NIDS Session 9

$\boxed{1}$ We have a Hamiltonian system:

$$\dot{p}(t) = -\frac{\partial H}{\partial q}(p(t), q(t))$$

$$\dot{q}(t) = \frac{\partial H}{\partial p}(p(t), q(t))$$

Recall the Symplectic Euler method:

$$p_1 = p_0 - h\frac{\partial H}{\partial q}(p_1, q_0)$$

$$q_1 = q_0 + h\frac{\partial H}{\partial p}(p_1, q_0)$$

We must verify that $\frac{\partial \varphi_h}{\partial y_0}(y_0)^T J \frac{\partial \varphi_h}{\partial y_0} = J$

$$= \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

$$\varphi_h(y_0) = \begin{pmatrix} p_1 \\ q_1 \end{pmatrix}$$

$$\frac{\partial \varphi_h}{\partial y_0}(y_0) = \begin{pmatrix} \frac{\partial p_1}{\partial p_0} & \frac{\partial p_1}{\partial q_0} \\ \frac{\partial q_1}{\partial p_0} & \frac{\partial q_1}{\partial q_0} \end{pmatrix}$$

(1) $$\frac{\partial p_1}{\partial p_0} = I - h\frac{\partial^2 H}{\partial p \partial q}(p_1, q_0)\frac{\partial p_1}{\partial p_0}$$

(2) $$\frac{\partial q_1}{\partial p_0} = h\frac{\partial^2 H}{\partial^2 p}(p_1, q_0)\frac{\partial p_1}{\partial p_0}$$

(3) $$\frac{\partial p_1}{\partial q_0} = -h\frac{\partial^2 H}{\partial^2 q}(p_1, q_0) - h\frac{\partial^2 H}{\partial p \partial q}(p_1, q_0)\frac{\partial p_1}{\partial q_0}$$

$$(4) \quad \frac{\partial q_1}{\partial q_0} = I + h \frac{\partial^2 H}{\partial q \partial p}(p_1, q_0) + h \frac{\partial^3 H}{\partial^2 p}(p_1, q_0) \frac{\partial p_1}{\partial q_0}$$

To simplify notations, denote $\frac{\partial^2 H}{\partial p \partial q}(p_1, q_0)$ as $\frac{\partial^2 H}{\partial p \partial q}$

(and similarly for the others)

Rewrite (2) as

$$\left(I + h \frac{\partial^2 H}{\partial p \partial q} \right) \frac{\partial p_1}{\partial p_0} = I$$

Rewrite (3) as

$$\left(I + h \frac{\partial^2 H}{\partial p \partial q} \right) \frac{\partial p_1}{\partial q_0} = -h \frac{\partial^2 H}{\partial q^2}$$

Additionally, observe that since H is smooth (at least C^2) $(\nabla^2 H = \nabla^2 H^T)$

$$\frac{\partial^2 H}{\partial p^2} = \frac{\partial^2 H}{\partial p^2}^T \qquad \frac{\partial^2 H}{\partial p \partial q} = \frac{\partial^2 H}{\partial q \partial p}^T$$

$$\frac{\partial^2 H}{\partial q^2} = \frac{\partial^2 H}{\partial q^2}^T$$

$$\frac{\partial \varphi_h(q_0)}{\partial q_0}^T J \frac{\partial \varphi_h(q_0)}{\partial q_0} = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}$$

For the (1,1) block

$$C_{11} = \frac{\partial p_1}{\partial p_0}^T \frac{\partial q_1}{\partial p_0} - \frac{\partial q_1}{\partial p_0}^T \frac{\partial p_1}{\partial p_0}$$

$$= h \frac{\partial p_1}{\partial p_0}^T \frac{\partial^2 H}{\partial p^2} \frac{\partial p_1}{\partial p_0} - h \frac{\partial p_1}{\partial p_0}^T \frac{\partial^2 H}{\partial p^2}^T \frac{\partial p_1}{\partial p_0}$$

$$= 0$$

For the (2,1) block

$$C_{21} = \frac{\partial p_1}{\partial q_0}^T \frac{\partial q_1}{\partial p_0} - \frac{\partial q_1}{\partial q_0}^T \frac{\partial p_1}{\partial p_0}$$

$$= h \frac{\partial p_1}{\partial q_0}^T \frac{\partial^2 H}{\partial p^2} \frac{\partial p_1}{\partial p_0} - \left(I + \frac{h \partial^2 H}{\partial q \partial p} + h \frac{\partial^2 H}{\partial p^2} \frac{\partial p_1}{\partial q_0} \right)^T \frac{\partial p_1}{\partial p_0}$$

$$= - \left(I + \frac{h \partial^2 H}{\partial q \partial p} \right)^T \frac{\partial p_1}{\partial p_0} = - I$$

For the (1,2) block:

$$C_{12} = \frac{\partial p_1}{\partial p_0}^T \frac{\partial q_1}{\partial q_0} - \frac{\partial q_1}{\partial p_0}^T \frac{\partial p_1}{\partial q_0}$$

$$= \frac{\partial p_1}{\partial p_0}^T \left(I + \frac{h \partial^2 H}{\partial q \partial p} + h \frac{\partial^2 H}{\partial p^2} \frac{\partial p_1}{\partial q_0} \right) - h \frac{\partial p_1}{\partial p_0}^T \frac{\partial^2 H}{\partial p^2} \frac{\partial p_1}{\partial q_0}$$

$$= \left(\left(I + h \frac{\partial^2 H}{\partial p \partial q} \right) \frac{\partial p_1}{\partial p_0} \right)^T = I$$

For the (2, 2) block

$$C_{22} = \frac{\partial p_1}{\partial q_0}^T \frac{\partial q_1}{\partial q_0} - \frac{\partial q_1}{\partial q_0}^T \frac{\partial p_1}{\partial q_0}$$

$$= \frac{\partial p_1}{\partial q_0}^T \left(I + h \frac{\partial^2 H}{\partial q \partial p} + h \frac{\partial^2 H}{\partial p^2} \frac{\partial p_1}{\partial q_0} \right)$$

$$- \left(I + h \frac{\partial^2 H}{\partial q \partial p} + h \frac{\partial^2 H}{\partial p^2} \frac{\partial p_1}{\partial q_0} \right)^T \frac{\partial p_1}{\partial q_0}$$

$$= \underbrace{\left(\left(I + h \frac{\partial^2 H}{\partial q \partial p} \right) \frac{\partial p_1}{\partial q_0} \right)^T}_{= -h \frac{\partial^2 H}{\partial q^2}} - \left(I + h \frac{\partial^2 H}{\partial q \partial p} \right) \frac{\partial p_1}{\partial q_0}$$

$$= 0$$

Then $\frac{\partial \varphi_h}{\partial y_0}(y_0)^T J \frac{\partial \varphi_h}{\partial y_0}(y_0) = J$

and the symplectic Euler method is indeed symplectic!

2 We consider again a Hamiltonian system

$$(1)\begin{cases} \dot{p}_i(t) = -\dfrac{\partial H}{\partial q_i}(p(t), q(t)) \\ \dot{q}_i(t) = \dfrac{\partial H}{\partial p_i}(p(t), q(t)) \end{cases}$$

with $H(p,q) = p - \int_0^q g(t)\,dt$ with $g(t)$ a polynomial

We are given a RK method $\{a_{ij}, b_i\}$ with $\sum_i b_i = 1$

Applying this method to (1)

$$\begin{pmatrix} k_i^p \\ k_i^q \end{pmatrix} = \begin{pmatrix} g(q_0 + h\sum_j a_{ij} k_j^q) \\ 1 \end{pmatrix} = \begin{pmatrix} g(q_0 + h\sum_j a_{ij}) \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} p_1 \\ q_1 \end{pmatrix} = \begin{pmatrix} p_0 + h\sum_i b_i k_i^p \\ q_0 + h\underbrace{\sum_i b_i k_i^q}_{=\sum_i b_i = 1} \end{pmatrix} = \begin{pmatrix} p_0 + h\sum b_i g(q_0 + h\sum_j a_{ij}) \\ q_0 + h \end{pmatrix}$$

$$H(p_1, q_1) - H(p_0, q_0)$$

$$= p_1 - p_0 - \int_{q_0}^{q_1} g(t)\,dt$$

$$= h\sum_i b_i g(q_0 + h\sum_j a_{ij}) - \int_{q_0}^{q_0+h} g(t)\,dt$$

$$= h\sum_i b_i g(q_0 + hc_i) - h\int_0^1 g(q_0 + \theta h)\,d\theta$$

when $c_i = \sum_j a_{ij}$

the best we can do is using a Gauss method of order $2s$

(degree of exactness $2s-1$)

Consequently for any polynomial of degree $k > 2s-1$,

the Hamiltonian is not preserved

ii) We know that the fixed point equation

$x = F(x)$ has a unique solution if F is a

contraction (i.e. $\|F(x) - F(y)\| \leq c\|x - y\|$ $c < 1$)

(Banach's fixed point theorem)

We have in our case $F(x) = y_n + h\int_0^1 f(\theta x + (1-\theta) y_n) d\theta$

We compute

$$\|F(x) - F(y)\| = h\left\| \int_0^1 f(\theta x + (1-\theta) y_n) - f(\theta y + (1-\theta) y_n) d\theta \right\|$$

$$\leq hL \int \theta \|x - y\| d\theta$$

$$= hL\|x - y\| \int \theta \, d\theta$$

$$= \frac{hL}{2} \|x - y\|$$

F is a contraction if $\frac{hL}{2} < 1$ (i.e. $h < \frac{2}{L}$)

for h small enough, the average vector field (AVF) method is well-posed.

(iii) Clearly $\int_0^1 \frac{d}{d\theta}\left(H(\theta y_{n+1} + (1-\theta)y_n)\right) d\theta$

$$= H(\theta y_{n+1} + (1-\theta)y_n)\Big|_0^1$$

$$= H(y_{n+1}) - H(y_n)$$

Moreover $\int_0^1 \frac{d}{d\theta}\left(H(\theta y_{n+1} + (1-\theta)y_n)\right) d\theta$

$$= \int_0^1 \nabla H(\theta y_{n+1} + (1-\theta)y_n) \cdot (y_{n+1} - y_n)\, d\theta$$

$$(1) = h^{-1} J \int_0^1 h J^{-1} \nabla H(\theta y_{n+1} + (1-\theta)y_n) \cdot (y_{n+1} - y_n)\, d\theta$$

Recall that $f(y) = J^{-1}\nabla H(y)$

Thus $(1) = h^{-1} J \int_0^1 h f(\theta y_{n+1} + (1-\theta)y_n) \cdot (y_{n+1} - y_n)\, d\theta$

Recall from ii) $h\int_0^1 f(\theta y_{n+1} + (1-\theta)y_n)\, d\theta = y_{n+1} - y_n$

Hence (9) becomes

$$h^{-1} J(y_{n+1} - y_n) \cdot \underbrace{(y_{n+1} - y_n)}_{B} = h^{-1} B^T J B$$

Since J is skew-symmetric,

$$B^T J B = \frac{1}{2}\left(B^T J B + (B^T J B)^T \right)$$

$$= \frac{1}{2}\left(B^T J B - B^T J B \right) = 0 \quad \forall B \in \mathbb{R}^n$$

Finally we obtain that

$$H(y_{n+1}) - H(y_n) = 0$$

iv) If H is a polynomial of degree k, then $f = J^{-1} \nabla H$ is a polynomial of degree $k-1$.

Therefore, if $(b_i, c_i)_{i=1}^{s}$ has order $2s \geq k$ (i.e. degree of exactness $2s-1 \geq k-1$), then the quadrature rule is exact and

$$\int_0^1 f(y_n + \theta(y_{n+1} - y_n))\, d\theta = \sum_{i=1}^{s} b_i f(y_n + c_i(y_{n+1} - y_n))$$

v) Combining questions iv) and ii)

$$y_{n+1} = y_n + h\int_0^1 f(\theta y_{n+1} + (1-\theta)y_n)\, d\theta$$

$$= y_n + h\sum_{i=1}^{s} b_i f(y_n + c_i(y_{n+1} - y_n))$$

Define $k_i = f(y_n + c_i(y_{n+1} - y_n))$ such that

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i k_i \qquad (1)$$

and $k_i = f(y_n + h\sum_{j=1}^{s} b_j c_i k_j)$

Now define $a_{ij} = c_i b_j$ such that

$$k_i = f(y_n + h\sum_{j=1}^{s} a_{ij} k_j) \qquad (2)$$

(1) and (2) define a RK method which coincides with the AVF method and since the latter preserves the Hamiltonian, so does the RK method.

$\boxed{3}$ We know that if the Cooper conditions are satisfied, then the method is symplectic

Consider a consistent RK method with $s = 2$

$$\begin{cases} \sum_{i=1}^{2} b_i = 1 \\ b_i a_{ij} + b_j a_{ji} = b_i b_j \qquad i,j = 1, \dots, s \end{cases}$$

for $s = 2$, we obtain

$$\begin{cases} b_1 + b_2 = 1 \\ 2 b_1 a_{11} = b_1^2 \\ b_1 a_{12} + b_2 a_{21} = b_1 b_2 \\ 2 b_2 a_{22} = b_2^2 \end{cases}$$

This is an underdetermined system

Let's try $b_1 = b_2 = 1/2$

$\Rightarrow$ $a_{11} = 1/4$

$a_{22} = 1/4$

$a_{12} + a_{21} = 1/2$

take

$a_{12} = 0$

$a_{21} = 1/2$

The Butcher tableau becomes

$$\begin{array}{c|cc} 1/4 & 1/4 & 0 \\ 3/4 & 1/2 & 1/4 \\ \hline & 1/2 & 1/2 \end{array}$$

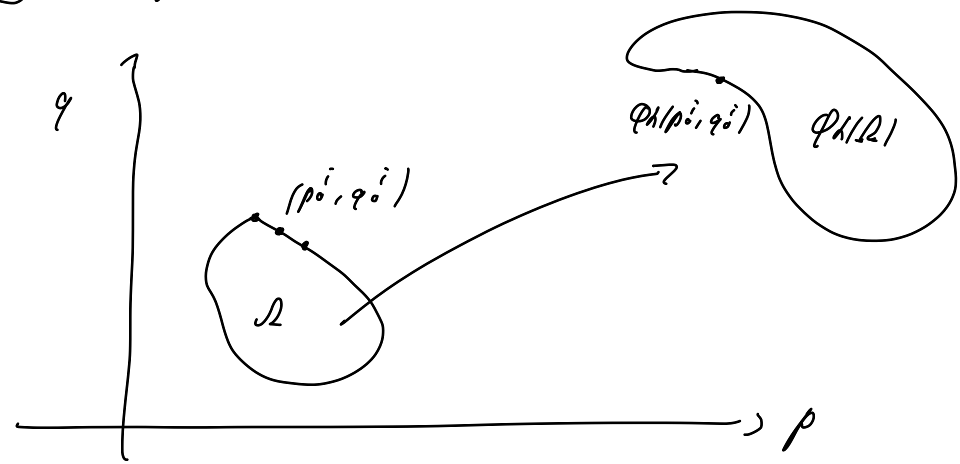
Remark: this method is irreducible (assume $k_1 = k_2$ and obtain a contradiction)

However the method is not equal to the 2 stage Gauss method

Recall the 2 stage Gauss method :

$$\left(\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & 1/4 & \frac{1}{4}-\frac{\sqrt{3}}{6} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4}+\frac{\sqrt{3}}{6} & 1/4 \\ \hline & 1/2 & 1/2 \end{array}\right)$$

$\boxed{4}$ Background :



If a numerical method is symplectic, then it is volume preserving $\quad Vol(\Omega) = Vol(\Phi_h(\Omega))$