Problem 12.1 Order of Leapfrog Method

Show that, Symplectic Euler method defined as (5.3) in lecture notes is a first order method, and Leapfrog method defined as (5.6) is a second order method.

**HINT:** When proving result for Leapfrog method, using result of symplectic euler could be helpful. Moreover you may need the result that the order of trapezoidal method is 2.

**Solution:**

First study the order of symplectic euler method. The element corresponding to $p^{k+1}$ in truncation error vector is

$$T_{eul}^p(\Delta t) := \frac{1}{\Delta t} [p(t_{k+1}) - p(t_k) + \Delta t \frac{\partial H}{\partial q}(p(t_{k+1}), q(t_k))].$$

So

$$\Delta t T_{eul}^p(\Delta t) = \int_{t_k}^{t_{k+1}} - \frac{\partial H}{\partial q}(p(t), q(t)) + \frac{\partial H}{\partial q}(p(t_{k+1}), q(t_k))dt$$

$$= \int_{t_k}^{t_{k+1}} \frac{\partial^2 H}{\partial q \partial p}(p(t_{k+1}), q(t_k))(p(t_{k+1}) - p(t)) + \frac{\partial^2 H}{\partial p^2}(p(t_{k+1}), q(t_k))(q(t_k) - q(t)) + O(\Delta t^2) dt$$

$$= \int_{t_k}^{t_{k+1}} - \frac{\partial^2 H}{\partial q \partial p}(p(t_{k+1}), q(t_k))(t - t_{k+1}) \frac{\partial H}{\partial q}(p(t_{k+1}), q(t_{k+1}))$$

$$+ \frac{\partial^2 H}{\partial q^2}(p(t_{k+1}), q(t_k))(t_{k+1} - t_k) \frac{\partial H}{\partial p}(p(t_k), q(t_k)) + O(\Delta t^2) dt$$

$$= \frac{\partial^2 H}{\partial q \partial p}(p(t_{k+1}), q(t_k)) \frac{\partial H}{\partial q}(p(t_{k+1}), q(t_{k+1})) \frac{\Delta t^2}{2}$$

$$+ \frac{\partial^2 H}{\partial q^2}(p(t_{k+1}), q(t_k)) \frac{\partial H}{\partial p}(p(t_k), q(t_k)) \frac{\Delta t^2}{2} + O(\Delta t^3),$$

this proves that symplectic euler method is of order 1.

The Leapfrog method could be rewritten as:

$$\begin{align*}
p^{k+1} &= p^k - \frac{\Delta t}{2} \left( \frac{\partial H}{\partial q}(p^{k+1/2}, q^{k+1}) + \frac{\partial H}{\partial q}(p^{k+1/2}, q^k) \right) \\
q^{k+1} &= q^k + \frac{\Delta t}{2} \left( \frac{\partial H}{\partial p}(p^{k+1/2}, q^{k+1}) + \frac{\partial H}{\partial p}(p^{k+1/2}, q^k) \right)
\end{align*}$$
The truncation error of element $p^k$ is defined to be
\[ T_p := \frac{1}{\Delta t} [p(t_{k+1}) - p(t_k) + \frac{\Delta t}{2} \left( \frac{\partial H}{\partial q} (\tilde{p}^{k+1/2}, q(t_{k+1})) + \frac{\partial H}{\partial q} (\tilde{p}^{k+1/2}, q(t_k)) \right) ] \]
and actually by the result of symplectic euler method, we learn that
\[ p(t_k + \Delta t/2) - \tilde{p}^{k+1/2} := p(t_k + \Delta t/2) - p(t_k) + \frac{\Delta t}{2} \frac{\partial H}{\partial q} (p(t_k + \frac{1}{2} \Delta t), q(t_k)) = O(\Delta t). \]

So
\[ \Delta t T_p = p(t_{k+1}) - p(t_k) + \frac{\Delta t}{2} \left( \frac{\partial H}{\partial q} (\tilde{p}^{k+1/2}, q(t_{k+1})) + \frac{\partial H}{\partial q} (\tilde{p}^{k+1/2}, q(t_k)) \right) \]
\[ = \int_{t_k}^{t_{k+1}} - \frac{\partial H}{\partial q} (p(t), q(t)) + \frac{1}{2} \left( \frac{\partial^2 H}{\partial q^2} (\tilde{p}^{k+1/2}, q(t_{k+1})) - \frac{\partial^2 H}{\partial q^2} (\tilde{p}^{k+1/2}, q(t_k)) + \frac{\partial^2 H}{\partial q^2} (q(t_{k+1}) - q(t)) \right) \]
\[ + \frac{\partial^2 H}{\partial q \partial p} (\tilde{p}^{k+1/2} - p(t)) + \frac{\partial^2 H}{\partial q^2} (q(t_k) - q(t)) \]dt + $O(\Delta t^3)
\[ = \int_{t_k}^{t_{k+1}} \frac{\partial^2 H}{\partial q \partial p} (p^{k+1/2} - p(t)) dt + \frac{1}{2} \int_{t_k}^{t_{k+1}} \frac{\partial^2 H}{\partial q^2} (q(t_{k+1}) + q(t_k) - 2q(t)) dt + O(\Delta t^3) \]
\[ = O(\Delta t^3), \]
and the last equality holds because $p^{k+1/2} - p(t) = O(\Delta t^2)$ and trapezoidal method is order 2. By the same method, we could prove that $T_q = O(\Delta t^2)$, and hence Leapfrog method is of order 2.

**Problem 12.2  Adjoint of numerical flow**

Consider the differential equation
\[ \frac{dx}{dt} = f(x), \quad x(0) = x_0. \]

We assume that $f$ is Lipschitz continuous. Consider the flow of the differential equation
\[ \Phi_t(x_0) = x(t). \]

(12.2a) Show that
\[ \Phi_t \circ \Phi_s(x_0) = \Phi_{t+s}(x_0), \quad \text{for all } t, s \in \mathbb{R} \]
and hence
\[ \Phi_t \circ \Phi_{-t} = I \quad \text{for all } t. \]

**Solution:** Consider
\[ \frac{d\tilde{x}}{dt} = f(\tilde{x}), \quad \tilde{x}(0) = x(s). \]
Then we have $\Phi_t \circ \Phi_s(x_0) = \Phi_t(x(s)) = \tilde{x}(t)$. Note that $x_{\cdot + s}$ satisfies the same equation for $\tilde{x}$. By the uniqueness of the solution (which follows from Cauchy-Lipschitz Theorem and the Lipschitz condition of $f$), we have $x(t+s) = \tilde{x}(t)$. Therefore, $\Phi_t \circ \Phi_s(x_0) = x(t+s) = \Phi_{t+s}(x_0)$. 

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(12.2b) Given a numerical method

\[ x^{k+1} = \Phi_{\Delta t}(x^k), \]

where \( \Delta t \) is the step size, its adjoint \( x^{k+1} = \Phi^*_{\Delta t}(x^k) \) is defined by

\[ x^k = \Phi_{-\Delta t}(x^{k+1}), \]
or equivalently

\[ x^{k+1} = \Phi^{-1}_{-\Delta t}(x^k). \]

We say that a numerical method is symmetric if it satisfies \( \Phi_{\Delta t} \circ \Phi_{-\Delta t} = I \). Show that

(i) \( \Phi_{\Delta t} \) symmetric \iff \( \Phi_{\Delta t} = \Phi^*_{\Delta t} \).
(ii) \( (\Phi^*_{\Delta t})^* = \Phi_{\Delta t} \).
(iii) \( (\Phi_{\Delta t} \circ \Psi_{\Delta t})^* = \Psi^*_{\Delta t} \circ \Phi^*_{\Delta t} \) for any one step methods \( \Psi_{\Delta t} \) and \( \Phi_{\Delta t} \).

Solution: (i) [\( \Phi_{\Delta t} \) is symmetric] \iff [\( \Phi^{-1}_{-\Delta t} = \Phi_{\Delta t} \)] \iff [\( \Phi^*_{\Delta t}(x^k) = \Phi^{-1}_{-\Delta t}(x^k) = \Phi(x^k) \)]
\iff [\( \Phi_{\Delta t} = \Phi^*_{\Delta t} \)].
(ii) \( (\Phi^*_{\Delta t})^* = (\Phi^{-1}_{-\Delta t})^* = (\Phi^{-1}_{-\Delta t})^{-1} = \Phi_{\Delta t} \).
(iii) \( (\Phi_{\Delta t} \circ \Psi_{\Delta t})^* = (\Phi_{-\Delta t} \circ \Psi_{-\Delta t})^{-1} = \Psi^{-1}_{\Delta t} \circ \Phi_{-\Delta t} = \Psi^*_{\Delta t} \circ \Phi^*_{\Delta t} \).

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