

Geometric Numerical Integration, Serie 5

19.6.2012

Exercise 14: Prove the following theorem from the lecture.

Let U and V be open subsets of \mathbb{R}^{2d} and $\psi : U \rightarrow V$ a diffeomorphism. If ψ is symplectic, then the Hamiltonian system

$$\dot{y} = J^{-1} \nabla_y H(y)$$

transforms to

$$\dot{z} = J^{-1} \nabla_z K(z)$$

where $K(z) = H(y)$ with respect to the coordinate transform $z = \psi(y)$.

Exercise 15:

Show, that the symplectic Euler method applied to a Hamiltonian system

$$\begin{aligned} p_{n+1} &= p_n - hH_q(p_{n+1}, q_n) \\ q_{n+1} &= q_n + hH_p(p_{n+1}, q_n) \end{aligned}$$

is symplectic. Make use only of the definition of symplecticity and proceed as follows:

- (a) Consider the numerical flow $\Phi_h(p_n, q_n) = (p_{n+1}, q_{n+1})$ and compute the derivative with respect to (p_n, q_n) . Show that

$$\begin{pmatrix} I + hH_{qp} & 0 \\ -hH_{pp} & I \end{pmatrix} \Phi'(p_n, q_n) = \begin{pmatrix} I & -hH_{qq} \\ 0 & I + hH_{pq} \end{pmatrix}$$

holds, where

$$\Phi'(p_n, q_n) = \begin{pmatrix} \partial_{p_n} p_{n+1} & \partial_{q_n} p_{n+1} \\ \partial_{p_n} q_{n+1} & \partial_{q_n} q_{n+1} \end{pmatrix}.$$

- (b) Now check the symplecticity condition

$$\Phi'(p_n, q_n)^T J \Phi'(p_n, q_n) = J$$

using the representation of $\Phi'(p_n, q_n)$ from the previous part.

Note, that for the second version of the symplectic Euler method

$$\begin{aligned} p_{n+1} &= p_n - hH_q(p_n, q_{n+1}) \\ q_{n+1} &= q_n + hH_p(p_n, q_{n+1}) \end{aligned}$$

the proof works analogously.

Exercise 16:

Prove, that the Störmer-Verlet methods applied to a Hamiltonian system

$$\Phi_h^{SV1} := \begin{cases} p_{n+1/2} &= p_n - \frac{h}{2} H_q(p_{n+1/2}, q_n) \\ q_{n+1} &= q_n + \frac{h}{2} (H_p(p_{n+1/2}, q_n) + H_p(p_{n+1/2}, q_{n+1})) \\ p_{n+1} &= p_{n+1/2} - \frac{h}{2} H_q(p_{n+1/2}, q_{n+1}) \end{cases}$$

$$\Phi_h^{SV2} := \begin{cases} q_{n+1/2} &= q_n + \frac{h}{2} H_p(p_n, q_{n+1/2}) \\ p_{n+1} &= p_n - \frac{h}{2} (H_q(p_n, q_{n+1/2}) + H_q(p_n, q_{n+1/2})) \\ q_{n+1} &= q_{n+1/2} + \frac{h}{2} H_p(p_{n+1}, q_{n+1/2}) \end{cases}$$

are symplectic. Prove this only for Φ_h^{SV1} and proceed as follows:

- (a) The composition of symplectic methods is again symplectic.
- (b) The Störmer-Verlet methods are compositions of the symplectic Euler methods with their adjoint methods;

$$\begin{aligned}\Phi_h^{SV1} &= (\Phi_{h/2}^{SE1})^* \circ \Phi_{h/2}^{SE1} = \Phi_{h/2}^{SE2} \circ \Phi_{h/2}^{SE1} \\ \Phi_h^{SV2} &= (\Phi_{h/2}^{SE2})^* \circ \Phi_{h/2}^{SE2} = \Phi_{h/2}^{SE1} \circ \Phi_{h/2}^{SE2}\end{aligned}$$

where

$$\Phi_h^{SE1} := \begin{cases} p_{n+1} &= p_n - hH_q(p_{n+1}, q_n) \\ q_{n+1} &= q_n + hH_p(p_{n+1}, q_n) \end{cases} \quad \text{and} \quad \Phi_h^{SE2} := \begin{cases} p_{n+1} &= p_n - hH_q(p_n, q_{n+1}) \\ q_{n+1} &= q_n + hH_p(p_n, q_{n+1}) \end{cases}.$$

Exercise 17:

Let Φ_h be the numerical flow for a given numerical scheme applied to the differential equation

$$y'(t) = f(y(t)). \tag{*^1}$$

This yields the modified equation

$$\tilde{y}'(t) = f(\tilde{y}(t)) + hf_2(\tilde{y}(t)) + h^2f_3(\tilde{y}(t)) + \dots, \tag{*^2}$$

such that the numerical solution of (*¹) computed with the numerical scheme described by Φ_h coincides with the exact solution of the modified equation (*²).

- (a) Compute the modified equation for the adjoint method $\Phi_h^* = \Phi_{-h}^{-1}$.
- (b) Using the first part, compute the modified equation for a symmetric method, where $\Phi_h^* = \Phi_h$.

Programming Exercise 6: Consider the differential equation

$$y'(t) = y^2(t), \quad y(0) = 1$$

for $t < 1$.

- (a) Compute the exact solution of the equation.
- (b) Consider the explicit Euler method for the numerical approximation of the solution of the above problem. Compute the modified equation for this problem up to order h^2 and h^3 .

Hint: The modified equation reads

$$\tilde{y}' = \tilde{y}^2 - h\tilde{y}^3 + h^2\frac{3}{2}\tilde{y}^4 - h^3\frac{8}{3}\tilde{y}^5 + \dots$$

- (c) Compute the numerical solution of the original problem with the explicit Euler method and time step size $h = 0.04$.
- (d) For $h = 0.04$ compute the exact solution of the truncated modified equations. For this, use the Matlab solver ode45 with a high precision.
- (e) Plot the exact solution of the original problem, the solution computed with the explicit Euler method and all exact solutions of the modified equation.

Discussion in the exercise class on 28.6.2012.