



NTNU

Norwegian University of Science and Technology

TMA4125 Matematikk 4N

Organisation & Preliminaries

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Team

Lecturer.

Lecturer: Ronny Bergmann (office hour: Wed. 16:15-17:15, online)
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Tue 12:15 – 14:00 & Wed 14:15 – 16:00 online for now

The lecture will be in english.

Teaching Assistants.

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Resources

We have

- ▶ the wiki for all information
<https://wiki.math.ntnu.no/tma4125/2022v/>
- ▶ the course description
<https://www.ntnu.edu/studies/courses/TMA4125/>
- ▶ the forum for feedback and questions
<https://mattelab2022v.math.ntnu.no/c/tma4125/>
- ▶ the blackboard group (mainly) for announcements
<https://ntnu.blackboard.com/>
- ▶ Panopto for recordings (link later in wiki)
- ▶ a JupyterHub <http://tma4125.apps.stack.it.ntnu.no>
- ▶ ovsys2 to hand in exercises <https://ovsys.math.ntnu.no/>

Reference group

I need a [reference group](#):

- ▶ at least 3 students
- ▶ diverse group (study subjects, gender, ...)

What that means:

- ▶ 3 meetings, each about 30-60 minutes, digital or in my office
- ▶ a student makes a summary of the meeting (posted on Blackboard)
- ▶ **goal:** collect reactions, advice, opinions from the class
- ▶ write a short report about the class for the Quality Assurance System of NTNU
- ▶ You will receive a certificate that your participation

Please email me (ronny.bergmann@ntnu.no) if you are willing to be in the reference group (subject "[TMA4125] Reference group")

Let's get started – with three short questions

<https://www.menti.com/ye259f1zcy>

menti.com Code 2729 9665



TMA4125 Matematikk 4N – What is it about?

In a nutshell, the lecture is about

We want to look at **analytical** and **numerical** techniques for solving ordinary differential equations (**ODEs**) as well as partial differential equations (**PDEs**).

We further introduce some numerical concepts in general.

Mathematical Modelling and Scientific Computing

In many engineering and science problems, we need to go through the following **six** steps to arrive at a solution

- 1. Mathematical Modelling** How can we describe the problem in mathematical terms?
- 2. Analysis of the model** Is the model **well-posed** in the sense that
 - a)** there is a solution? (**Existence**)
 - b)** there is only one solution? (**Uniqueness**)
 - c)** the model depends continuously on the data?
(**Continuity/Stability**)
- 3. Solve the resulting model** Two approaches are typically considered:
 - a)** **Analytical methods** compute the exact solution
 - b)** **Numerical methods** compute a solution computational means.
The obtained solution can be either **exact** or (just)
an **approximation** to the exact solution.

Mathematical Modelling and Scientific Computing II

- 4. Realization** Devise an efficient algorithmic realization of the chosen solution method.
- 5. Postprocessing** of the computed solution to make it interpretable e.g. through visualization
- 6. Verification and Validation**
 - a)** Verification: "Do I solve the problem correctly?", i.e.:
Does the realization from (3.) solve the model problem (2.)?
 - b)** Validation: "Do I solve the correct problem?", i.e.:
Does the model (2.) describe the problem (1.) correctly/sufficiently?

Our focus: Steps 3(b), 4 and 5. Especially

- ▶ well-posedness of a numerical method itself
- ▶ the complexity of the proposed method/algorithm.
- ▶ the accuracy of the proposed method (in comparison to its complexity)

TMA4125 Matematikk 4N

We consider analytical and numerical methods e. g. for algebraic equations, ordinary differential equations (ODEs), partial differential equations (PDEs) :

1. Introduction to numerical mathematics

- ▶ Interpolation of functions (N)
- ▶ Numerical integration a.k.a quadrature (N)
- ▶ Solving non-linear algebraic equations numerically (N)

2. Analytical & numerical methods for ODEs

- ▶ Laplace transform (A)
- ▶ Runge-Kutta methods (N)

3. Analytical & numerical methods for PDEs

- ▶ Fourier series and transforms (A)
- ▶ Fourier-based methods to solve the heat and wave equation analytically (A)
- ▶ Finite-difference methods to solve the heat and wave equation numerically (N)

Preliminaries

Let's recap concepts from earlier lectures and extend them slightly.

Real vector spaces

A **real vector space** is a set V together with operations $+$ (addition) and \cdot (multiplication with a scalar) that satisfy

1. $x + y \in V$ for all $x, y \in V$
2. $x + y = y + x$ for all $x, y \in V$
3. $x + (y + z) = (x + y) + z$ for all $x, y, z \in V$
4. There exists some element $0 \in V$ such that $x + 0 = x$ for all $x \in V$
5. For all $x \in V$, there exists some element $(-x) \in V$ s.t. $x + (-x) = 0$
6. $\alpha \cdot x \in V$ for all $x \in V$ and $\alpha \in \mathbb{R}$
7. $\alpha \cdot (\beta \cdot x) = (\alpha\beta) \cdot x$ for all $x \in V$ and $\alpha, \beta \in \mathbb{R}$
8. $1 \cdot x = x$ for all $x \in V$
9. $\alpha \cdot (x + y) = \alpha \cdot x + \alpha \cdot y$ for all $x, y \in V$ and $\alpha \in \mathbb{R}$
10. $(\alpha + \beta) \cdot x = \alpha \cdot x + \beta \cdot x$ for all $x \in V$ and $\alpha, \beta \in \mathbb{R}$

Complex vector spaces

A **complex vector space** is defined in exactly the same way as a real vector space, just replacing \mathbb{R} with \mathbb{C} in the definition from the last slide, so that the scalars are now allowed to be complex numbers.

Examples of vector spaces

The following examples we will see throughout the course

- ▶ The set \mathbb{R}^m of real vectors with m components
- ▶ The set $\mathbb{R}^{m \times n}$ of real-valued $m \times n$ matrices
- ▶ The set \mathbb{P}_n of polynomials of degree n or less
- ▶ The set $C^m[a, b]$ of all functions with continuous first m derivatives on the interval $[a, b]$.
we write $C[a, b]$ for $C^0[a, b]$, i.e. the set of all continuous functions.

Note that $C^n[a, b] \subset C^m[a, b]$ for $n > m$. Further, $\mathbb{P}_n \subset C^\infty[\mathbb{R}]$.

Exercise. Let's verify that \mathbb{P}_n and $C^m[a, b]$ are actually vector spaces.

Exercise: Vector spaces of Polynomials \mathbb{P}_n

What are “+” and “.” for polynomials $f, g \in \mathbb{P}_n$?

$$(f + g)(x) =$$

$$(\alpha \cdot f)(x) =$$

Exercise: Vector spaces of smooth functions $C^m[a, b]$

What are “+” and “.” for $f, g \in C[a, b]$?

$$(f + g)(x) =$$

$$(\alpha \cdot f)(x) =$$

Norms

Let V be a vector space. A **norm** $\|\cdot\|$ is a function such that the following properties hold

1. $\|x\| \geq 0$ for all $x \in V$
2. $\|x\| = 0$ if and only if $x = 0$
3. $\|\alpha \cdot x\| = |\alpha| \|x\|$ for all $x \in V$ and $\alpha \in \mathbb{R}$
4. $\|x + y\| \leq \|x\| + \|y\|$ for all $x, y \in V$ (triangle inequality)

Remarks.

- ▶ the norm $\|\cdot\|$ of $x \in V$ is essentially **a measure of the size** of x
- ▶ the norm $\|x - y\|$, $x, y \in V$, is **a measure for the distance** between x and y or put differently, how **similar** they are.
- ▶ there are usually different meaningful norms for a vector space V

Norms for \mathbb{R}^n

On \mathbb{R}^n , $n \in \mathbb{N}$ we denote elements by $\mathbf{x} = (x_1, \dots, x_n)^T \in \mathbb{R}^n$.

Then we have the following norms

► The **maximum norm** $\|\mathbf{x}\|_\infty = \max_{i=1,2,\dots,n} |x_i|$

► The **Euclidean norm** $\|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^n x_i^2}$

► more generally the **ℓ^p norm** $\|\mathbf{x}\|_p = \left(\sum_{i=1}^n |x_i|^p \right)^{1/p}, \quad 1 \leq p \leq \infty$

Note. For $n = 1$ all these are equal and we just use $\|x\| = |x|$.

Norm of functions $C[a, b]$

On $C[a, b]$, $a < b$, we can similarly define for a function $f \in C[a, b]$ the following norms

- ▶ The **maximum-norm** $\|f\|_\infty = \max_{x \in [a, b]} |f(x)|$
- ▶ The **L^2 -norm** $\|f\|_2 = \sqrt{\int_a^b f(x)^2 dx}$
- ▶ more generally **the L^p -norm** $\|f\|_p = \left(\int_a^b |f(x)|^p dx \right)^{1/p}, \quad 1 \leq p \leq \infty$

For two functions $f, g \in C[a, b]$

- ▶ $\|f - g\|_\infty$ measures the **maximal** pointwise difference
- ▶ $\|f - g\|_2$ measures the **average** (quadratic) difference

Exercise. Check that $\|f\|_2$ is a norm.

Examples of norms

For the \mathbb{R}^n let's look at a small Python code example.

Let $f(x) = \sin(x)$ on $[0, 2\pi]$ be given. Then $f \in C[0, 2\pi]$.

We obtain

$$\|f\|_2 = \sqrt{\int_0^{2\pi} \sin^2(x) \, dx} = \sqrt{\pi} \approx 1.7725$$

$$\|f\|_\infty = \max_{x \in [0, 2\pi]} |\sin(x)| = 1$$

Scalar product

A **scalar product** (also called inner product) $\langle \cdot, \cdot \rangle$ on a real vector space V is a **symmetric, positive definite bilinear form** on V , that is, it is a mapping $\langle \cdot, \cdot \rangle: V \times V \rightarrow \mathbb{R}$ which is

bilinear

1. $\langle \alpha x + \beta y, z \rangle = \alpha \langle x, z \rangle + \beta \langle y, z \rangle$ for all $x, y, z \in V$ and $\alpha, \beta \in \mathbb{R}$
2. $\langle z, \alpha x + \beta y \rangle = \alpha \langle z, x \rangle + \beta \langle z, y \rangle$ for all $x, y, z \in V$ and $\alpha, \beta \in \mathbb{R}$

symmetric

3. $\langle x, y \rangle = \langle y, x \rangle$ for all $x, y \in V$

and **positive definite**

4. $\langle x, x \rangle \geq 0$ for all $x \in V$ and $\langle x, x \rangle = 0 \Leftrightarrow x = 0$.

Note. A scalar product induces a norm given by $\|x\| = \sqrt{\langle x, x \rangle}$

Examples of scalar products

We know already on \mathbb{R}^n : $\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^T \mathbf{y} = \sum_{i=1}^n x_i y_i$ is a scalar product.

For $f, g \in C[a, b]$ we obtain a scalar product by

$$\langle f, g \rangle := \int_a^b f(x)g(x) \, dx$$

Clearly this is **symmetric** and **bilinear** (Why? Verify!)

But is it positive definite? Sure. Looking at

$$\langle f, f \rangle = \int_a^b f(x)^2 \, dx$$

we see that the argument is the same as for the L^2 -norms definiteness since $\|f\|_2 = \sqrt{\langle f, f \rangle}$.

Orthogonal vectors

Let V be a vector space with scalar product $\langle \cdot, \cdot \rangle$ and $x, y \in V$. Then x and y are said to be **orthogonal** if $\langle x, y \rangle = 0$.

Example 1. We know e. g. $V = \mathbb{R}^3$: $\mathbf{x} = (1, 2, 3)^T$ and $\mathbf{y} = (3, 0, -1)^T$ are orthogonal.

Example 2. on $V = C[-1, 1]$ with inner product $\langle f, g \rangle = \int_{-1}^1 f(x)g(x) dx$.

Then the two functions $f(x) = x$ and $g(x) = x^2$ are orthogonal, i. e.
 $\langle f, g \rangle = 0$

Let's convince ourselves with a little Python.

Cauchy-Schwarz inequality

Assume we have a vector space V with inner product $\langle \cdot, \cdot \rangle$.
Then for $f, g \in V$ it holds that

$$|\langle f, g \rangle| \leq \|f\| \|g\|$$

This is the [Cauchy-Schwarz inequality](#) (CSI) and holds for any abstract inner product.

More precisely we have

$$|\langle f, g \rangle| < \|f\| \|g\|$$

unless $f = \lambda g$ for some $\lambda \in \mathbb{R}$

Gram-Schmidt orthogonalization

Let $\{\mathbf{a}_1, \dots, \mathbf{a}_n\} \in \mathbb{R}^m$ n linearly independent vectors in \mathbb{R}^m .

The **Gram-Schmidt orthogonalization** process allows to orthogonalize the set: This means, we can construct a set $\{\mathbf{q}_1, \dots, \mathbf{q}_n\}$ of orthogonal (orthonormal) vectors which have the same span as the original set.

Algorithm.

$$\mathbf{y}_1 := \mathbf{a}_1, \quad \mathbf{q}_1 := \frac{\mathbf{y}_1}{\|\mathbf{y}_1\|}$$

$$\mathbf{y}_2 := \mathbf{a}_2 - \langle \mathbf{q}_1, \mathbf{a}_2 \rangle \mathbf{q}_1, \quad \mathbf{q}_2 := \frac{\mathbf{y}_2}{\|\mathbf{y}_2\|}$$

and so on. the eneral formula for $k = 2, \dots, n$:

$$\mathbf{y}_k := \mathbf{a}_k - \sum_{i=1}^{k-1} \langle \mathbf{q}_i, \mathbf{a}_k \rangle \mathbf{q}_i, \quad \mathbf{q}_k := \frac{\mathbf{y}_k}{\|\mathbf{y}_k\|}$$

Gram-Schmidt orthogonalization

Note. The Gram-Schmidt orthogonalization **only** requires a vector space V (to do the multiplication and subtraction) and a scalar product to make sense.

\Rightarrow Given any linearly independent $f_1, f_2, \dots, f_n \in V$ we can orthogonalize them with Gram-Schmidt!

Orthogonal projection

Let V be a vector space endowed with an inner product $\langle \cdot, \cdot \rangle$. Let $V_n \subset V$ be a finite dimensional subspace. Due to Gram-Schmidt we can construct an orthonormal basis $\{e_1, \dots, e_n\}$ of V_n .

We define the **orthogonal projection**

$$\Pi_{V_n} := \Pi_n: V \rightarrow V_n$$

by requiring that for $v \in V$ its projection $\Pi_n v$ must satisfy

$$\langle \Pi_n v, w \rangle = \langle v, w \rangle \quad \text{for all } w \in V_n.$$

Rephrased we obtain, that the **projection error** $\Pi_n v - v$ must satisfy a **orthogonal property** with respect to V_n :

$$\langle \Pi_n v - v, w \rangle = 0 \quad \text{for all } w \in V_n.$$

Is it well-defined? How to compute it?

The orthogonal projection is well defined.

Since $\{e_1, \dots, e_n\}$ is an ONB of V_n , we can write $\Pi_n v$ and $w \in V$ as

$$\Pi_n v = \sum_{i=1}^n \tilde{v}_i e_i \quad \text{and} \quad w = \sum_{j=1}^n w_j e_j$$

Plugging this in (and using linearity of $\langle \cdot, \cdot \rangle$) yields for both sides

$$\langle \Pi_n v, w \rangle = \sum_{j=1}^n w_j \langle \Pi_n v, e_j \rangle = \sum_{j=1}^n w_j \sum_{i=1}^n \tilde{v}_i \langle e_i, e_j \rangle \quad \text{and} \quad \langle v, w \rangle = \sum_{j=1}^n w_j \langle v, e_j \rangle$$

For $\langle \Pi_n v, w \rangle = \langle v, w \rangle$ we need for $j = 1, \dots, n$ that

$$\sum_{i=1}^n \tilde{v}_i \langle e_i, e_j \rangle = \sum_{i=1}^n \tilde{v}_i \langle e_j, e_i \rangle = \langle v, e_j \rangle =: b_j$$

Since $\langle e_i, e_j \rangle = \delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{else,} \end{cases}$ we get $\text{Id}(\tilde{v}_1, \dots, \tilde{v}_n)^T = (b_1, \dots, b_n)^T$

Best approximation theorem

Theorem. For any $v \in V$ we have for the approximation error

$$\|\Pi_n v - v\| = \min_{w \in V_n} \|w - v\|.$$

Proof.

Taylor expansions

Given a function $f \in C^\infty[a, b]$, a point x_0 , and an increment $h = x - x_0$ such that $x_0, x_0 + h \in [a, b]$, the **Taylor series expansion** of f around x_0 is given by

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

The function f is called **analytic** in x_0 if the series converges for sufficiently small values of h , i. e. if

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

Interlude: the big \mathcal{O} -notation

Let f and g be some real valued function and $a \in \mathbb{R}$. We say that

$$f(x) = \mathcal{O}(g(x)) \quad \text{as } x \rightarrow a$$

if there exist $\delta > 0$ and $M > 0$ such that

$$|f(x)| \leq M|g(x)| \quad \text{when } 0 < |x - a| < \delta$$

That is: **locally** around a the function f can be **bounded** (up to a constant, M) by the function g .

Taylor Polynomial

In numerics we usually truncate the sum after m summands.

We obtain the **Taylor polynomial** (and a Remainder) for any $f \in C^{m+1}[a, b]$ defined as

$$f(x) = \sum_{k=0}^m \frac{f^{(k)}(x_0)}{k!} (x - x_0)^k + R_{m+1}(x_0)$$

where the remainder term is given by

$$R_{m+1}(x_0) = \frac{f^{m+1}(\xi)}{(m+1)!} (x - x_0)^{m+1},$$

for some unknown ξ between x_0 and x .

We often write this using the big \mathcal{O} -notation

$$f(x_0 + h) = \sum_{k=0}^m \frac{f^{(k)}(x_0)}{k!} h^k + \mathcal{O}(h^{m+1})$$

Some other useful results

Theorem 1. Let $f \in C[a, b]$ and let u be a number between $f(a)$ and $f(b)$. Then there exists at least one $\xi \in (a, b)$ such that $f(\xi) = u$

Theorem 2. (Rolle's theorem) Let $f \in C^1[a, b]$ and $f(a) = f(b) = 0$. Then there exists at least one $\xi \in (a, b)$ such that $f'(\xi) = 0$.

Theorem 3. Let $f \in C^1[a, b]$. Then there exists at least one $\xi \in (a, b)$ such that

$$f'(\xi) = \frac{f(b) - f(a)}{b - a}.$$