Weeks 12-14

Numerical methods for physicists, 2018/19 autumn semester

Numerical integration - `integral`

Problem 1. Calculate the Newton–Cotes coefficients $N_c^{4,k}$ and give an approximate value to the integral

$$\int_0^\pi \sin x \, \mathrm{d}x$$

with them. Use Matlab's `integral` command to calculate the integral.

Problem 2. Let us apply the composite Simpson's rule to estimate the integral of the previous problem. Let us verify the order of the convergence of the method using Matlab. How small should the length of the subintervals be to achieve an error less than 10^{-6}?

Problem 3. Let us construct the four-point Gauss-Chebyshev formula on the interval $[-1, 1]$! What is the order of the exactness of the method? Verify the result with Matlab. (The nodes are the zeros of the 4th degree Chebyshev polynomial and all weights are $\pi/4$.)

Problem 4. Let us apply the three-point Gauss–Legendre formula in a composite way to estimate the integral $\int_0^1 e^{-x^2} \, \mathrm{d}x$. What is the order of the convergence? Check it! (The third degree Legendre polynomial is $(5x^3 - 3x)/2$ and the weights are 5/9, 8/9, 5/9, respectively.)

Solution of initial value problems - `ode45, ode23s`

Problem 5. Solve the initial value problem $y' = \mathrm{arctg} y, y(0) = 1$ with the explicit Euler method on the interval $[0, 1]$. Give an estimate to the step size to guarantee an error below 10^{-4}. (The error formula is

$$\|\overline{\mathbf{e}}_k\| \leq e^{(x_{\max} - x_0)L} h(x_{\max} - x_0) M_2/2 \quad .)$$

Problem 6. Solve the initial value problem $y' = x^2(1 + y), y(0) = 3$ with the RK4 method. Verify the order of the convergence of the method. Repeat the investigation with the Heun method.

Problem 7. Consider the following problem of reaction kinetics on the interval [0,50], where we use the initial values 1,1,0, respectively. Solve the problem with Matlab's `ode45, ode23s` functions and with the implicit Euler method. Compare the results.

$$\begin{aligned}
c_1' &= -0.013c_1 - 1000c_1c_3 \\
c_2' &= -2500c_2c_3 \\
c_3' &= -0.013c_1 - 1000c_1c_3 - 2500c_2c_3
\end{aligned}$$

Problem 8. Construct the two-step BDF formula (BDF2). Investigate its stability, consistency and convergence. Verify its order of convergence on the initial value problem $y' = x^2(1 + y), y(0) = 3$ ($x \in [0, 1]$). Calculate the first step using the RK2 method.

PROBLEM 9. Construct the two-step Adams–Bashforth formula and perform similar analysis to that of the previous problem.

Solution of boundary value problems

PROBLEM 10. Using the shooting method, solve the boundary value problem $y'' = y + 4e^x, y(0) = 1, y(1/2) = 2e^{1/2}$! Solve the initial value problems with the Heun method, and apply the bisection method to solve the nonlinear equations. (Exact solution: $y(x) = (2x + 1)e^x$.)

PROBLEM 11. Solve the boundary value problem in the previous problem using the finite difference method.

HOMEWORK FOR WEEKS 12-14 - to be submitted until the next computer lab (The detailed solutions can be submitted either on A4 sheets of paper (printed or written) or in a pdf file (e.g. in an exported Matlab livescript) to rhorvath@math.bme.hu. Do not send Matlab files. Answer all questions with a sentence at the end of each problem.)

1. (2p) Solve Problem 2 again but with the composite midpoint rule.
2. (2p) Solve the equation of the damped harmonic oscillator with the RK4 method:

$$my'' + cy' + ky = 0, \quad x \in [0, 15],\ y(0) = 1(m),\ y'(0) = 0(m/s).$$

Let $m = 20kg$, $k = 20N/m$, $c = 5(40\ \mathit{and}\ 200)Ns/m$. Plot the solution for the three different c values.