_0) = \frac{1}{(m-1)!} \lim_{z \to z_0} \frac{d^{m-1}}{dz^{m-1}} \left((z - z_0)^m f(z) \right).$$

Example.

1. The function
$$f(z) = \frac{\sin(z)}{z^2} = \frac{1}{z} \frac{\sin(z)}{z}$$
has a first order pole at $z = 0$ (since by the previous example the singularity of $\frac{\sin(z)}{z}$ is removable). Therefore, the previous theorem gives
$$\mathrm{Res}(f, 0) = \lim_{z \to 0} z f(z) = \lim_{z \to 0} \frac{\sin(z)}{z} = 1.$$

2. The function
$$f(z) = \frac{e^{iz}}{(z^2+1)} = \frac{e^{iz}}{(z+i)^2(z-i)^2}$$
has two poles of second order at $z = i$ and $z = -i$. Using the previous theorem, we compute the residue at $z = i$ as
$$\frac{d}{dz}\left[(z-i)^2 f(z)\right] = \frac{d}{dz}\left(\frac{e^{iz}}{(z+i)^2}\right) = \frac{(z+i)^2 i e^{iz} - 2e^{iz}(z+i)}{(z+i)^4}.$$
Now, taking the limit $z \to i$ gives the residue
$$\mathrm{Res}(f, i) = \lim_{z\to i} \frac{d}{dz}\left[(z-i)^2 f(z)\right] = -\frac{i}{2e}.$$

3. The function $f(z) = e^{1/z}$ has an essential singularity at $z = 0$. Therefore, we cannot apply the previous theorem. However, we have already determined the Laurent series expansion in a previous example. This gives
$$\mathrm{Res}(f, 0) = 1.$$

■

The following theorem, called the **residue theorem** is the most important result of this subsection, and it states that the complex line integral of a function with singularities can be evaluated by only computing the residues.

Theorem 8.11. *Let $f : \mathbb{C} \to \mathbb{C}$ be an analytic function except at a finite number of singularities $z_0, z_1, \ldots, z_N$ in a region bounded by a closed curve C. Then,*
$$\oint_C f(z)\, dz = 2\pi i \sum_{j=0}^{N} \mathrm{Res}(f, z_j).$$

Remark. At the beginning of this chapter we assumed that the curve C only circles once around each point in the interior. This is important in the formulation of the residue theorem (and also Cauchy's integral formula). Otherwise, one would have to multiply the residues with the so called **winding number**, which measures how often the curve C moves around a point. ■

Example. Let $C := \{z \in \mathbb{C} \,:\, |z| = 1\}$ be the unit disc and
$$f(z) = \frac{\sin(z)}{z^2}.$$
We want to compute the integral $\oint_C f\, dz$. By the previous example, we have $\mathrm{Res}(f, 0) = 1$ and the function f is everywhere else analytic in the unit circle. Therefore, the residue theorem implies
$$\oint_C f(z)\, dz = 2\pi i \,\mathrm{Res}(f, 0) = 2\pi i.$$

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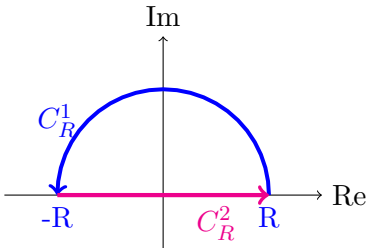
Evaluation of infinite integrals

The residue theorem is a powerful tool to also evaluate some difficult real valued integrals.
In the following, we consider integrals

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

where $f = \frac{p}{q}$ is a rational function without poles on the real axis that also satisfies $\lim_{|x|\to\infty} xf(x) = 0$ (which guarantees that the infinite integral exists).

Now, we take the curve $C_R = C_R^1 \cup C_R^2$, where $C_R^1 := \{z \in \mathbb{C} \,:\, |z| = R, \mathrm{Im}(z) > 0\}$ is the upper half circle of radius R and $C_R^2 := \{z \in \mathbb{C} \,:\, \mathrm{Im}(z) = 0, \mathrm{Re}(z) \in [-R, R]\}$ (the real interval $[-R, R]$ as subset of $\mathbb{C}$) orientated as drawn in the picture.



Now, taking R big enough, we can ensure that all poles of f (which must be zeros of the polynomial q) in the upper half plane $\mathrm{Im}(z) > 0$ lie inside the half circle of radius R. Thus, the residue theorem implies

$$\oint_{C_R} f(z)\, dz = \int_{C_R^1} f(z)\, dz + \int_{-R}^{R} f(x)\, dx.$$

Therefore, taking the limit $R \to \infty$ would produce the sought integral on the right-hand side. In order to do so, we need to analyze what happens with the integral $\int_{C_R^1} f(z)\, dz$. Using polar coordinates, we write

$$\int_{C_R^1} f(z)\, dz = \int_0^{\pi} f(R, \varphi) R d\varphi \leq \pi \max_{|z|=R} f(z) R \to 0 \qquad \text{for } R \to \infty,$$

due to the assumption $\lim_{|x|\to\infty} xf(x) = 0$ together with the fact that f is rational. Consequently, we have that

$$\lim_{R\to\infty} \oint_{C_R} f(z)\, dz = \int_{-\infty}^{\infty} f(x)\, dx.$$

The integral on the left-hand side can be computed using the residue theorem and we finally arrive at

$$\int_{-\infty}^{\infty} f(x)\, dx = 2\pi i \sum_{j=0}^{N} \mathrm{Res}(f, z_j),$$

where z_j are the complex poles of f in the upper half plane (i.e. those with positive imaginary part).

Example. We want to compute the integral

$$\int_{-\infty}^{\infty} \frac{1}{x^2+1}\, dx.$$

We have a rational function $\frac{1}{x^2+1}$ that satisfies the additional assumption $\lim_{|x|\to\infty} xf(x) = 0$ and has two non-real poles of first order at $z_1 = i$ and $z_2 = -i$, where only z_1 lies in the upper half-plane (therefore, z_2 is irrelevant for the computations). We can easily compute the residue by

$$\operatorname{Res}(f, i) = \lim_{z\to i}(z-i)\frac{1}{z^2+1} = \lim_{z\to i}\frac{1}{z+i} = \frac{1}{2i}.$$

Therefore, by the preceding discussion, we get the value of the integral as

$$\int_{-\infty}^{\infty} \frac{1}{x^2+1}\, dx = 2\pi i \operatorname{Res}(f, i) = \pi.$$

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Obviously, the previous example could also easily be solved by knowing the principal integral of the function (here the function $\operatorname{atan}(x)$). However, the shown technique applies also to functions, whose principal integrals are not that clear.

In fact, we can also compute integrals with singularities at the real axis, if the curve is chosen differently.

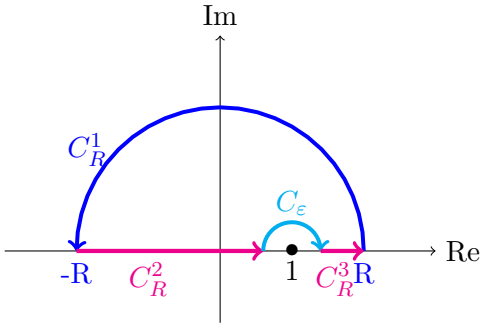
Example. We want to compute the principal value (this was defined in the exercise part and is needed here, since the integral does not exist in a classical sense) of

$$P.V. \int_{-\infty}^{\infty} \frac{\sin(x)}{x-1}\, dx.$$

Thus, the function $f(z) = \frac{e^{iz}}{(z-1)}$ has exactly one pole at $z = 1$ and we have that

$$\operatorname{Im} \int_{-\infty}^{\infty} \frac{e^{ix}}{x-1}\, dx = \int_{-\infty}^{\infty} \frac{\sin(x)}{x-1}\, dx.$$

We chose our curve as drawn below, where C_R^1 is a half circle of radius R centered at the origin and C_ε is a half circle (orientated the other way round) of radius ε centered at $(1, 0)$.



Therefore, the function $f(z)$ is analytic inside the curve $C = C_R^1 \cup C_R^2 \cup C_\varepsilon \cup C_R^3$ for $R > 1$ and by the residue theorem (or Cauchy's integral theorem), we obtain

$$0 = \oint_C f(z)\, dz = \int_{C_R^1} f(z)\, dz + \int_{-R}^{1-\varepsilon} f(x)\, dx + \int_{C_\varepsilon} f(z)\, dz + \int_{1+\varepsilon}^{R} f(x)\, dx$$

Now, it can be shown that $\left|\int_{C_R^1} f(z)\, dz\right| \to 0$ for $R \to \infty$ by parametrization of the half circle. Finally, we compute with the parametrization $z = \varepsilon e^{i\varphi} + 1$ with $\varphi \in [0, \pi]$ of the circle half circle $-C_\varepsilon$ that

$$\int_{C_\varepsilon} f(z)dz = \int_{\pi}^{0} \frac{\exp(i\varepsilon(e^{i\varphi}+1))}{\varepsilon e^{i\varphi}} i\varepsilon e^{i\varphi} d\varphi = -i\int_{0}^{\pi} \exp(i\varepsilon(e^{i\varphi}+1))d\varphi.$$

Taking the limit $\varepsilon \to 0$ this converges to $-i\pi$ (we note that this integral could have also been computed using the residue theorem). Consequently, we obtain

$$P.V. \int_{-\infty}^{\infty} \frac{e^{ix}}{x-1}\, dx = \lim_{\varepsilon \to 0} \lim_{R \to 0} \left(\oint_C f(z)\, dz - \int_{C_\varepsilon} f(z)\, dz \right) = i\pi.$$

Now, taking the imaginary part, we have shown

$$P.V. \int_{-\infty}^{\infty} \frac{\sin(x)}{x-1}\, dx = \pi.$$

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