

Lecture 1

What is the Topic of this Course?

The ultimate aim of these notes is quickly formulated: We would like to develop those functional analytic tools that allows us to adopt methods for ordinary differential equations (ODEs) to solve some classes of time-dependent partial differential equations (PDEs) numerically.

Let us illustrate this idea by recalling first the most trivial one of all ODEs. For a matrix $A \in \mathbb{R}^{d \times d}$ consider the initial value problem

$$\begin{cases} \dot{u}(t) = Au(t), \\ u(0) = u_0. \end{cases}$$

We know that the solution to such an ordinary differential equation is given by

$$u(t) = e^{tA}u_0,$$

where e^{tA} is the exponential function of the matrix tA defined by the power series

$$e^{tA} = \sum_{n=0}^{\infty} \frac{t^n A^n}{n!},$$

which converges absolutely and uniformly on every compact interval of \mathbb{R} . Here the numerical challenge is, especially for large matrices, to calculate this exponential function in an effective and accurate way.

The exponential function of a matrix plays an important role not only because it solves the linear problem above, but it also occurs in more complicated problems where a nonlinearity is present, like in the equation

$$\dot{v}(t) = Av(t) + F(t, v(t)).$$

To solve such an equation by iterative methods the variation of constants formula plays an essential role, stating that the solution $v(t)$ of this nonlinear equation satisfies

$$v(t) = e^{tA}v(0) + \int_0^t e^{(t-s)A}F(s, v(s)) ds.$$

Here again the exponential function of a matrix appears. Of course, here further numerical issues arise, such as the calculation of integrals.

There is a multitude of theoretical methods for the calculation of such exponentials, each of them leading to some possible numerical treatment of the problem. We mention those that will be important for us in this course:

1. by means of the Jordan normal form,

2. by means of the Cauchy's integral formula, more precisely, by using the identity

$$\frac{1}{2\pi i} \oint \frac{e^\lambda}{\lambda - z} d\lambda = e^z,$$

3. by using other formulae for the exponential function, say

$$e^x = \lim_{n \rightarrow \infty} \left(1 + \frac{x}{n}\right)^n = \lim_{n \rightarrow \infty} \left(1 - \frac{x}{n}\right)^{-n}.$$

Let us start by looking at the first of the suggestions on the above list. Theory tells us that we "only" have to bring A to Jordan normal form, and then the exponential function can be simply read off. The situation is even better if we can find a basis of orthogonal eigenvectors. Then we can bring the matrix A to diagonal form by a similarity transformation $S^{-1}AS = D = \text{diag}(\lambda_1, \dots, \lambda_d)$, and hence the exponential becomes

$$e^{tA} = S e^{tD} S^{-1} = S \text{diag}(e^{t\lambda_1}, \dots, e^{t\lambda_d}) S^{-1}.$$

Of course, other numerical difficulties are hidden in calculating the Jordan normal form or the similarity transformation S . Still this very idea proves itself to be useful for partial differential equations. Let us illustrate this idea on the next example.

1.1 The heat equation

Consider the one-dimensional heat equation, say, on the interval $(0, \pi)$

$$\begin{aligned} \partial_t w(t, x) &= \partial_{xx} w(t, x), \quad t > 0 \\ w(0, x) &= w_0(x), \end{aligned}$$

with homogeneous Dirichlet boundary conditions

$$w(t, 0) = w(t, \pi) = 0.$$

We can rewrite this equation (without the initial condition) as a linear ordinary differential equation

$$\dot{u}(t) = Au(t), \quad t > 0 \tag{1.1}$$

in the infinite dimensional Hilbert space $L^2(0, \pi)$. To do this define the operator

$$(Ag)(x) := g''(x) = \frac{d^2}{dx^2} g(x)$$

with domain

$$\begin{aligned} D(A) := \left\{ g \in L^2(0, \pi) : g \text{ cont. differentiable on } [0, \pi], \right. \\ \left. g'' \text{ exists a.e., } g'' \in L^2, g'(t) - g'(0) = \int_0^t g''(s) ds \text{ for } t \in [0, \pi] \right. \\ \left. \text{and } g(0) = g(\pi) = 0 \right\}. \end{aligned}$$

Note that the definition of the domain has two ingredients: a condition that the differential operator on the right-hand side of the equation has values in the underlying space (in this case L^2), and

boundary conditions. The initial value is a function $f \in L^2(0, \pi)$, $f = w_0$, and we look for a continuous function $u : [0, \infty) \rightarrow L^2(0, \pi)$ that is differentiable on $(0, \infty)$ and satisfies equation (1.1) with $u(0) = f$. Formally the solution of this problem is given by the exponential function “ e^{tA} ” applied to the initial value f . Our aim is now to give a mathematical meaning to the expression “ $u(t) = e^{tA}f$ ”.

First of all, we calculate the eigenvalues of this operator. These are $-n^2$ with corresponding eigenvectors

$$f_n(x) = \sqrt{\frac{2}{\pi}} \sin(nx) \quad \text{for } n \in \mathbb{N},$$

that is,

$$Af_n = -n^2 f_n. \quad (1.2)$$

Note that we have normalised the eigenvectors so that $\|f_n\|_2 = 1$. It is also easy to see that these eigenfunctions are mutually orthogonal with respect to the L^2 scalar product, i.e.,

$$\langle f_n, f_m \rangle := \int_0^\pi f_n(x) \overline{f_m(x)} dx = \begin{cases} 1, & \text{for } n = m \\ 0, & \text{otherwise.} \end{cases}$$

The linear span $\text{lin}\{f_n : n \in \mathbb{N}\}$ of these functions is dense in $L^2(0, \pi)$, so altogether we obtain an orthonormal basis of eigenvectors of A . As a consequence, every function $f \in L^2(0, \pi)$ can be written as a series

$$f = \sum_{n=1}^{\infty} \langle f, f_n \rangle f_n, \quad (1.3)$$

where the convergence has to be understood in the L^2 norm. We call $\langle f, f_n \rangle$ the (generalised) **Fourier coefficients** of f .

For $f \in \text{lin}\{f_n : n \in \mathbb{N}\}$, $f = \sum_{n=1}^N a_n f_n$, the action of A is simple:

$$Af = \sum_{n=1}^N a_n Af_n = \sum_{n=1}^N -n^2 a_n f_n.$$

One expects that such a formula should hold true for functions for which the series on the right-hand side converges in $L^2(0, \pi)$.

Proposition 1.1. *Consider the linear operator M on $L^2(0, \pi)$ with domain*

$$D(M) := \left\{ f \in L^2(0, \pi) : \sum_{n=1}^{\infty} n^4 |\langle f, f_n \rangle|^2 < \infty \right\}$$

defined by

$$Mf := \sum_{n=1}^{\infty} -n^2 \langle f, f_n \rangle f_n.$$

Then $A = M$, i.e., $D(A) = D(M)$, and for $f \in D(A)$ we have $Af = Mf$. In particular we have

$$Af = \sum_{n=1}^{\infty} -n^2 \langle f, f_n \rangle f_n \quad \text{for all } f \in D(A) = D(M).$$

Proof. Suppose $f \in D(A)$. Then we integrate by parts twice(!) and obtain

$$\begin{aligned} \sqrt{\frac{\pi}{2}} \langle Af, f_n \rangle &= \int_0^\pi f''(x) \sin(nx) \, dx = f'(x) \sin(nx) \Big|_{x=0}^{x=\pi} - n \int_0^\pi f'(x) \cos(nx) \, dx \\ &= -n \int_0^\pi f'(x) \cos(nx) \, dx \\ &= -nf(x) \cos(nx) \Big|_{x=0}^{x=\pi} - n^2 \int_0^\pi f(x) \sin(nx) \, dx = -n^2 \sqrt{\frac{\pi}{2}} \langle f, f_n \rangle, \end{aligned}$$

where in the last step we used the boundary conditions $f(0) = f(\pi) = 0$. Since $Af \in L^2$, its Fourier coefficients are square summable. Whence, $f \in D(M)$ follows. This shows $D(A) \subseteq D(M)$. We also see that

$$Af = \sum_{n=1}^{\infty} -n^2 \langle f, f_n \rangle f_n \quad \text{holds for all } f \in D(A).$$

It only remains to show the other inclusion $D(M) \subseteq D(A)$. To see that, it suffices to note that A is surjective (this is “classical”) and M is injective, so $A = M$ because M extends A (see Exercises 3 and 4.) \square

Intuitively, the result above states that A has diagonal form with respect to the basis of eigenvectors, and is given by

$$A = \text{diag}(-1, -2^2, \dots, -n^2, \dots).$$

Thus, the exponential of this operator can be immediately defined as

$$e^{tA} := \text{diag}(e^{-t}, e^{-t4}, \dots, e^{-tn^2}, \dots),$$

meaning that

$$e^{tA} f = \sum_{n=1}^{\infty} e^{-tn^2} \langle f, f_n \rangle f_n.$$

We have to show that this is a meaningful definition. As a first step, let us show that the formula above gives rise to a continuous function.

Proposition 1.2. *Let $f \in L^2(0, \pi)$. Then for every $t \geq 0$ the series*

$$e^{tA} f := \sum_{n=1}^{\infty} e^{-tn^2} \langle f, f_n \rangle f_n$$

is convergent and defines a function $u(t) = e^{tA} f$ which is continuous on $[0, \infty)$ with values in $L^2(0, \pi)$.

Proof. Since for every $n \in \mathbb{N}$ and $t \geq 0$ the inequality $|e^{-tn^2}| \leq 1$ holds, the sequence $(e^{-tn^2} \langle f, f_n \rangle)$ is square summable, and the series

$$\sum_{n=1}^{\infty} e^{-tn^2} \langle f, f_n \rangle f_n$$

that defines $u(t) = e^{tA} f$ converges in $L^2(0, \pi)$.

We now prove the continuity at a given $t \geq 0$. Let $\varepsilon > 0$ be given, and choose $n_0 \in \mathbb{N}$ so that

$$\sum_{n=n_0+1}^{\infty} |\langle f, f_n \rangle|^2 \leq \varepsilon.$$

If $t = 0$, then in the following we consider only $h \geq 0$, and if $t > 0$ we additionally suppose $|h| \leq t$. This way we can write

$$\begin{aligned} \|e^{tA} f - e^{(t+h)A} f\|_2^2 &= \langle e^{tA} f - e^{(t+h)A} f, e^{tA} f - e^{(t+h)A} f \rangle \\ &= \sum_{n=1}^{\infty} |e^{-(t+h)n^2} - e^{-tn^2}|^2 |\langle f, f_n \rangle|^2 \leq \sum_{n=1}^{n_0} |e^{-(t+h)n^2} - e^{-tn^2}|^2 |\langle f, f_n \rangle|^2 + 2\varepsilon \\ &\leq \sum_{n=1}^{n_0} |e^{-hn^2} - 1|^2 |\langle f, f_n \rangle|^2 + 2\varepsilon. \end{aligned}$$

We can finish the proof by choosing $|h|$ so small that the first finitely many terms contribute at most ε . \square

Hence, this exponential function provides a candidate to be the solution of (1.1). Let us prove that it is indeed the solution.

Proposition 1.3. *For $f \in L^2(0, \pi)$ we define $u(t) := e^{tA} f$. Then $u(t) \in D(A)$ holds for all $t > 0$, and u is differentiable on $(0, \infty)$ with derivative $Au(t)$. That is, u solves the initial value problem*

$$\begin{aligned} \dot{u}(t) &= Au(t), \quad t > 0 \\ u(0) &= f. \end{aligned}$$

Proof. The initial condition is fulfilled by (1.3). Note that for all $t > 0$ and $n \in \mathbb{N}$ we have

$$|e^{-tn^2} n^2| \leq e^{-\frac{t}{2}n^2} \frac{2e^{-1}}{t} \quad \text{for all } n \in \mathbb{N}. \quad (1.4)$$

From this estimate, using the characterisation in Proposition 1.1, we obtain that $u(t) \in D(M) = D(A)$ for each $t > 0$. Define

$$\begin{aligned} v(t) &:= Au(t), \\ u_n(s) &:= e^{-sn^2} \langle f, f_n \rangle f_n, \end{aligned}$$

and

$$v_n(s) := -n^2 e^{-sn^2} \langle f, f_n \rangle f_n.$$

Then $\dot{u}_n = v_n$, and both functions are continuous on $[t/2, 3t/2]$ with values in L^2 . From inequality (1.4) we obtain that the following two series

$$u(s) = \sum_{n=1}^{\infty} u_n(s) \quad \text{and} \quad v(s) = \sum_{n=1}^{\infty} \dot{u}_n(s)$$

have summable numerical majorants for $s \in [t/2, 3/2t]$. This implies that u is differentiable and that we can interchange summation and differentiation, whence $\dot{u}(t) = v(t) = Au(t)$ follows. \square

Let us put the above in an abstract, operator theoretic perspective.

Proposition 1.4. For $t \geq 0$ define $T(t)f := e^{tA}f$. Then $T(t)$ is a bounded linear operator on $L^2(0, \pi)$ for each $t \geq 0$. The mapping T satisfies

$$T(t+s) = T(t)T(s) \quad \text{and} \quad T(0) = I, \text{ the identity operator on } L^2.$$

For each $f \in L^2(0, \pi)$ the function $t \mapsto T(t)f$ is continuous on $[0, \infty)$.

Proof. As we saw in Proposition 1.2, the inequality

$$\|e^{tA}f\|_2^2 = \langle e^{tA}f, e^{tA}f \rangle \leq \sum_{n=1}^{\infty} e^{-2tn^2} |\langle f, f_n \rangle|^2 \leq \sum_{n=1}^{\infty} |\langle f, f_n \rangle|^2 = \|f\|_2^2$$

holds. It is moreover clear that the mapping $f \mapsto e^{tA}f$ is linear, and from the previous inequality we obtain that it is bounded with operator norm

$$\|e^{tA}\| \leq 1.$$

The identity $T(t+s) = T(t)T(s)$ follows from the properties of the exponential function and the definition of e^{tA} . The relation $T(0) = I$ was discussed in Proposition 1.3, the continuity of the mapping $t \mapsto T(t)f$ follows from Proposition 1.2. \square

From the properties above we can coin a new definition.

Definition 1.5. Let X be a Banach space, and let the mapping $T : [0, \infty) \rightarrow \mathcal{L}(X)$ have¹ the properties:

a) For all $t, s \in [0, \infty)$

$$\begin{cases} T(t+s) = T(t)T(s) \\ T(0) = I, \text{ the identity operator on } X. \end{cases}$$

b) For all $x \in X$ the mapping

$$t \mapsto T(t)x \in X$$

is continuous.

Then T is called a **strongly continuous** one-parameter **semigroup**² of bounded linear operators on the Banach space X . We abbreviate this long expression sometimes to *strongly continuous semigroup*, or simply to *semigroup*.

The semigroup constructed in Proposition 1.4 is called the (Dirichlet) **heat semigroup** on $[0, \pi]$. To sum up, we can state the following.

Conclusion 1.6. Initial value problems lead to semigroups.

¹Here and later on, $\mathcal{L}(X)$ denotes the set of bounded linear operators on X .

²By an alternative terminology one may call such an object a C_0 -semigroup.

1.2 The shift semigroup

Now that we have the new mathematical notion of *one-parameter semigroups* we want to study them in detail. This, as a matter of fact, is one of the aims of this course. Before doing so let us consider another example.

Take

$$X = \text{BUC}(\mathbb{R}) := \{f : \mathbb{R} \rightarrow \mathbb{R} : f \text{ is uniformly continuous and bounded}\},$$

which is a Banach space with the supremum norm

$$\|f\|_\infty := \sup_{s \in \mathbb{R}} |f(s)|.$$

The additive (semi)group structure of \mathbb{R} naturally induces a semigroup on this Banach space by setting

$$(S(t)f)(s) = f(t + s), \quad \text{for } f \in X, s \in \mathbb{R}, t \geq 0.$$

One readily sees that $S(t)$ is a bounded linear operator on X , in fact a linear isometry. The semigroup property follows immediately from the definition. From the uniform continuity of $f \in X$ we conclude that

$$t \mapsto S(t)f$$

is continuous, i.e., that S is a strongly continuous semigroup on $X = \text{BUC}(\mathbb{R})$, called the **left shift semigroup**.

Let us investigate whether this semigroup S solves some initial value problem such as (1.1). Again the heuristics of exponential functions helps: Given e^{tA} for a matrix $A \in \mathbb{R}^{d \times d}$, we can “calculate” the exponent by differentiating this exponential function at 0:

$$A = \left. \frac{d}{dt} e^{tA} \right|_{t=0}.$$

What happens in the case of the shift semigroup S ? The semigroup S is not even continuous for the operator norm (why?). So let us look at differentiability of the **orbit map** $t \mapsto S(t)f$ for some given $f \in X$, called **strong differentiability**. The limit

$$\lim_{h \rightarrow 0} \frac{1}{h} (S(h)f - f) = \lim_{h \rightarrow 0} \frac{f(h + \cdot) - f(\cdot)}{h}$$

must exist in the sup-norm of X . We immediately find a suitable candidate for the limit: Since the limit must exist pointwise on \mathbb{R} , it cannot be anything else than f' . Hence, the function f must be at least differentiable so that the limit can exist. For f differentiable with f' being uniformly continuous we have

$$\sup_{s \in \mathbb{R}} \left| \frac{f(h + s) - f(s)}{h} - f'(s) \right| = \sup_{s \in \mathbb{R}} \left| \frac{1}{h} \int_s^{s+h} (f'(r) - f'(s)) dr \right| \leq \varepsilon,$$

for all h with $|h| \leq \delta$, where $\delta > 0$ is sufficiently small, chosen for the arbitrarily given $\varepsilon > 0$ from the uniform continuity of f' . This shows that if $f, f' \in X$, then we have

$$\lim_{h \rightarrow 0} \left\| \frac{f(h + \cdot) - f(\cdot)}{h} - f'(\cdot) \right\|_\infty = \lim_{h \rightarrow 0} \sup_{s \in \mathbb{R}} \left| \frac{f(h + s) - f(s)}{h} - f'(s) \right| = 0.$$

Note that for the derivative of $S(t)f$ at arbitrary $t \in \mathbb{R}$ we obtain by the same argument

$$\frac{d}{dt}(S(t)f) = S(t)f'.$$

This means that for $f, f' \in X$ the orbit function $u(t) = S(t)f$ solves the differential equation

$$\begin{cases} \dot{u}(t) = Au(t) \\ u(0) = f, \end{cases}$$

where $(Af)(s) = f'(s)$ with domain

$$D(A) := \{f : f, f' \in \text{BUC}(\mathbb{R})\}.$$

We can therefore formulate the parallel of Conclusion 1.6:

Conclusion 1.7. To a semigroup there exists a corresponding initial value problem.

1.3 What is the topic of this course?

At this point we hope to have motivated the study of strongly continuous semigroups from the analytic or PDE point of view. To solve an initial value problem $\dot{u}(t) = Au(t)$, one has to define a semigroup e^{tA} .

The numerical analysis aspects are now the following:

- The operator A is complicated, and numerically impossible to treat, so one approximates it via a sequence of operators A_m and hopes that the corresponding solutions (expected to be easily calculated) e^{tA_m} converge to the solution of the original problem e^{tA} (in a sense yet to be made precise). This procedure is called *space discretisation*, and may indeed come from a spatial mesh (e.g., for a finite element method) or from some not so space-related discretisation, like for Fourier-Galerkin methods, an instance of which we have seen in Section 1.1.
- Equally hard is to determine the exponential function of a matrix (or operator) A (see the list of suggestions on page 1). So a different idea is to approximate the exponential function $z \mapsto e^z$ by functions r that are easier to handle. A typical example, known also from basic calculus courses, is that of the implicit Euler scheme $r(z) = (1 - z)^{-1}$. In this case the approximation means $r(0) = 1$ and $r'(0) = 1$, i.e., the first two Taylor coefficients of the two functions coincide. Heuristically we obtain that $r(tA)$ for a small t is approximately the same as e^{tA} (up to an error of magnitude t^2), we may take the n^{th} power and to compensate the growing error we would obtain, we take the time step smaller and smaller as n grows. We obtain

$$\left(r\left(\frac{t}{n}A\right)\right)^n \approx \left(e^{\frac{t}{n}A}\right)^n = e^{tA},$$

where the semigroup property was used. This procedure is called *time discretisation*.

- Due to numerical reasons one is usually forced to combine the two methods above, and sometimes even by adding a further spice to the stew: operator splitting. This is usually done when operator A has a complicated structure, but decomposes into a finite number of parts that are easier to handle.

- The theory presented above is the basis in extending known ODE methods to time dependent partial differential equations and will allow us to use the variation of constants formula for inhomogeneous or semilinear equations. Hence the convergence analysis of various iteration methods will depend on this theory.

In semigroup theory the above methods culminate in the famous Lax-Chernoff Equivalence Theorem that describes precisely the situation when these methods work. In this course we shall develop the basic tools from operator semigroup theory needed for such an abstract treatment of discretisation procedures.

Exercises

1. Prove that $\sin(nx)$, $n \in \mathbb{N}$, form a complete orthogonal system in $L^2(0, \pi)$, compute the L^2 norms.
2. Analogously to what is presented in Section 1.1, study the heat equation with **Neumann boundary conditions**:

$$\begin{aligned}\partial_t u(t, x) &= \partial_{xx} u(t, x), \quad t > 0 \\ u(0, x) &= f(x), \\ \partial_x u(t, 0) &= \partial_x u(t, \pi) = 0.\end{aligned}$$

3. Let X be a Banach space and $A_1 : X \rightarrow X$ and $A_2 : X \rightarrow X$ linear maps such that
 - $D(A_1) \subset D(A_2)$ and A_1 is a restriction of A_2
 - A_1 is surjective and A_2 is injective.

Show that $A_1 = A_2$.

4. Consider the Hilbert space ℓ^2 of square summable complex sequences.

a) Prove that

$$c_{00} = \{(x_n) \in \ell^2 : x_n = 0 \text{ except for finitely many } n\}$$

is a dense linear subspace of ℓ^2 .

b) For $m = (m_n)$ an arbitrarily fixed sequence of complex numbers, and $x = (x_n) \in c_{00}$ define

$$(M_m x)_n = (m_n x_n), \quad \text{i.e., componentwise multiplication.}$$

Give such a necessary and sufficient condition on m that $M_m : c_{00} \rightarrow c_{00}$ becomes a continuous linear operator with respect to the ℓ^2 norm.

- c) Under this condition, prove that M_m extends continuously and linearly to ℓ^2 , give a formula for this linear operator, and compute its norm.
- d) Give a necessary and sufficient condition on m so that M_m has a continuous inverse.
- e) Give a necessary and sufficient condition on m so that e^{tM_m} is defined analogously to Section 1.1.

5. Let $p \in [1, \infty)$ and consider the Banach space $L^p(\mathbb{R})$. Prove that the formula

$$(S(t)f)(s) := f(t + s) \quad \text{for } f \in L^p, s \in \mathbb{R}, t \geq 0$$

defines a strongly continuous semigroup on L^p . What happens for $p = \infty$?

6. Let $F_b(\mathbb{R})$ denote the linear space of all bounded $\mathbb{R} \rightarrow \mathbb{R}$ functions. Define

$$(S(t)f)(s) := f(t + s) \quad \text{for } f \in F_b(\mathbb{R}), s \in \mathbb{R}, t \geq 0.$$

Prove that S is a semigroup, i.e., satisfies Definition 1.5.a). Prove that each of the following spaces is a Banach space with the supremum norm $\|\cdot\|_\infty$ and invariant under $S(t)$ for all $t \geq 0$. Is S a strongly continuous semigroup on these spaces?

a) $F_b(\mathbb{R})$.

b) $C_b(\mathbb{R})$ = the space bounded and continuous functions.

c) $C_0(\mathbb{R})$ = the space bounded and continuous functions vanishing at infinity.

7. Determine the set of those $f \in BUC(\mathbb{R})$ for which $t \mapsto S(t)f$ is differentiable (S denotes the left shift semigroup).

8. Let S be the left shift semigroup on $BUC(\mathbb{R})$, and T be the heat semigroup from Section 1.1. Prove the following assertions:

a) $t \mapsto S(t)$ is nowhere continuous for the operator norm.

b) $t \mapsto T(t)$ is not continuous for the operator norm at 0.

c) $t \mapsto T(t)$ is continuous for the operator norm on $(0, \infty)$.

9. Explain why it is not possible to define the heat semigroup for negative time values.