Universität Tübingen
Mathematisches Institut
Prof. Dr. Christian Lubich

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1. Exercise Sheet to Numerical Methods for Quantum Dynamics

Exercise 1: Let $f \in C^p(\mathbb{R})$ for $p \geq 2$ be 2π-periodic. Show, under this condition, the following statements.

(a) The Fourier coefficients decay at least polynomially, namely it holds that

$$\left|\widehat{f}(n)\right| \leq \frac{1}{2\pi n^p} \int_0^{2\pi} \left|f^{(p)(t)}\right| dt.$$

(b) The discrete Fourier transformation $\widehat{f}_N(n)$ fulfills the following approximation result for $n \leq N/2$: There exists a constant $C_{p,f} > 0$, which only depends on p and f, such that

$$\left|\widehat{f}_N(n) - \widehat{f}(n)\right| \leq C_{p,f} N^{-p}.$$

Exercise 2: Let $f \in C^p(\mathbb{R})$ for $p \geq 2$ be 2π-periodic. Show that $I_N f$, the trigonometric interpolation of f, fulfills the following error bound

$$\sup_{t \in [0,2\pi]} |I_N f(t) - f(t)| \leq C N^{-p+1}.$$

The constant C may depend on p and f, but crucially not on N.

Programming Exercise 1: In the lecture, the following spatially discrete approximation to the Schrödinger equation in 1D has been introduced: Find $U(t) \in \mathbb{C}^N$ for all $t \in [0, T]$, such that

$$\begin{aligned} i\partial_t U(t) &= -\mathcal{F}_K^{-1} D_K^2 \mathcal{F}_K U(t) + V U(t), \\ U(0) &= U_0. \end{aligned}$$

Note that $\mathcal{F}_K$ denotes the discrete Fourier transform and $D_K = \operatorname{diag}(ik)_{k=-K/2}^{K/2-1}$.

The most basic time-stepping scheme is the explicit Euler, which locally uses the Taylor expansion

$$U(t+\tau) \approx U(t) + \tau \partial_t U(t) = U(t) - \tau i (i\partial_t U(t)).$$

Inserting the discrete Schrödinger equation on the right-hand side recursively yields the following fully discrete scheme: Find $U_n \in \mathbb{C}^N$ for all $n \leq N$, such that

$$\begin{aligned} U_{n+1} &= U_n + \tau i \mathcal{F}_K^{-1} D_K^2 \mathcal{F}_K U_n - \tau i V U_n, \\ U(0) &= U_0, \end{aligned}$$

where $\tau = T/N$. Consider $U_0 = e^{-10x^2+10ix}$, on the interval $[-\pi, \pi]$, with the potential $V(x) = 100(1-\cos(x))$. Implement this scheme, compute the solutions $(U_n)_{n=1}^N$ and plot the scaled euclidian norm of the solutions $\frac{1}{K}|U_n|$ for all $n \leq N$, for the following sets of parameters with $T = \frac{1}{5}$:

- $N = 1000$, $K = 16$;
- $N = 1000$, $K = 64$;
- $N = 10000$, $K = 64$.

Try to interpret the result. (If the result is unreasonable for all parameter sets, then there is an error in the implementation.) The use of libraries is generally permitted, but be wary of the conventions of the authors for the Fourier transformations.

Discussed in the exercise in S07, on wednesday the 2.11.2022 from 10.15–12.