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Aspects of numerical time integration — Exercise Sheet 3 April 25, 2014

The purpose of this exercise sheet is to get used to the application of numerical methods for space discretization. Therefore we learn how to use the method of finite differences and spectral methods to compute spatial derivatives of a function $g : [a, b] \to \mathbb{R}$ numerically.

Let $N \in \mathbb{N}$, $h = \frac{b-a}{N}$, $x_j = jh$ and $g_j := g(x_j)$, $j = 0, \ldots, N$. Furthermore we assume g to be periodic such that $g(x_0) = g(x_N)$. Define $G := [g_0, \ldots, g_{N-1}]^T$.

Finite differences are based on central difference quotients derived by Taylor expansion of g such that

$$\begin{aligned} \frac{d}{dx} g(x_j) &\approx \frac{g_{j+1} - g_{j-1}}{2h} \\ \frac{d^2}{dx^2} g(x_j) &\approx \frac{g_{j+1} - 2g_j + g_{j-1}}{h^2}, \end{aligned} \qquad j = 0, \ldots, N-1. \tag{1}$$

Spectral methods make use of the discrete Fourier transform $\mathcal{F}_N$ such that for $j = 0, \ldots, N-1$ we can approximate the derivatives of g by

$$\begin{aligned} \frac{d}{dx} g(x_j) &\approx \left\{ \mathcal{F}_N^{-1} \left(iK * \mathcal{F}_N G \right) \right\}_j, & K &= \left[-\frac{N}{2} + 1, \ldots, \frac{N}{2} - 1, 0 \right]^T, \\ \frac{d^2}{dx^2} g(x_j) &\approx \left\{ \mathcal{F}_N^{-1} \left(-K^2 * \mathcal{F}_N G \right) \right\}_j, & K &= \left[-\frac{N}{2} + 1, \ldots, \frac{N}{2} - 1, \frac{N}{2} \right]^T, \end{aligned} \tag{2}$$

where $*$ is the pointwise product and K^2 has to be understood likewise.

Exercise 6: (numerical differentiation)

a) Consider g to be smooth.
Show the representation of the derivatives in (1) using Taylor expansion. What is the order of the error by this discretization?

b) write MATLAB functions `dx_fd(funvec,h)` and `dxx_fd(funvec,h)` respectively in order to compute the first and second derivative of g using **finite differences** (1).
The vector `funvec` contains the evaluations $f_0, \ldots, f_{N-1}$, the second argument h is the spatial step size

c) write MATLAB functions `dx_sp(funvec)` and `dxx_sp(funvec)` respectively in order to compute the first and second derivative of g using the **spectral method** (2).
(HINT: use the MATLAB command `fft()` and `ifft()` for $\mathcal{F}_N$ and $\mathcal{F}_N^{-1}$ respectively and note that in MATLAB the Fourier modes k are arranged in the order $0, \ldots, \frac{N}{2}, -\frac{N}{2} + 1, \ldots, -1$.)

Exercise 7: (differentiation examples)

Consider the function $f(x) = e^{\sin(x)}$ and the so called "hat"function $g(x) = \max(0, 1 - \frac{1}{2}|x - \pi|)$ with formal derivative $g'(x) = -(g(x) > 0) \cdot 0.5 \cdot sign(x - \pi)$ on the interval $[0, 2\pi]$. Set $N = 32$.

a) compute $\frac{d}{dx} f$ and $\frac{d^2}{dx^2} f$ analytically.

b) compute $\frac{d}{dx} f$ and $\frac{d^2}{dx^2} f$ numerically using the MATLAB functions of Exercise 6 b) and c). Plot the results.

c) For $N \in \{8, 16, 32\}$ compare the L^2 error of the finite difference method with the L^2 error of the spectral method.

d) compute $g'(x)$ numerically and compare the L^2 error of the finite difference method with the L^2 error of the spectral method.

e) plot the exact formal derivative $g'(x)$ using $\tilde{N} \gg N$ together with the numerical results for $N = 32$ in one figure.

Discussion in the exercises tuesday 3:45 pm, the 29.04.2014 in room K2 (Kronenstraße 32).