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Numerical Analysis and Simulation I: Ordinary Differential Equations (ODEs)

Sheet 9 - DAEs and Geometric Integrators

Return of the Exercise Sheet: Tuesday, January 6th before the lecture

Exercise 19: *Störmer/Verlet (= Leapfrog)*
Mechanical problems often yield systems of second order

$$y''(x) = f(x, y), \quad y(x_0) = y_0,\ y'(x_0) = u_0$$

where two initial conditions are imposed (usually position and velocity). A straightforward discretisation is the symmetric difference quotient: given the time points $x_j = x_0 + j \cdot h$ and $y_j \doteq y(x_j)$, we have

$$\frac{y_{i-1} - 2y_i + y_{i+1}}{h^2} \qquad (\star)$$

as an approximation of the second derivative. A numerical scheme is obtained by demanding formula $(\star)$ to be equal to $y''(x_j) = f(x_j, y_j)$ (where the choice of index j is discussed in part (a) below).

Remark: For $f \equiv 0$, the recursion defined by the aforementioned approach reads

$$y_{i+1} - 2y_i + y_{i-1} = 0.$$

The corresponding characteristic polynomial exhibits the double root $\lambda = 1$. Hence, this method is unstable in view of Dahlquist's criterion. However, errors are amplified only linearly. Moreover, the scheme is often applied for boundary value problems, where these stability difficulties do not occur. The stability of the according methods is not investigated in this exercise.

a) Let the index j be equal to i, i.e. $i = j$. The resulting method does not include the velocity $u = y'$. Usually, the following numerical scheme for the overall system is used:

$$\begin{aligned} y_1 &= y_0 + h\big(u_0 + \frac{h}{2} f(t_0, y_0)\big) && \text{(start step)} \\ y_{k+1} &= 2y_k - y_{k-1} + h^2 f(x_k, y_k), && (k = 1, \ldots, l-1) \\ u_l &= \frac{y_l - y_{l-1}}{h} + \frac{h}{2} f(x_l, y_l) && \text{(final step).} \end{aligned}$$

(This scheme is very popular and often called Störmer-discretisation, or in physics Leapfrog method, or especially in molecular dynamics Verlet-discretisation.)

Of which consistency order is the approximation y_1 for the solution in the start-up step and the velocity approximation u_l in the final step?

b) The best choice for the index j is i, i.e. $(\star)$ is an approximation for $f(x_i, y_i)$. In order to understand that assignment, compute the local error of the numerical scheme for $f(x_j, y_j)$ with arbitrary j. To this end, plug the exact solutions $y(x_{i-1})$, $y(x_i)$, $y(x_{i+1})$ into formula $(\star)$ and perform the Taylor expansion up to rest terms $\mathcal{O}(h^4)$ at an unspecified point x_j. Determine the order of consistency w.r.t. $y''(x_j)$.

Exercise 20: *Mathematical Pendulum*
The DAE model of the mathematical pendulum reads (see also script)

$$\xi' = u, \quad \eta' = v, \quad u' = -\tfrac{2}{m}\lambda\xi, \quad v' = -\tfrac{2}{m}\lambda\eta - g, \quad 0 = \xi^2 + \eta^2 - l^2$$

with the unknown functions ξ, η, u, v, λ and constants $g, l, m > 0$.
Show that this system can be written in the semi-explicit form according to exercise 18.

Hint: The semi-explicit system will have the form

$$\begin{aligned} y_1' &= F(y_1, y_2, z) \\ y_2' &= G(y_1, y_2) \\ 0 &= H(y_2). \end{aligned}$$

Homework 17: *Mathematical Pendulum as Hessenberg System* (10 Points)
A Hessenberg system of (differential) index 3 is a semi-explicit system of DAEs

$$\begin{aligned} y_1' &= F(y_1, y_2, z) \\ y_2' &= G(y_1, y_2) \\ 0 &= H(y_2) \end{aligned}$$

with $y_1 \in \mathbb{R}^{n_1}, y_2 \in \mathbb{R}^{n_2}, z \in \mathbb{R}^{n_3}$ and $F \in \mathbb{R}^{n_1}, G \in \mathbb{R}^{n_2}, H \in \mathbb{R}^{n_3}$, where the matrix $\frac{\partial H}{\partial y_2}\frac{\partial G}{\partial y_1}\frac{\partial F}{\partial z} \in \mathbb{R}^{n_3 \times n_3}$ is regular, i.e. non-singular.
Show that the DAE model of the mathematical pendulum

$$\xi' = u, \quad \eta' = v, \quad u' = -\tfrac{2}{m}\lambda\xi, \quad v' = -\tfrac{2}{m}\lambda\eta - g, \quad 0 = \xi^2 + \eta^2 - l^2$$

with unknowns ξ, η, u, v, λ and constants $g, l, m > 0$ is a Hessenberg system of index 3.

Homework 18: *Geometric Integrators: First Integral* (10 Points)
A non-constant function $I(y)$ is called first integral or invariant of a differential equation $y' = f(y)$ if

$$\frac{d}{dx} I(y) = I'(y) f(y) = 0 \, .$$

Show the following statements for the Lotka-Volterra problem and the pendulum equation:

a) The Lotka-Volterra problem

$$\begin{aligned} u' &= u(v-2) \\ v' &= v(1-u) \end{aligned}$$

has the first integral of $I(u, v) = \ln u - u + 2\ln v - v$.

b) The pendulum equation

$$\begin{aligned} p' &= -\sin q \\ q' &= p \end{aligned}$$

has the invariant $H(p, q) = p^2/2 - \cos q$.