Universität Tübingen
Mathematisches Institut
Prof. Dr. Christian Lubich

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2. Exercise Sheet to Numerical Methods for Quantum Dynamics

Programming Exercise 2: Oh no! A signal has been heavily polluted by (additive) noise. We provided the measurements on the website. Taken at the points **x_equid.csv**, the signal is saved in **noisy_signal.csv**. Can you reconstruct the original signal (which is suspected to be e^{-cx^2} for some constant $c > 0$)? You can assume that the original signal is smooth and 2π-periodic.

Hint: The function **np.genfromtext** reads .csv files into vectors. Use the discrete Fourier Transformation!

Programming Exercise 3: The following approximation to the Laplace operator in 1−D is derived from collocation

$$\Delta \approx \mathcal{F}_K^{-1} D_K^2 \mathcal{F}_K.$$

Implement this operator, by using library functions for the fft, for example in the form of the following functionality. The function **approx_lap**(v) takes a vector v, assumed to be evaluations of a 2π-periodic function at equidistant points, and returns a vector with approximations at those equidistant points. (Other reasonable functions are accepted, as long as the above functionality is implemented.)

Test your implementation with the test function $f(x) = e^{-10x^2}$ on the interval $[-\pi, \pi]$. Plot the errors (e.g. the maximum error in space), in a reasonable way, for several values of K. (Note that you can compute an exact solution easily by hand).

Programming Exercise 4: Consider the spatially discrete formulation of the free Schrödinger equation (i.e. $V = 0$)

$$i\partial_t U(t) = -\mathcal{F}_K^{-1} D_K^2 \mathcal{F}_K U(t),$$
$$U(0) = U_0.$$

We can directly realize the exact solution via

$$U(t) = e^{it\mathcal{F}_K^{-1} D_K^2 \mathcal{F}_K} U_0 = \mathcal{F}_K^{-1} e^{itD_K^2} \mathcal{F}_K U_0.$$

The matrix exponential on the right-hand side is easy to compute, since D_K is a diagonal matrix. Write a code that computes the solution on the time interval $[0, 0.2]$, for $U_0 = e^{-10x^2+10ix}$, on the space interval $[-\pi, \pi]$. Visualize the solution with $K = 128$ space points and $N = 100$ time points.

Programming Exercise 5: Implement the Strang splitting discussed in the lectures, for the Schrödinger equation in the setting of Programming exercise 1. Compute the solution with $K = 128$ and $N = 50$. Do you observe a qualitative difference to the explicit Euler? Make a time convergence plot with a reference solution through the following steps:

- Compute a reference solution with $K = 128$ and $N = 1024$;
- Compute the numerical solutions with $K = 128$ and $N = 8, 16, 32, 64, 128, 256$;
- Compute the maximal absolute differences of the solutions with the reference solution (at the final time T) and store them in a vector;
- Plot (double logarithmically through **loglog**), the error of the scheme against the different τ.

Try to interpret the result.

Discussed in the exercise in S08, on wednesday the 16.11.2022, from 10.15–12.