Function spaces and functional frameworks

and their usefulness in applied mathematics and engineering

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Preface

This course is designed for students and doctoral researchers mainly from engineering. Applied mathematicians are welcome though.

The **goal** is to provide an overview about **function spaces**, and more generally speaking **functional frameworks** that include metric spacs, normed spaces, inner product spaces, and convex sets for variational inequalities. Throughout, the implication to algorithms and practical applications is made and sometimes illustrated with numerical simulations from my own work.

This course is organized into three parts:

A) **What I do:** 60 minutes presentation, exercises

→ **What you learn:** organizing a given engineering problem statement into a mathematical framework, guiding questions to be asked, implications to algorithms and numerical simulations

B) **What I do:** 90 minutes presentation, exercises

→ **What you learn:** metric spaces, normed spaces, inner product spaces (Hilbert spaces), completeness, convergence, Cauchy sequence, L^2, H^1, space-time spaces (Bochner spaces), outlook to further abstract spaces (e.g., nonlinear PDEs) such as Sobolev spaces

C) **What I do:** 60 minutes presentation, exercises

→ **What you learn:** convex sets for variational inequalities, relaxation via penalization, obstacle problem, a long exercise from mathematical modeling, over discretization to the numerical solution

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Overview

Motivation I

1. We are given some problem from engineering, physics, chemistry, biology, economy, and so forth

→ **Problem statement**

2. Often such a problem statement results into a **differential equation**[1]

Definition

A differential equation is a mathematical equation that relates a function with its derivatives such that the solution satisfies both the function and the derivatives.

[1] e.g., Wick; Numerical Methods for Partial Differential Equations, Leibniz University Hannover, 2022, https://doi.org/10.15488/11709

Motivation II

1. Often, three equivalent formulations:

   strong, weak, energy

2. Strong form: differential equation
3. Weak form: principle of virtual work
4. Energy form: related to physical energy (exists only for symmetric problems)
5. **Example (Poisson):**

$$\text{Find } u : \Omega \to \mathbb{R} : \quad -\Delta u = f \quad \text{in } \Omega \quad u = 0 \quad \text{on } \partial\Omega$$

$$\text{Find } u \in X : \quad \int_\Omega \nabla u \cdot \nabla \varphi \, dx = \int_\Omega f \varphi \, dx \quad \forall \varphi \in X$$

$$\text{Find } u \in X : \quad \min_{u \in X} \left(\frac{1}{2} \int_\Omega |\nabla u|^2 \, dx - \int_\Omega f u \, dx \right)$$

6. **Exercise:** what is Ω? What is X? What is φ? How is f called? How is $u = 0$ on $\partial\Omega$ called? How are the three problems formally related?

Motivation III

1. We want to **organize** and **structure** the problem statement

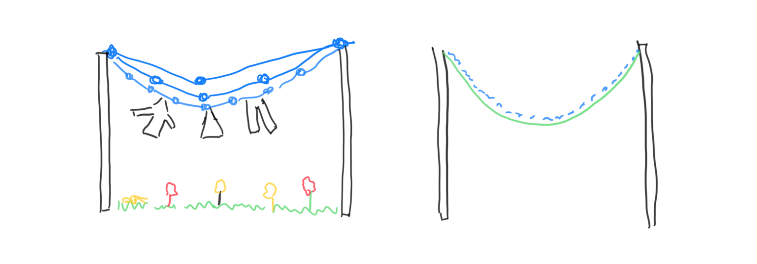
→ **Better understanding** how it 'works' and how it is driven by right hand side data, boundary conditions, initial conditions, geometry, and so forth

2. **Final goal:** We want to have accurate, efficient (fast), and robust numerical simulations that we can trust

Example of differential equation: Poisson's problem

Find $u : \Omega \to \mathbb{R}$ such that

$$\begin{aligned} -\Delta u &= f \quad \text{in } \Omega \\ u &= g \quad \text{on } \partial\Omega \end{aligned}$$



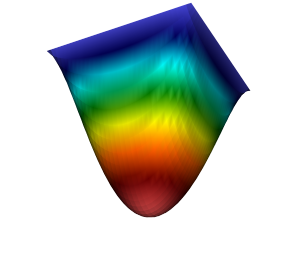


Figure: Poisson problem in 1D (left and middle). Poisson problem in 2D (right).

Questions we can ask

1. What does this (Poisson's problem) differential equation describe?
2. Is it useful for 'some' application?
3. Can we solve the differential equation analytically?
4. Does there exist a solution?
5. Is such a solution unique?
6. How does the solution change, if we change boundary conditions or initial data?
7. If not analytically, can we make use of the computer?
8. **Computer:** design an algorithm, implement that algorithm into some software, run the software, analyze the outcome (numerical result)
9. Is there only one such algorithm? Or more? Do they differ in their **accuracy, efficiency, robustness**?

These questions lead to ...

→ **Seven concepts of numerics:**[2] [3] approximation, convergence, convergence order, errors, error estimation, efficiency, stability (robustness)

→ **Scientific computing**: Mathematical modeling (of problem statments), design and analysis of algorithms (in functional frameworks), implementation into software (including debugging), analysis and interpretation of the results, feedback loop to applications and/or improvements of math. modeling and/or improvements of algorithms and/or improvements of software/code

[2] Richter, Wick; Springer, 2017 (german), first and original version of these seven concepts
[3] Wick; NumPDE lecture notes, 2022; `https://doi.org/10.15488/11709`, Chapter 2 (english)

What do these questions have to do with function spaces?

1. Well, how can we mathematically investigate questions of well-posedness, efficiency (convergence) of algorithms, approximation (discretization) errors?
2. We need **mathematical structures**
3. For instance, for approximation errors, we need to measure **distances**

→ Distances between two numerical solutions (do they come closer; convergence)? Distances between manufactured and numerical solutions

4. **Concept:** Metric
5. **Concept:** Norm
6. **Example:** Usual metric we all know is the Euclidian metric
7. But with respect to what? In which **space**?
8. Well, in our well-known 3d (three-dimensional) space in which we all live
9. Aha: this is our first function space: $\mathbb{R}^3$

Functional frameworks[4]

1. Function spaces with norms are vector spaces
2. In the presence of inequality constraints, we rather deal with convex sets

→ **Functional frameworks** help in better understanding engineering problem statements

→ **Functional frameworks** help in the choice of discretizations and numerical (linear and nonlinear) solution algorithms

[4] The original title was 'function spaces'. However, since also metric spaces, measure spaces, convex sets, and so forth exist, 'functional framework' is a more general wording that I prefer to use.

Consequences in scientific computing and engineering

1. Studying convergence rates (speed of algorithms)

→ Different norms (different spaces) may yield difference convergence rates

2. **Example:** 2D Poisson: Bilinear FEM with Q_c^1 elements. Evaluate the L^2 and H^1 norms using bilinear FEM. The results are (which norm is 'better'?):

Level	Elements	DoFs (N)	h	L2 err	H1 err
2	16	25	1.11072	0.0955104	0.510388
3	64	81	0.55536	0.0238811	0.252645
4	256	289	0.27768	0.00597095	0.126015
5	1024	1089	0.13884	0.00149279	0.0629697
6	4096	4225	0.06942	0.0003732	0.0314801
7	16384	16641	0.03471	9.33001e-05	0.0157395
8	65536	66049	0.017355	2.3325e-05	0.00786965
9	262144	263169	0.00867751	5.83126e-06	0.00393482
10	1048576	1050625	0.00433875	1.45782e-06	0.00196741
11	4194304	4198401	0.00216938	3.64448e-07	0.000983703

3. Analyzing algorithms in terms of accuracy, efficiency, robustness

4. Do we converge with our numerical scheme to the correct limit?

Algorithm

Definition (Algorithm)

An algorithm is an instruction for a **schematic solution** of a mathematical problem statement. The main purpose of an algorithm is to formulate a scheme that can be implemented into a **computer** to carry out so-called **numerical simulations**.

1. Direct schemes solve the given problem up to round-off errors (for instance Gaussian elimination).
2. Iterative schemes approximate the solution up to a certain accuracy (for instance Richardson iteration for solving linear equation systems, or fixed-point iterations).
3. Algorithms differ in terms of **accuracy, robustness**, and **efficiency**.
4. Algorithms can be (sometimes/often?) rigorously **analyzed within a functional framework**

- In many numerical examples and applications it is a trade-off of a 'rough' approximation (some kind of 'guess' about the solution) which might be relatively cheap in the computational cost, and on the other hand, high-accuracy or robust (with respect to all parameters) numerical simulations.

→ One challenge (at least to me in scientific computing) is to address all three aspects of accuracy, efficiency, robustness simultaneously.

L'art de bien faire des erreurs[5]

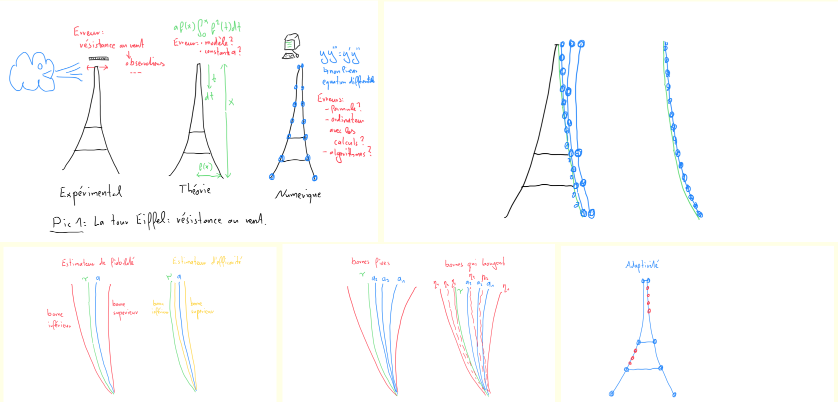


Figure: From modeling over a 'mesh' (discretization) to finer discretizations (all top row), up to graphical error bounds until adaptivity (bottom row). Modeling, discretization, error analysis require to choose **function spaces**.

[5]Fau, Wick; Revue du Palais de la découverte, Vol. 436, pp. 50-55, 2022

Important to notice I

1. These concepts are defined with respect to **spaces**
2. Why can we not work always with the **same space**?

→ Answer: we want to represent the 'physics' of a given problem statement, and this requires, specifically-tailored spaces, numerical methods, preconditioners, and numerical solution algorithms

3. Is there some **optimal norm or optimal space**?

→ Answer: often yes, but not always (fortunately, unfortunately)

4. Unfortunately: it often requires new analyses of problem statements in (new) function spaces
5. Fortunately: there is always something to do for us

Important to notice II

1. Why does it often work out successfully not to analyze specifically in applications again function spaces and algorithms?
2. Well, somebody (most likely from mathematics) already did it somewhere else

$\rightarrow$ **literature research/knowledge is so crucial!**

3. Very, very often not exactly 'our' problem has been analyzed, but similar related problems (in their correct function space framework)

$\rightarrow$ intuitively we can hope that known algorithms work

4. Mathematical functional frameworks help to analyze new algorithms

Exercises

1. Give examples where you have been in touch with function spaces so far
2. If not, how did you treat so far PDE problem statements? Explain the procedure how you come from a given PDE to a numerical simulation results (which steps need to be done in your case?)
3. Give an example of an algorithm that you recently implemented (how did it perform? Were you fully satisfied with the performance? Why yes, why not?)

End Part I

Introduction

1. There is a zoo of function spaces
2. They need to be chosen according to the characterization of the problem statement (see some slides before: ‘physics’ of the problem)

→ linear, nonlinear, stationary, nonstationary, coupled, systems, inequality constraints, continuous level, discretization after time and/or space

Infinite-dimensional spaces versus finite-dimensional spaces

1. Main purpose of **functional analysis**: studying problems in infinite-dimensional spaces
2. Surprising things may happen: norms are not equivalent, compactness results (existence of solutions) become technical, weak convergence
3. **Why should we care?**
4. Discretizations (such as finite differences or finite elements) yield finite-dimensional problems

$\rightarrow$ What is the correspondance between our original problem statement and the discretized one? Do we really converge to the correct solution?

Three spatial meshes, three time step sizes

1. **Computational convergence analysis:** compute discretized solution on at least three different spatial meshes

→ Having finer meshes, does the error between two subsequent solutions become smaller? Do the curves come closer together?

2. **Computational convergence analysis:** compute discretized solution on at least three different temporal meshes / time step sizes

→ Having finer meshes, does the error between two subsequent solutions become smaller? Do the curves come closer together?

3. At least for linear problems, do we even detect some order of convergence?

Three time step sizes for three schemes for ODE model problem

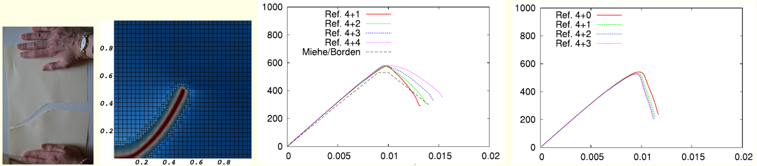
1. ODE model problem $y' = ay$ and $y(t_0) = y_0$ taken from Amstutz/Wick[6]
2. Goal: (absolute) end time error of an ODE problem on three mesh levels (different time step sizes k)
3. In addition: three schemes (FE - forward Euler, BE - backward Euler, CN - Crank-Nicolson):
4. Computational findings:

```
Scheme          #steps  k      Error at t_N
===========================================
FE err.:        8       0.36   0.13786
BE err.:        8       0.36   0.16188
CN err.:        8       0.36   0.0023295
FE err.:        16      0.18   0.071567
BE err.:        16      0.18   0.077538
CN err.:        16      0.18   0.00058168
FE err.:        32      0.09   0.036483
BE err.:        32      0.09   0.037974
CN err.:        32      0.09   0.00014538
===========================================
```

5. Interpretation: We monitor that doubling the number of intervals (i.e., halving the step size k) reduces the error in the forward and backward Euler scheme by a factor of 2. This is (almost) linear convergence, with $\alpha = 0.91804$.
   The CN scheme is much more accurate (for instance using $n = 8$ the error is 0.2% rather than $13 - 16\%$) and we observe that the error is reduced by a factor of 4. Thus quadratic convergence is detected. Here the 'exact' order on these three mesh levels is $\alpha = 1.9967$.

[6] Amstutz, Wick; Refresher course in maths and a project on numerical modeling done in twos, Hannover : Institutionelles Repositorium der Leibniz Universität Hannover, 2022, https://doi.org/10.15488/11629

Example and counter example[7]



1. 3rd figure: no (qualitative) convergence, since curves have same distance
2. 4th (last) figure: convergence: on finer meshes, curves become closer
3. **What is the problem in the 3rd figure?**
4. Answer not fully clear: on the left we vary both a regularization parameter ε and the spatial mesh size h
5. Possibility 1: The limit $\varepsilon \to 0$ **does not lie** anymore in the usual **Hilbert space $H^1(\Omega)$**
6. Possibility 2: The goal functional that we measure is $\int_\Gamma \sigma \cdot n \, ds$ over the top boundary Γ. We **have not checked**, whether this quantity is **well-defined in the underlying function space**

[7] Heister, Wheeler, Wick; CMAME, Vol. 290, pp. 466-495, 2015; Fig. 9 and Fig. 8

Convergence in different function spaces

1. What is better: L^2 error $\|u - u_h\|_{L^2}$ with $O(h^2)$ or H^1 error $\|u - u_h\|_{H^1}$ with $O(h)$?

Convergence in different function spaces

1. What is better: L^2 error $\|u - u_h\|_{L^2}$ with $O(h^2)$ or H^1 error $\|u - u_h\|_{H^1}$ with $O(h)$?
2. Answer: **it depends!**
3. Convergence in L^2 is faster, but we only 'know' something about the function values themselves
4. Convergence in H^1 is slower, but we know function values and function gradients (so we have more information about the numerical solutions)

Metric spaces[11]

1. A **metric space**[8] is a set X with a metric on it
2. A generalization of metric spaces are topological spaces[9] [10]
3. Metric associates with any pair of elements of X a **distance**
4. **Example:** $\mathbb{R}$ with a distance function

$$d = d(x, y) = |x - y|, \quad x, y \in \mathbb{R} \tag{1}$$

5. Functional analysis: more general spaces and functions
6. Replace set X (here real numbers $\mathbb{R}$) with some abstract set X
7. **In exactly the same fashion, we can define a distance on the abstract set X**

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[8] Metric spaces were first considered by Fréchet in 1906

[9] Topological spaces were first introduced by Hausdorff in 1914

[10] Dirk Werner; Funktionalanalysis, 8. Auflage, Springer, 2018; Anhang B

[11] Erwin Kreyszig; Introductory functional analysis with applications, Wiley, 1978

Metric spaces[12]

Definition (Metric space, metric)

A metric space is a pair (X, d), where X is a set and d is a metric on X, i.e., d is a distance function on X, that is, a function on $X \times X$ such that for all $x, y, z \in X$, it holds:

1. d is real-valued, finite, non-negative
2. $d(x, y) = 0$ if and only if $x = y$
3. $d(x, y) = d(y, x)$, symmetry
4. $d(x, y) \leq d(x, z) + d(z, y)$, triangle inequality

Exercise:

1. Take $X := \mathbb{R}$
2. Take for example $1, 4, 7 \in X$
3. Double-check the above four conditions for the metric $d(a, b) := |a - b|$.

[12] Erwin Kreyszig; Introductory functional analysis with applications, Wiley, 1978

Solution to the exericse

Euclidian space $\mathbb{R}^3$

1. The daily space we live in
2. $X := \mathbb{R}^3$
3. Ordered triples $x, y \in X$ with

$$x = (x_1, x_2, x_3)^T, \quad y = (y_1, y_2, y_3)^T \tag{2}$$

4. Euclidian metric defined by

$$d(x,y) = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2 + (x_3 - y_3)^2} \tag{3}$$

Function space $C[a, b]$

1. C = set of continuous functions $u_1, u_2, \ldots$
2. Independent variable t
3. We have $u_1(t), \ldots$; thus u_1 is the dependent variable
4. Set $X := C[a, b]$ where $t \in [a, b]$ and $u_1, u_2, \ldots \in X$
5. Metric defined by

$$d(u_1, u_2) = \max_{[a,b]} |u_1(t) - u_2(t)| \tag{4}$$

6. $C[a, b]$ is a **function space** because every 'point' of $C[a, b]$ is a function

Function space: definition and properties

Definition

A set X that contains functions as its **elements** $u_i \in X$ for $i = 1, 2, 3, \ldots$ is a **function space**. In analogy to $\mathbb{R}$ (previous example), functions are considered as 'points' in that space. To those points, a metric d can be associated to measure distances. In discretizations, these distances represent for example so called **discretization errors**. Further properties such as norms, possibly inner products, are introduced later and apply in the same fashion to X and u_i.
It is a **general concept** to view functions, measures, and so forth in any abstract space (we get to know many more later) as such elements with such properties.

Convergence

Definition

A sequence $(x_n)_{n\in\mathbb{N}}$ in a metric space X with distance function d is said to converge if there is a limit $x \in X$ such that

$$\lim_{n\to\infty} d(x_n, x) = 0 \tag{5}$$

or in another notation

$$\lim_{n\to\infty} x_n = x \tag{6}$$

If $(x_n)_{n\in\mathbb{N}}$ does not converge, then the sequence is said to diverge

Why should we care in engineering and scientific computing?

1. The elements $x_1, x_2, \ldots$ are in our case often FEM numerical solutions
2. Compare our previous example with three meshes and three time step sizes
3. Principle and key interest whether taking more and more numerical solutions whether we really converge to something (i.e., the limit) useful (not clear at all! See counter example from before)

Cauchy sequence and completeness

Definition

A sequence $(x_n)_{n\in\mathbb{N}}$ in a metric space X with distance function d is said to be a **Cauchy sequence** if for every $\varepsilon > 0$ there exists an N such that

$$d(x_m, x_n) < \varepsilon \quad \forall m, n > N \tag{7}$$

The space X is said to be **complete** if every Cauchy sequence in X converges.

1. Each convergent sequence $(x_n)_{n\in\mathbb{N}}$ is a Cauchy sequence. Due to convergence the above criterion is naturally fulfilled.
2. **However,** not each Cauchy sequence does converge!
3. We are now at a fundamental ground of the choice of the **correct function space**

Example I

1. The rational line $\mathbb{Q}$ is incomplete.
2. Between each two $x, y \in \mathbb{Q}$, we will find an irrational number $z \in \mathbb{R}$.
3. Thus, we can construct sequences $(x_n)_{n\in\mathbb{N}} \subset \mathbb{Q}$ that converge to a limit $x \in \mathbb{R}$
4. **Why should we care?**
5. Again: assume $(x_n)_{n\in\mathbb{N}}$ is a sequence of numerical solutions in a certain function space, say FEM in H^1. When the limit $x \neq H^1$ what can we say about our numerics?

→ Drastically speaking, in this case, our numerics is useless and **not robust**

6. **In practice:** Why very often we do not 'see' these phenomena?
7. Two reasons:
    1. Our functional framework is correct and everything behaves well
    2. We are too far away from the (asymptotic) limits. Sometimes FEM meshes are too coarse to 'see' problems in the convergence

→ The last point is sometimes the reason what we observe in high performance computing, when we can we have much finer meshes, and now - suddenly - convergence problems arise

Example II: a Cauchy sequence that does not converge

1. Take $X := (0, 1]$; left-half open interval
2. Usual metric $d(x, y) := |x - y|$
3. Define sequence $(x_n), n = 1, 2, 3, \ldots$ with

$$x_n = \frac{1}{n} \tag{8}$$

4. This is clearly a Cauchy sequence: $d(x_m, x_n) < \varepsilon$ for $m, n > N$ is fulfilled!
5. But **it does not converge!** The limit $x = 0$ (since $x_n \to 0$ for $n \to \infty$) is not an element of X (because we excluded 0)
6. This shows **convergence is not an intrinsic property of the sequence, but requires also the correct design of the function space X such that the limit x is included.**
7. In FA (functional analysis)[13] these concepts are further generalized in abstract spaces

[13] Kreyszig (1978), Werner (2018), Ciarlet (2013), and many more

Example III

1. $X := \mathbb{R}$ is complete (each Cauchy sequence converges)
2. $X := \mathbb{Q}$ is not complete
3. $X := C[a,b]$ is complete w.r.t. to the maximum norm we had earlier
4. $X := C[a,b]$ with the metric

$$d(u,v) := \int_a^b |u(t) - v(t)|\, dt \tag{9}$$

is **not complete**

5. Proof: See Kreyszig (1978) on page 38
6. **Why should we care?**
7. Well, in FEM we work with weak forms (principle of virtual work) and consequently, we work with integrals.

→ The space $C[a,b]$ is not appropriate for FEM

8. This is the reason, why L^2 spaces must be introduced (later more)

Normed spaces

1. So far no linear algebra structure; arbitrary metric spaces
2. Now let X be a **vector space**
3. Define a metric by means of a **norm**
4. **A norm generalizes the length of a vector in abstract spaces**
5. Complete normed spaces are known as **Banach spaces**

Vector spaces[14]

Definition

A **vector space**, also known as **linear space**, over a field K (often $K = \mathbb{R}$) is a nonempty set X of elements $x, y, \dots$ (called vectors) together with two algebraic operations:

1. Vector addition: for $x, y \in X$, we have $x + y \in X$
2. Multiplication by scalars: for $x \in X$ and $a \in K$, we have $ax \in X$

Moreover, we then have commutative, associative, and distributive laws.

[14] e.g., Gerd Fischer; Lineare Algebra, Springer, 2014

Examples

1. $X := \mathbb{R}^n$, then

$$x + y \in X \tag{10}$$
$$ax \in X \tag{11}$$

for $x, y \in X$ and $a \in \mathbb{R}$ (little exercise write down detailed version of vectors yourself)

2. $X := C[a,b]$, then for $u, v \in X$ and $t \in [a,b]$

$$(u+v)(t) = u(t) + v(t) \tag{12}$$
$$(au)(t) = au(t) \tag{13}$$

Dimension of a vector space

Definition

A vector space X is said to be finite dimensional if there exists a positive integer n such that X contains a linearly independent set of n vectors, while $n+1$ (or more) vectors are linearly dependent. The integer n is called the dimension of X, written $n = dim(X)$. Such a n-tuple of X is called a basis, which spans X and each element of X can be obtained by a linear combination of the n basis vectors. If X is not finite dimensional, then X is infinite dimensional.

Examples:

1. $dim(\mathbb{R})$ has the dimension 1
2. $dim(\mathbb{R}^n)$ has the dimension n
3. $dim(C[a,b])$ is infinite dimensional, because we have infinite many $t \in [a,b]$ to insert into $u(t)$ in order to span $C[a,b]$
4. The main purpose of FA (functional analysis) is to investigate infinite-dimensional spaces

Dimension of a vector space

Why should we care? (About infinite-dimensional vector spaces)

1. Answer 1: Nearly all engineering problem statements take place in infinite-dimensional spaces, $C[a,b], L^2, H^1, \ldots$
2. Answer 2: Norms are not anymore equivalent (we cannot switch simply from one norm to another)
3. Answer 3: Convergence is not anymore obvious
4. Answer 4: Numerical simulations must be analyzed with care (as before: is limit $x \in X$? Etc.)

Example

1. Take $X := \mathbb{R}^3$
2. Dimension: $dim(X) = 3$
3. Basis: canonical basis: $e_1 = (1,0,0)^T, e_2 = (0,1,0)^T, e_3 = (0,0,1)^T$
4. Each vector from $x \in X$ can be represented as a linear combination of e_1, e_2, e_3:

$$x = a_1 e_1 + a_2 e_2 + a_3 e_3, \tag{14}$$

for the scalars $a_1, a_2, a_3 \in K = \mathbb{R}$

Normed spaces

Definition

A normed (vector) space X is a vector space with a norm. A Banach space is a complete (each Cauchy sequence converges) normed space. A norm is a real-valued function on X with the notation $\|x\|$ for $x \in X$ and the properties:

1. $\|x\| \geq 0$
2. $\|x\| = 0$ if and only if $x = 0$
3. $\|ax\| = |a|\|x\|$ for $x \in X$ and $a \in K$ (K being the field as before)
4. $\|x + y\| \leq \|x\| + \|y\|$

A norm defines a metric d on X via

$$d(x, y) := \|x - y\| \tag{15}$$

Clearly, we see that a norm measures the distance in X.

Normed spaces

Examples:

1. The norm on $X := \mathbb{R}^n$ is defined by $\|x - y\| := \sqrt{|x_1 - y_1|^2 + \ldots + |x_n - y_n|^2}$
2. The norm on $X := C[a, b]$ is defined by $\|u\| := \max_{t \in [a,b]} |u(t)|$

Completion of $C[a,b]$ resulting into $L^2[a,b]$

1. Recall from before $C[a,b]$ with $\|u\| := \sqrt{\int_a^b u(t)^2\,dt}$ is not complete. Limit may not be in $C[a,b]$
2. Choice of norm is important!
3. But of course: norm must fit to the problem statement: weak forms of PDEs require integrals. Maximum norm is not good!
4. PDEs in strong form discretized with FD (finite differences) can be treated however with $\|u\| := \max_{t\in[a,b]} |u(t)|$

$\rightarrow$ Given the **same problem statement**, different numerical methods, may require different functional frameworks, i.e., different function spaces and/or different norms

5. Back to the problem, take $[a,b] = [0,1]$ w.l.o.g

$$\|u_n - u_m\| = \int_0^1 [u_n(t) - u_m(t)]^2\,dt = \frac{(n-m)^2}{3mn^2} < \frac{1}{3m} - \frac{1}{3n} \tag{16}$$

6. This Cauchy sequence does not converge! Limit u does result into a discontinuous function (Kreyszig, p. 38), and thus $u \neq C[0,1]$.

Inner product spaces; Hilbert spaces

1. So far no orthogonality, two vectors are perpendicular

→ $x, y \in X$ result into $x \cdot y = 0$

2. Euclidian spaces have an inner product, Pythagoras
3. Complete spaces (Banach spaces) with inner product are called **Hilbert spaces** [15]

[15] Hilbert spaces were initiated by David Hilbert in 1912

Hilbert space

Definition

An inner product space (pre-Hilbert space) is a vector space X with an inner product defined on X. A **Hilbert space** is a complete inner product space. The metric is defined by the inner product. The inner product is a mapping of $X \times X$ into the scalar field K, often denoted by $\langle x, y \rangle$ or (x, y). It holds

1. $(x + y, z) = (x, z) + (y, z)$
2. $(ax, y) = a(x, y)$
3. $(x, y) = \overline{(y, x)}$
4. $(x, x) \geq 0$ and $(x, x) = 0$ if and only if $x = 0$

Hilbert space (cont'd)

Definition (cont'd)

The norm is defined by

$$\|x\| := \sqrt{(x,x)} \tag{17}$$

and the resulting metric is given by

$$d(x,y) := \|x-y\| = \sqrt{(x-y,x-y)} \tag{18}$$

Thus: inner product spaces are normed spaces. Hilbert spaces are Banach spaces.

Examples

1. The Euclidian space $\mathbb{R}^n$ is a Hilbert space with inner product
$$(x, y) = \sum_{i=1}^{n} x_i y_i \tag{19}$$
2. In $\mathbb{R}^3$ let e_1, e_2, e_3 be the canonical basis. The inner product of two of them is for instance
$$(e_1, e_2) = 1 \cdot 0 + 0 \cdot 1 + 0 \cdot 0 = 0.$$
Thus, e_1 and e_2 are orthogonal (was clear; school knowledge!)
3. In $\mathbb{R}^3$ let, $a = (4, 1, 0)^T$ and $b = (1, 56, 3)^T$, then
$$(a, b) = 4 \cdot 1 + 1 \cdot 56 + 0 \cdot 3 = 60.$$
4. The space $L^2[a, b]$ is a Hilbert space with inner product
$$(u, v) = \int_a^b u(t)v(t)\, dt \tag{20}$$

Lebesgue space L^2

Definition (L^2 space in $\mathbb{R}^n$)

Let $\Omega \subset \mathbb{R}^n$ be a Lebesgue-measurable open domain. The space $L^2 = L^2(\Omega)$ contains all square-integrable functions in Ω:

$$L^2 = \{v \text{ is Lebesgue measurable} \mid \int_\Omega v^2 \, dx < \infty\}.$$

The space L^2 is complete (each Cauchy sequence converges in the norm defined below) and thus a Banach-space. For a proof see for instance Kreyszig 1989 [Section 2.2-7] or Werner 2018 [Kapitel I]. Moreover, we can define an inner product:

$$(u, v) = \int_\Omega vu \, dx$$

such that L^2 is even a Hilbert space with norm

$$\|u\|_{L^2} = \sqrt{(u, u)}.$$

Convergence of CG (conjugate gradients)[16]

1. Background: solve linear equation system $Ax = b$
2. Let $A \in \mathbb{R}^{n\times n}$ symmetric, positive, definite
3. Then, we can define a weighted inner product (Ax, x) with induced norm (energy norm)

$$\|x\|_A := \sqrt{(Ax, x)} \tag{21}$$

4. Convergence results are shown in this norm:

$$\|x_n - x\|_A \le 2\left(\frac{1 - 1/\sqrt{\kappa}}{1 + 1/\sqrt{\kappa}}\right)^n \|x_0 - x\|_A, \quad n = 1, 2, 3, \ldots \tag{22}$$

where $\kappa := cond_2(A)$ is the spectral condition of A

[16] e.g., Saad; Iterative methods for sparse linear systems, SIAM, 2003

Linear stationary PDEs

1. Let Ω be a domain (with certain assumptions)
2. Our problem statement takes geometrically place in that domain; e.g., car simulation, aircraft, ship, screw, ...
3. Hilbert space $L^2(\Omega)$ (we had before)
4. Hilbert space $H^1(\Omega)$
5. Hilbert space $H_0^1(\Omega)$
6. Roughly (but each new equation, requires new thinking), **second-order PDEs** (in strong form) result (by integration by parts) into **weak first-order derivatives** on trial and test functions, for which we need H^1 spaces:

$$-\Delta u \quad \to \quad \int_\Omega \nabla u \cdot \nabla \varphi \, dx$$

7. For non-symmetric problems, e.g., $b \cdot \nabla u$, it depends whether integration by parts is applied or not (e.g., pressure term in Navier-Stokes or transport equations)

Hilbert spaces H^1

Definition (The space H^1)

Let $\Omega \subset \mathbb{R}^n$ be an open, measurable, domain. The space $H^1 := H^1(\Omega)$ is defined by

$$H^1 := \{v \in L^2(\Omega) |\, \partial_{x_i} v \in L^2, \quad i = 1, \ldots, n\}$$

In compact form:

$$H^1 := \{v \in L^2(\Omega) |\, \nabla v \in L^2\}.$$

Remark

In physics and mechanics, the space H^1 is also called the ***energy space*** *. The associated norm is called* ***energy norm****.*

Hilbert spaces H^1

Proposition (H^1 is a Hilbert space)

We define the inner product

$$(u, v)_{H^1} := \int_\Omega (uv + \nabla u \cdot \nabla v)\, dx$$

which induces the norm:

$$\|u\|_{H^1} = \sqrt{(u, u)_{H^1}}.$$

The space H^1 equipped with the norm $\|u\|_{H^1}$ is a Hilbert space.

- In the above definition $(u, v)_{H^1}$, constants such as material parameters are hidden, but do exist, since otherwise the physical units of u and ∇u would not match in the definition of the inner product

Hilbert spaces H^1

Proof.

It is tivial to see that $(u, v)_{H^1}$ defines a inner product. It remains to show that H^1 is complete. Let $(u_n)_{n\in N}$ be a Cauchy sequence in H^1. We need to show that this Cauchy sequence converges in H^1. Specifically $(u_n)_{n\in N}$ and $(\partial_{x_i} u_n)_{n\in N}$ are Cauchy sequences in L^2. Since L^2 is complete, see Definition 12, there exist two limits u and w_i with

$$u_n \to u \quad \text{in } L^2 \quad \text{for } n \to \infty$$

$$\partial_{x_i} u_n \to w_i \quad \text{in } L^2 \quad \text{for } n \to \infty.$$

We employ now the weak derivative:

$$\int_\Omega u_n(x)\partial_{x_i}\varphi(x)\,dx = -\int_\Omega \partial_{x_i} u_n(x)\varphi(x)\,dx \quad \varphi \in C_c^\infty$$

Passing to the limit $n \to \infty$ yields

$$\int_\Omega u(x)\partial_{x_i}\varphi(x)\,dx = -\int_\Omega w_i(x)\varphi(x)\,dx.$$

Hilbert spaces H_0^1

Definition (H_0^1)

The space $H_0^1(\Omega)$ contains vanishing function values on the boundary $\partial\Omega$. The space $H_0^1(\Omega)$ is the closure of $C_c^\infty(\Omega)$ in H^1.

One often writes:

Definition (H_0^1)

The space H_0^1 (spoken: 'H,1,0' and **not** 'H,0,1') is defined by:

$$H_0^1(\Omega) = \{v \in H^1 \,|\, v = 0 \text{ on } \partial\Omega\}.$$

Embedding theorems[17]

1. Lebesgue and Sobolev spaces generalize solution concepts
2. But sometimes basic needs cannot be guarenteed, e.g., evaluation of point values
3. Embedding theorems tell us which function spaces can be embedded, i.e., $Y \subset X$
4. Depends on the dimension of the problem statement
5. Curious things happen (only on the first view; on the second view, one can learn that these facts can be rigorously mathematically established)

Proposition (Singularities of H^1 functions)

Let $\Omega \subset \mathbb{R}^n$ be open and measurable. It holds:

- *For $n = 1$, $H^1(\Omega) \subset C(\Omega)$.*
- *For $n \geq 2$, functions in $H^1(\Omega)$ are in general neither continuous nor bounded.*

[17] e.g., Evans; Partial differential equations, AMS, 2010

Well-posedness of Poisson's problem

Proposition

Let Ω be a bounded domain of class C^1 and let $f \in L^2$. Let $V := H_0^1$. Then, the Poisson problem has a unique solution $u \in V$ and it exists a constant c_p (independant of f) such that the stability estimate

$$\|u\|_{H^1} \leq c_p \|f\|_{L^2}$$

holds true.

Proof.

Apply Lax-Milgram lemma. E.g., my NumPDE lecture notes. □

A priori error FEM estimates of Poisson

Theorem

Let $\mathcal{T}_h$ be a quasi-uniform decomposition of Ω. Then it holds for $u_h \in V_h^{(k)}, k = 1, 2, 3$ and triangular or quadrilaterals elements:

$$\|u - u_h\|_{H^1} \leq ch\|u\|_{H^2} \leq ch\|f\|_{L^2} = O(h).$$

Using a duality argument (Aubin-Nitsche[18]), we obtain:

Theorem

Let the previous assumptions hold true, then:

$$\|u - u_h\|_{L^2} \leq ch^2\|f\|_{L^2} = O(h^2).$$

[18] e.g., Braess; Finite Elemente, 4. Auflage, Springer, 2007

A priori error FD estimates of Poisson

Proposition

The five-point stencil approximation of the Poisson problem in two dimensions satisfies the following a priori error estimate:

$$\max_{ij} |u(x_{ij}) - u_{ij}| \leq \frac{1}{96} h^2 \max_{\Omega}(|\partial_x^4 u| + |\partial_y^4 u|).$$

Main differences between FEM and FD

1. Different norms
2. Different spaces (FEM H^1 and FD $C^4(\Omega)$)
3. FD requires more derivatives (up to 4 than FEM up to 2)

Linear nonstationary PDE modeling

1. Bochner spaces: time-dependent function spaces
2. **Space-time formulations**
3. Let $I := (0, T)$ with $0 < T < \infty$ a bounded time interval with end time value T.
4. For any Banach space X and $1 \le p \le \infty$, the space

$$L^p(I, X) \tag{23}$$

   denotes the space of L^p integrable functions f from the time interval I into X.
5. This is a Banach space, the so-called Bochner space, with the norm, see Wloka[19]

[19] Wloka; Partial differential equations, Cambridge University Press, 1987

Linear nonstationary PDE modeling

Definition (Weak derivative of space-time functions)

Let $u \in L^1(I;X)$. A function $v \in L^1(I;X)$ is the weak derivative of v, denoted as

$$\partial_t u = v$$

if

$$\int_0^T \partial_t \varphi(t) u(t)\, dt = -\int_0^T \varphi(t) v(t)\, dt$$

for all test functions $\varphi \in C_c^\infty(I)$.

Linear nonstationary PDE modeling

In particular, the following result holds (Evans; 2010)

Theorem

Assume $v \in L^2(I, H_0^1)$ and $\partial_t v \in L^2(I, H^{-1})$. Then, v is continuous in time, i.e.,

$$v \in C(I, L^2)$$

(after possible redefined on a set of measure zero). Furthermore, the mapping

$$t \mapsto \|v(t)\|^2_{L^2(X)}$$

is absolutely continuous with

$$\frac{d}{dt}\|v(t)\|^2_{L^2(X)} = 2\langle \frac{d}{dt} v(t), v(t)\rangle$$

for a.e. $0 \le t \le T$.

Mixed systems and electro-magnetic problems (Maxwell)

1. H_{div} spaces; normally-continuous, well-suited for mixed problems

→ Raviart-Thomas finite elements[20] [21]

2. H_{curl} spaces; tangentially-continuous, well-suited for Maxwell's equations

→ Nédélec finite elements[22] [23]

[20] Raviart, Pierre-Arnaud and Thomas, Jean-Marie. A mixed finite element method for 2nd order elliptic problems, in Mathematical aspects of finite element methods (eds: Galligani, Ilio and Magenes, Enrico), 1977

[21] https://defelement.com/

[22] J.-C. Nédélec; Mixed finite elements in $\mathbb{R}^3$, Numerische Mathematik, Vol. 35, pp. 315-341, 1980

[23] J.-C. Nédélec; A new family of mixed finite elements in $\mathbb{R}^3$, Numerische Mathematik, Vol. 50, pp. 57-81, 1986

Space-time heat equation

Formulation

Find $u := u(x,t) : \Omega \times I \to \mathbb{R}$ *such that*

$$\begin{aligned} \rho\partial_t u - \nabla\cdot(\alpha\nabla u) &= f \quad \text{in } \Omega\times I,\\ u &= a \quad \text{on } \partial\Omega\times[0,T],\\ u(0) &= g \quad \text{in } \Omega\times t=0, \end{aligned}$$

where $f : \Omega \times I \to \mathbb{R}$ *and* $g : \Omega \to \mathbb{R}$ *and* $\alpha \in \mathbb{R}$ *and* ρ *are material parameters, and* $a \geq 0$ *is a Dirichlet boundary condition. More precisely,* g *is the initial temperature and* a *is the wall temperature, and* f *is some heat source.*

Space-time heat equation

Definition (Inner products)

The spatial inner product on H is denoted by

$$(u, \varphi)_H = \int_\Omega u \cdot \varphi \, dx$$

The temporal inner product on a space-time space X is denoted by

$$(u, \varphi) := (u, \varphi)_X = \int_0^T (u, \varphi)_H \, dt$$

Space-time heat equation

1. Let us now define the function spaces.
2. In space, we choose our well-known canditates:

$$V := H_0^1(\Omega), \quad H := L^2(\Omega)$$

3. On the time interval I, we introduce the Hilbert space $X := W(0,T)$ with

$$W(0,T) := \{v | v \in L^2(I,V),\ \partial_t v \in L^2(I,V^*)\}$$

4. The notation $L^2(I,V)$ means that v is square-integrable in time using values from I and mapping to the image space V.
5. The space X is embedded in $C(\bar{I},H)$, which allows to work with well-defined (continuous) initial conditions u^0 (theorem from a few slides before).

Space-time heat equation

Definition (Bilinear forms)

We define the spatial bilinear form $\bar{a} : V \times V \to \mathbb{R}$ as usually. The time-dependent semi-linear form is as follows: $a : X \times X \to \mathbb{R}$:

$$a(u, \varphi) := \int_0^T \bar{a}(u(t), \varphi(t))\, dt.$$

Formulation (Space-time weak form)

Then the space-time parabolic problem is given by: Find $u \in X$ such that

$$\int_0^T (\partial_t u, \varphi) + a(u, \varphi) = \int_0^T (f, \varphi) \quad \forall \varphi \in X$$
$$u(0) = u^0$$

with $f \in L^2(I, V^*)$ and $u^0 \in H$.

Nonlinear PDE modeling

1. Recall: $L^p(\Omega)$ denotes Lebesgue spaces for which $\int_\Omega |u(x)|^p\,dx < \infty$
2. Sobolev space $W^{l,p}(\Omega)$, which consists of the functions $\varphi : \Omega \to \mathbb{R}$ such that their weak derivatives $D^\alpha \varphi$ with $|\alpha| \leq l$ belong to $L^p(\Omega)$.
3. Norms: $\varphi \in W^{l,p}(\Omega)$, then its norm is defined by

$$\|\varphi\|_{W^{l,p}(\Omega)} = \Big(\sum_{0\leq|\alpha|\leq l} \|D^\alpha \varphi\|^p_{L^p(\Omega)} \Big)^{\frac{1}{p}} \quad \text{and} \quad \|\varphi\|_{W^{l,\infty}(\Omega)} = \max_{0\leq|\alpha|\leq l} \|D^\alpha \varphi\|_{L^\infty(\Omega)},$$

for $1 \leq p < \infty$ and $p = \infty$, respectively.

Example: regularized p-Laplacian [24] [25]

1. Assume Ω being a bounded polygonal domain in $\mathbb{R}^d$, with $d = 2$ and $\Gamma_D = \partial\Omega$.
2. Consider the following scalar p-type problem

$$-\operatorname{div}\mathbf{A}(\nabla u) = f \quad \textit{in } \Omega, \qquad u = u_D \quad \textit{on } \Gamma_D, \tag{24}$$

   where $f : \Omega \to \mathbb{R}$ and $u_D : \Gamma_D \to \mathbb{R}$ are given smooth functions.
3. The operator $\mathbf{A}(\nabla u) : \mathbb{R}^2 \to \mathbb{R}^2$ has the following p-power law form

$$\mathbf{A}(\nabla u) = (\varepsilon^2 + |\nabla u|^2)^{\frac{p-2}{2}} \nabla u, \tag{25}$$

   where $p \in (1, \infty)$ and $\varepsilon > 0$ are model parameters and $|\cdot|^2 = (\cdot, \cdot)$.
4. The function $a(\nabla u) = (\varepsilon^2 + |\nabla u|^2)^{\frac{p-2}{2}}$ is the diffusivity term of (24).

[24] Wick; Numerical Methods for Partial Differential Equations, Leibniz University Hannover, `https://doi.org/10.15488/11709`, Sec. 13.15

[25] Toulopoulos, Wick; Numerical methods for power-law diffusion problems, SIAM J. Sci. Comput., Vol. 39(3), 2017, pp. A681-A710

Example: regularized p-Laplacian

The weak formulation for (24) reads as follows: Find $u \in W_D^{1,p}$ such that

$$B(u,\varphi) = l_f(\varphi),\ \forall \varphi \in W_0^{1,p}(\Omega), \quad \text{where } B(u,\varphi) = \int_\Omega \mathbf{A}(\nabla u)\cdot \nabla \varphi\, dx,\ l_f(\varphi) = \int_\Omega f\varphi\, dx. \tag{26}$$

Theorem

Let $u \in V$ be the solution of (26) under some assumptions, and let $u_h \in V_{D,h}^{(k)}$ be the solution of the discrete p-Laplacian. Then, there exist $C \geq 0$, independent of the grid size h, such that

$$\int_\Omega |\mathbf{F}(\nabla u) - \mathbf{F}(\nabla u_h)|^2\, dx \leq Ch^{2(l-1)} \|u\|^2_{W^{l,p}(\Omega)}. \tag{27}$$

Proof.

See Toulopoulos, Wick; Numerical methods for power-law diffusion problems, SIAM J. Sci. Comput., Vol. 39(3), 2017, pp. A681-A710. □

Example: regularized p-Laplacian

We obtain as numerical results for computational error analysis, nonlinear Newton solver, and linear multigrid:

```
FE degree       eps     p       TOL (LinSolve) TOL(Newton)
==============================================================
1               0.1     1.01    1e-12           1e-10
--------------------------------------------------------------
Cells   DoFs    h               F-norm err      ConvRate        Min/MaxLinIter  Newton iter
============================================================================================
4096    4225    2.20971e-02     5.43340e-02     1.04683e+00     18/28           5
16384   16641   1.10485e-02     2.03360e-02     1.41782e+00     27/37           5
65536   66049   5.52427e-03     1.01906e-02     9.96804e-01     25/33           4
262144  263169  2.76214e-03     5.09674e-03     9.99587e-01     25/30           3
1048576 1050625 1.38107e-03     2.54855e-03     9.99899e-01     24/28           3
4194304 4198401 6.90534e-04     1.27430e-03     9.99975e-01     23/25           3
============================================================================================
```

Observations:

- The F norm is close to 1 as to be expected from the theory stated above
- The number of linear iterations is (nearly) mesh-independent and asymptotically stable. Therefore, the geometric multigrid preconditioner works very well.
- The number of nonlinear Newton iterations is as well mesh-independent and asymptotically stable

Nonlinear coupled PDE and limiting processes

1. Limiting processes[26]: plasticity[27] and fracture [28]

→ solution u may have discontinuities

2. **Measure spaces**: BD (bounded deformation) or BV (bounded variation)

[26] Limiting processes my own definition for these lecture notes
[27] Temam; Mathematical Problems in Plasticity, Dover, 2018
[28] Francfort, Larsen; Existence and convergence for quasi-static evolution in brittle fracture, Comm. Pure Appl. Math., Vol. 56(10), pp. 1465-1500, 2003

Broken Sobolev spaces [31] [32]

1. Problem statements with discontinuities (e.g., transport)
2. Broken Sobolev spaces
3. Jumps and averages to be added to bilinear/semi-linear forms
4. Discontinuous Galerkin finite elements as discretization
5. Interior penality Galerkin methods (IPG), symmetric IPG (SIPG), nonsymmetric IPG (NIPG), incomplete IPG (IIPG)
6. Applications in all fields: solid mechanics, fluid mechanics, porous media, and so forth
7. High flexibility in the discretization, but also higher cost (because more degrees of freedom)
8. Related is enriched Galerkin (EG)[29] [30]

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[29] S. Sun, J. Liu, A locally conservative finite element method based on piecewise constant enrichment of the continuous galerkin method, SIAM J. Sci. Comput. 31 (4) (2009) 2528-2548

[30] S. Lee, M.F. Wheeler, Enriched Galerkin approximations for two phase flow in porous media with capillary pressure, J. Comput. Phys. 367 (2018) 65-86.

[31] Rivière; Discontinuous Galerkin Methods for Solving Elliptic and Parabolic Equations, SIAM, 2008

[32] Di Pietro, Ern; Mathematical Aspects of Discontinuous Galerkin Methods, Springer, 2012

Stochastic PDEs[33] [34]

1. Stochastic Lebesgue and Sobolev spaces
2. Schwartz space
3. Brownian motion, white noise (Hida, 1980)
4. Stochastic Poisson, stochastic heat equation

[33] e.g., Holden, Oksendal, Uboe, Zhang; Stochastic Partial Differential Equations, Springer, 2010
[34] e.g., Evans; An Introduction to Stochastic Differential Equations, AMS, 2013

Lebesgue and Sobolev spaces with variable exponents[35]

1. Variable exponent spaces
2. Variable expondent Lebesgue spaces
3. Weighted variable exponent Lebesgue spaces
4. Orlicz spaces

[35] Diening, Harjulehto, Hästö, Ruzicka; Lebesgue and Sobolev spaces with variable exponents, Springer, 2010

Exercises

1. Short question: what is the difference between a metric space and a normed space?
2. Short question: why is completeness important?
3. Short question: define the inner product of $L^2(\Omega)$
4. Let $-\Delta u = f$ in Ω with $u = 0$ on $\partial\Omega$:
    1. Formulate the weak form
    2. Design the trial/test spaces X
    3. Write down explicitly the norm
5. Let $-\Delta u = f$ in Ω with $u = 0$ on $\partial\Omega_D$ and $\partial_n u = 0$ on $\partial\Omega_{N1}$ and $\partial_n u = g$ on $\partial\Omega_{N2}$, where the three boundary parts are non-overlapping (as usual).
    1. Formulate the weak form
    2. Design the trial/test spaces X
    3. Write down explicitly the norm
6. Design formally an FEM scheme in X_h with $dim(X_h) = N$

End Part II

Motivation

1. Many PDEs are subject to variational inequality constraints
2. **Example:** Obstacle problem[36 37], fracture with irreversibility[38]
3. Obstacle problem: Find $u : \Omega \to \mathbb{R}$ such that

$$-\Delta u \geq f, \quad u \geq g, \quad (f - \Delta u)(u - g) = 0 \quad \text{in } \Omega$$
$$u = 0 \quad \text{on } \partial\Omega$$

Figure: Obstacle problem $-u'' = -1$ in Ω and $u(0) = u(1) = 0$: deformation u of a line that is constraint by the obstacle g. In the green area with $u > g$, the PDE is solved. In the red area $u = g$ we 'sit' on the obstacle.

[36] Kinderlehrer, Stampacchia; An Introduction to Variational Inequalities and Their Applications, SIAM, 2000
[37] Kikuchi, Oden; Contact problems in elasticity, SIAM, 1988
[38] Wick, Multiphysics phase-field fracture, de Gruyter, 2020

Obstacle problem I

1. Solution u in a convex set K (rather a linear function space)

$\rightarrow$ cannot apply standard FEM as discretization

2. Either special algorithms from optimization
3. One other possibility: regularize inequality constraint:

$$u \geq g \quad \rightarrow \gamma[g-u]^+ \tag{28}$$

where $[x]^+ = \max\{0, x\}$ and $\gamma > 0$

Obstacle problem II

1. Introducing the penalization relaxes the inequality contraint (relaxation means it is not enforced that strictly anymore), but enlarges from the convex set K to a linear function space X (here $X = H_0^1(\Omega)$)
2. Now, classical FEM works again
3. **Prize to pay:** nonlinear problem with a high dependence on γ
4. γ too high: enforces better inequality, but nonlinear solution algorithm suffers
5. γ too small: inequality constraint more and more violated, better performance of solution algorithm (balance between accuracy and efficiency)

Obstacle problem III (Poisson versus obstacle)

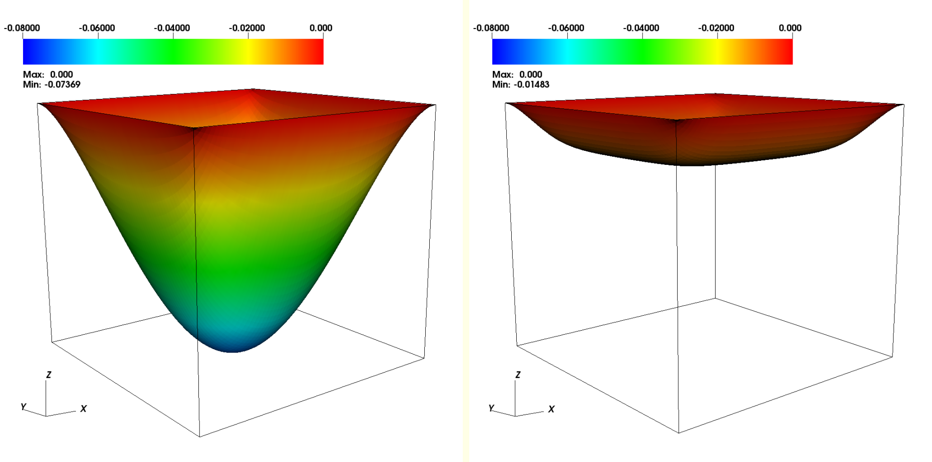

Figure: Left: 3d surface plot solution of the classical Poisson problem in $(0,1)^2$ and right hand side $f = -1$. Right: obstacle problem with $g = -0.01$ and simple penalization.

Obstacle problem IV

The nonlinear solver (Newton's method) behaves as follows (**Convergence in 5 steps**):

```
Newton step: 0  Residual (abs.):   2.4414e-04
Newton step: 0  Residual (rel.):   1.0000e+00
Newton step: 1  Residual (rel.):   9.7262e-01   LineSearch {2}
Newton step: 2  Residual (rel.):   4.8631e-01   LineSearch {1}
Newton step: 3  Residual (rel.):   2.6331e-01   LineSearch {0}
Newton step: 4  Residual (rel.):   5.1674e-03   LineSearch {0}
Newton step: 5  Residual (rel.): < 1.0000e-11   LineSearch {0}
```

As comparison, we briefly state the results for the classical Poisson problem (**Convergence in 1 step - linear problem!**)

```
Newton step: 0  Residual (abs.):   2.4414e-04
Newton step: 0  Residual (rel.):   1.0000e+00
Newton step: 1  Residual (rel.): < 1.0000e-11   LineSearch {0}
```

Obstacle: energy minimization problem

1. Let $\Omega \subset \mathbb{R}$ (all developements in this section hold also for $\Omega \subset \mathbb{R}^n$) be open and $u : \Omega \to \mathbb{R}$ and $f : \Omega \to \mathbb{R}$.
2. The (nonlinear) potential energy is defined as
$$E(u) = \int_\Omega \left(\mu(\sqrt{1 + |\nabla u|^2} - 1) - fu \right) dx$$
where $\mu > 0$ is a material parameter.
3. Taylor linearization yields:
$$E(u) = \frac{1}{2} \int_\Omega (\mu |\nabla u|^2 - fu)\, dx$$
4. The physical state without constraints is given by
$$\min_{u \in V} E(u)$$
with $V = \{v \in H^1(\Omega) |\ v = u_0 \text{ on } \partial\Omega\}$.
5. So far, all is equivalent to Poisson

Obstacle: constraint and convex set

1. We introduce the constraint (for instance a table that blocks the further deformation of the membrane):

$$u \geq g, \quad g \in L^2$$

2. Then:

$$\min_{u \in V, u \geq g} E(u)$$

3. The admissible space is the convex set

$$K = \{v \in H^1 | v = u_0 \text{ on } \partial\Omega, \ v \geq g \text{ in } \Omega\}.$$

4. We recall the definition of a convex set:

$$u, v \in K : \quad \theta u + (1 - \theta) v \in K.$$

Weak form with convex sets

1. If $u \in K$ is a minimum, it holds:
$$E(u) = \min_{v \in K} E(v).$$

2. We now derive a variational formulation. Let $\theta v + (1-\theta)u = u + \theta(v-u) \in K$ for $\theta \in [0,1]$. Then it clearly holds:
$$E(u + \theta(v-u)) \geq E(u)$$

3. We derive now the first-order optimality condition (i.e., the PDE in weak form):

    - Differentiate w.r.t. θ;
    - Set $\theta = 0$.

Directional derivative (first-order necessary condition)

Then:

$$
\begin{aligned}
\frac{d}{d\theta}E(u+\theta(v-u))|_{\theta=0} &\geq \frac{d}{d\theta}E(u) \\
\Leftrightarrow \frac{d}{d\theta}E(u+\theta(v-u))|_{\theta=0} &\geq 0 \\
\Leftrightarrow \frac{d}{d\theta}\int_\Omega \mu\nabla u\cdot\nabla(u+\theta(v-u))|_{\theta=0}\,dx - \int_\Omega f(v-u)\,dx &\geq 0 \\
\Rightarrow \int_\Omega \mu\nabla u\cdot\nabla(v-u)\,dx - \int_\Omega f(v-u)\,dx &\geq 0
\end{aligned}
$$

for all $v\in K$.

Weak form with convex sets

In summary:

Formulation (Obstacle problem: variational formulation)

We have

$$(\mu \nabla u, \nabla (v-u)) \geq (f, v-u)$$

for

$$K = \{v \in H^1 |\, v = u_0 \text{ on } \partial\Omega,\ v \geq g \text{ in } \Omega\}.$$

1. Recall that $(\cdot,\cdot)$ is the inner product on L^2, i.e.,

$$(\mu \nabla u, \nabla (v-u)) := \int_\Omega \mu \nabla u \cdot \nabla (v-u)\, dx$$

and

$$(f, v-u) := \int_\Omega f \cdot (v-u)\, dx$$

Extensions

1. Irrevesible processes, bounds on the solution (as in obstacle), e.g., damage/fracture

→ e.g., space-time material modeling using an extended Hamilton functional[39]

2. Optimal control problems with control and/or state constraints[40]

[39] Junker, Wick; Space-time variational material modeling: a new paradigm demonstrated for thermo-mechanically coupled wave propagation, visco-elasticity, elasto-plasticity with hardening, and gradient-enhanced damage, 2023

[40] Hinze, Pinnau, Ulbrich, Ulbrich; Optimization with PDE constraints, Springer, 2009

Exercises

1. Go to the NumPDE lecture notes `https://doi.org/10.15488/11709` and do Section 13.4 (Exercise) on page 321ff.
2. Formulate the functional framework for phase-field fracture.
   Hint: Wick, 2020 `https://doi.org/10.1515/9783110497397` in Chapter 4.

Take away in a few words

1. **Function spaces**, more general **functional frameworks** give **mathematical structure** to engineering problem statements
2. **Function spaces**, more general **functional frameworks** are needed to study **well-posedness** (existence, uniqueness, data dependencies) and **error estimates**
3. **Function spaces**, more general **functional frameworks** help **analyzing numerical algorithms** in terms of their **accuracy, efficiency, robustness** and can consequently suggest **improvements**