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Computer Lab 2 supporting chapter 3

Numerical Solution of Initial Value Problems

Here IVPs are solved numerically and the following items are studied:

- accuracy and stability
- constant stepsize and adaptive (variable) stepsize
- stiff and non-stiff problems
- parameter study of the solutions of a system of ODEs

A) Accuracy of a Runge-Kutta method

In chapter 3 different Runge-Kutta methods are presented. Make a numerical experiment to find the order of accuracy of the following RK-method:

$$u_k = u_{k-1} + \frac{h}{6}(k_1 + k_2 + 4k_3), \quad t_k = t_{k-1} + h, \quad k = 1, 2, \ldots, N$$

$$k_1 = f(t_{k-1}, u_{k-1})$$

$$k_2 = f(t_{k-1} + h, u_{k-1} + hk_1)$$

$$k_3 = f(t_{k-1} + h/2, u_{k-1} + hk_1/4 + hk_2/4)$$

Implement the method on Van der Pol's differential equation

$$\frac{d^2y}{dt^2} + \epsilon(y^2 - 1)\frac{dy}{dt} + y = 0, \quad y(0) = 1, \frac{dy}{dt}(0) = 0, \quad \epsilon = 1, \quad t \in [0, 1]$$

Run the problem with constant stepsizes using $N =$ 10,20,40,80,160,320 steps in the t-interval $[0, 1]$. Estimate the error at $t = 1$ by computation of $e_N = y_N - y(1)$, $N = 10, 20, 40, 80, 160$. Since $y(1)$ is not known exactly, use the approximation $y(1) \approx y_{Nmax}$, where $Nmax = 320$. Make a *loglog*-plot of $|e_N|$ as a function of h, and estimate the order of accuracy from the graph.

Hint 1: Treat the problem as a system on *vector form*, both when you rewrite the second order differential equation to a system of two first order ODEs and when you program the method.

Hint 2: Be careful to take the correct number of steps to reach $t = 1$. If you get the answer $order = 1$, there is some mistake in your Matlab-code!

B) Stability investigation of a Runge-Kutta method

The stability of a numerical method for IVPs is important when we want to solve *stiff* problems. The following ODE-system modeling the kinetics of a set of three reactions, known as Robertson's problem, is studied here:

$$A \to B \quad (k_1) \qquad B + C \to A + C \quad (k_2) \qquad 2B \to B + C \quad (k_3)$$

In the reactions above k_1, k_2 and k_3 denote the *rate constants* of the three reactions. The following set of ODEs describe the evolution of (scaled) concentrations of A, B and C as a function of time t:

$$\frac{dx_1}{dt} = -k_1x_1 + k_2x_2x_3, \qquad x_1(0) = 1$$

$$\frac{dx_2}{dt} = k_1x_1 - k_2x_2x_3 - k_3x_2^2, \qquad x_2(0) = 0$$

$$\frac{dx_3}{dt} = k_3x_2^2, \qquad x_3(0) = 0$$

The rate constants have the values: $k_1 = 0.04, k_2 = 10^4, k_3 = 3 \cdot 10^7$.

B1) Constant stepsize experiment

If Robertson's problem is solved with an explicit method the stepsize has to be very small to avoid numerical instability. Use the Runge-Kutta method given in A) on Robertson's problem when the t-interval is $[0, 1]$. Run the problem with constant stepsizes corresponding to $N = 125, 250, 500, 1000, 2000$ steps and find the smallest number of steps (from the 5 given) needed to obtain a stable solution. Plot the solution trajectory in a *loglog*-diagram for the solution computed with the smallest step.

B2) Adaptive stepsize experiment using Matlab functions

There are several IVP-solvers in Matlab. Use the command `>>help funfun` to see which are available. To get more information about one of them, say `ode23`, give the command `>>help ode23`. In order to control e.g. accuracy parameters you also need to read about the function `odeset`. When the problem is stiff you need a stiff IVP-solver, e.g. `ode23s`.

There are several ways to find demo examples in Matlab. If you give the command `>>demo` and follow the path MATLAB, Numerics, Differential Equations, you find a number of examples to look at, e.g. `vdpode` and `rigidode`. You can run the demo programs and see the graphical output and you can also see the Matlab code.

Make the following numerical experiments on Robertson's problem:

- Use the non-stiff IVP-solver `ode23` on the t-interval $[0, 1]$ for different relative tolerances: $RelTol = 10^{-3}, 10^{-4}, 10^{-5}, 10^{-6}$ and record the number of steps taken by `ode23`. Make a graph of the stepsize h as function of t for one of the tolerances.

- Run the stiff IVP-solver `ode23s` on the t-interval $[0, 1000]$ for the same relative tolerances as above and record the number of steps taken by `ode23s`. Make a graph of the stepsize h as function of t for one of the tolerances.

C) Parameter study of solutions of an ODE-system

Make a parameter study for the following problems taken from applications. Choose a method (order of accuracy must be at least two) yourself. Present the result graphically in a suitable way. Think about the following possibilities and choose what you think is best:

- one or several graphs (using `subplot`) in the figure window?
- linear or logarithmic scales?
- in the graphs: `title`, `x-label`, `y-label`

Problem 1: Particle flow past a cylinder

A long cylinder with radius $R = 2$ is placed in an incompressible fluid streaming in the direction of the positive x-axis. The axis of the cylinder is perpendicular to the direction of the flow. The position $(x(t), y(t))$ of a flow particle at time t is determined by the start position $(x(0), y(0))$ and the ODE-system:

$$\frac{dx}{dt} = 1 - \frac{R^2(x^2 - y^2)}{(x^2 + y^2)^2}, \quad \frac{dy}{dt} = -\frac{2xyR^2}{(x^2 + y^2)^2}$$

At $t = 0$ there are four flow particles at $x = -4$ with the y-positions $0.2, 0.6, 1.0$ and 1.6. Compute and make a graph of the flow curves of the particles in the t-interval $[0, 10]$. Use `axis equal` in the graph!

Problem 2: Motion of a particle

A particle is thrown from the position $(0, 1.5)$ with an elevation angle α and the velocity $v_0 = 20$. The trajectory of the particle depends on α, the air resistance coefficient k and the ODE-system

$$\frac{d^2x}{dt^2} = -k\frac{dx}{dt}\sqrt{(\frac{dx}{dt})^2 + (\frac{dy}{dt})^2}, \quad x(0) = 0, \quad \frac{dx}{dt}(0) = 20\cos(\alpha)$$

$$\frac{d^2y}{dt^2} = -9.81 - k\,|\frac{dy}{dt}|\sqrt{(\frac{dx}{dt})^2 + (\frac{dy}{dt})^2}, \quad y(0) = 1.5, \quad \frac{dy}{dt}(0) = 20\sin(\alpha)$$

For two different values of k, say $k = 0.020$ and $k = 0.065$, plot the solution trajectories for $\alpha = 30, 45$ and 60 (degrees). For the graphical presentation, observe that the model is valid only until the particle touches the ground, i.e. it is valid only while $y \geq 0$. The graph should show the motion in a xy-coordinate system with t as a parameter.