How to develop algorithms with $\det M = 1$

↳ canonical transformation

Four formulations of classical mechanics

1) Newtonian: $\vec{F} = m\vec{a} \Rightarrow \frac{d^2\vec{r}}{dt^2} = \frac{\vec{F}(\vec{r})}{m}$

↑ basis for Runge Kutta algorithm

2) Lagrangian: variational

↳ generalize coordinates (angles)

" momentum

3) Hamiltonian: momentum is a fundamental degree of freedom

ind. of $\vec{r}$.

$$\frac{d\vec{r}}{dt} = \frac{\vec{p}}{m} \ !$$

$$\underbrace{\frac{d\vec{p}}{dt} = -\frac{\partial H}{\partial \vec{r}} \qquad = \frac{\partial H}{\partial \vec{p}}}$$

Hamilton's Eq.

transformations of $(\vec{r}, \vec{p}) \to (\vec{r}', \vec{p}')$ which preserves the form of Han. Eq. are canonical transformation: $\det M = 1$

4) Poissonian: instead of equations of motion, operator form of the solution!

Recall Taylor expansion for $f(x,y)$

$$f(x+c,y) = f(x,y) + c\frac{\partial f}{\partial x} + \frac{1}{2}c^2\frac{\partial^2 f}{\partial x^2} + \cdots$$

$$= \left(1 + c\frac{\partial}{\partial x} + \frac{1}{2}c^2\frac{\partial^2}{\partial x^2} + \cdots\right) f(x,y)$$

$$+\frac{1}{3!}c^3\frac{\partial^3}{\partial x^3} + \frac{1}{4!}c^4\frac{\partial^4}{\partial x^4}$$

$$= \boxed{e^{c\frac{\partial}{\partial x}} f(x,y) = f(x+c,y)}$$

what is now

$$e^{c(y)\frac{\partial}{\partial x}} f(x,y) = \left(1 + c(y)\frac{\partial}{\partial x} + \frac{1}{2}\left(c(y)\frac{\partial}{\partial x}\right)^2 + \cdots\right) f(x,y)$$

$$\left(c(y)\frac{\partial}{\partial x}\right)^2 = c(y)\frac{\partial}{\partial x}\left[c(y)\frac{\partial}{\partial x}\right] = c(y)^2\frac{\partial^2}{\partial x^2}$$

$$= \left(1 + c(y)\frac{\partial}{\partial x} + \frac{1}{2}c^2\frac{\partial^2}{\partial x^2} + \cdots\right)$$

Lie operator

$$\boxed{\underbrace{e^{c(y)\frac{\partial}{\partial x}} f(x,y)}_{\text{Lie transform}} = f(x+c(y),y)}$$

Lie series

Hamiltonian Mechanics

independent q_i, p_i conjugated variables

generalized coordinates ↑ ↑ generalized momentum variables

Hamiltonian function $H(q_i, p_i) = \sum_i \frac{p_i^2}{2m} + V(q_i)$

Hamilton's equation of motion

$$\frac{dq_i}{dt} = \boxed{\begin{aligned} \dot{q}_i &= \frac{\partial H}{\partial p_i} \\ \dot{p}_i &= -\frac{\partial H}{\partial q_i} \end{aligned}} \begin{aligned} &= \frac{p_i}{m} \\ &= -\frac{\partial V}{\partial q_i} = F_i \end{aligned}$$

therefor $\ddot{q}_i = \frac{\dot{p}_i}{m} = \frac{F_i}{m}$ ← Newton's eq. of motion.

Consider the evolution of $f(q_i, p_i)$ any fct of q_i, p_i

$$\dot{f} = \sum_i \left(\frac{\partial f}{\partial q_i} \frac{\partial q_i}{\partial t} + \frac{\partial f}{\partial p_i} \frac{\partial p_i}{\partial t} \right)$$

Poisson bracket

for $H = \sum_i \frac{p_i^2}{m} + V(q_i)$

$$= \sum_i \left(\frac{\partial f}{\partial q_i} \dot{q}_i + \frac{\partial f}{\partial p_i} \dot{p}_i \right) = \sum_i \left(\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right)$$

$$\dot{f} = \sum_i \left(\frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i} \right) f = \{f, H\}_{q,p}$$

$$= \sum_i \left(\frac{p_i}{m} \frac{\partial}{\partial q_i} + F_i \frac{\partial}{\partial p_i} \right) f = \boxed{(T+V) f(q_i, p_i) = \dot{f}}$$

$$T = \sum_i \frac{p_i}{m} \frac{\partial}{\partial q_i} \qquad V = \sum_i F_i \frac{\partial}{\partial p_i}$$

$$\frac{df}{dt} = (T+V) f$$

Poisson Eq. of motion.

$$\Rightarrow \quad \frac{1}{f} \frac{df}{dt} = (T+V) \Rightarrow \frac{d}{dt} \ln f = (T+V) \Rightarrow \ln f = (T+V)t + C$$

$$\boxed{f(q_i, p_i, t) = e^{t(T+V)} f(q_i, p_i, 0)}$$

Poisson's solution !

Let's see a simple example

$$H = \frac{p^2}{2m} - ma\,q \quad \text{const}$$

$$T = \frac{\partial H}{\partial p}\frac{\partial}{\partial q} = \frac{p}{m}\frac{\partial}{\partial q} \qquad V = -\frac{\partial V}{\partial q}\frac{\partial}{\partial p} = ma\frac{\partial}{\partial p}$$

def $v \equiv \frac{p}{m}$ $\qquad T = v\frac{\partial}{\partial q} \qquad V = a\frac{\partial}{\partial v}$

$$f = e^{t(T+V)} f_0 \qquad \hat{H} = T+V$$

$Hv = a$

$$q(t) = \left(1 + tH + \frac{1}{2}t^2H^2 + \frac{1}{3!}t^3H^3 + \cdots\right) q$$

$$= q + tv + \frac{1}{2}t^2 a + 0 + 0 + 0.$$

$$= q + tv + \frac{1}{2}t^2 a$$

$$v(t) = v + ta$$

$Hq = v$

$H^2 q = Hv$
$= a$

what happens now if $a(q) = \frac{F(q)}{m}$ not a const. ?

$q(t) = e^{t\hat{H}} q \qquad v(t) = e^{t\hat{H}} v$

$= (1 + t\hat{H} + \frac{1}{2}t^2\hat{H} + \cdots) q \qquad \hat{H} = T + V$

However, one notes that ↑ inf series to sum $\qquad = v\frac{\partial}{\partial q} + a(q)\frac{\partial}{\partial v}$

$q(t) = e^{t(T+V)} q$

$e^{tT} q = e^{tv\frac{\partial}{\partial q}} q = (1 + tv\frac{\partial}{\partial q} + \frac{1}{2}(tv)^2\frac{\partial^2}{\partial q^2} + \cdots) q$

$= q + tv$ exactly

$e^{tv\frac{\partial}{\partial q}} f(q) = f(q + tv)$ The effect of each e^{tT}

$e^{tV} q = q$ are know e^{tV} exactly !

$e^{tT} v = v$

$e^{tV} v = e^{ta(q)\frac{\partial}{\partial v}} v = v + ta(q)$!

exactly

Since the effect of e^{tT}, e^{tV} are known exactly

$$e^{tT} f(q,v) = f(q+tv, v) \qquad v \equiv \frac{p}{m}$$

$$e^{tV} f(q,v) = f(q, v+ta(q))$$

the solution operator

$$e^{tT+tV} = \prod_i e^{t a_i T} e^{t b_i V}$$

Can be approximated by a product of operators

Algebratization of algorithms

The key to this product approximation is Baker-Campbell-Hausdorff formula:

$[A,B] \neq 0$

$$e^{\epsilon A} e^{\epsilon B} = e^{\epsilon A + \epsilon B + \frac{\epsilon^2}{2}[A,B] + \cdots}$$

$$e^{\epsilon A} e^{\epsilon B} = e^{\epsilon(A+B)} + O(\epsilon^2) \qquad e^{\epsilon\left[A+B+\frac{\epsilon}{2}[A,B]\right] \cdots}$$

first error in A+B

first-order symplectic algorithm $T_{1a} = e^{\Delta t V} e^{\Delta t T}$

$$q(\Delta t) = e^{\Delta t V} e^{\Delta t T} q$$
$$= e^{\Delta t V}(q + \Delta t v)$$
$$= q + \Delta t(v + \Delta t\, a(q))$$

In reverse order of the operators

This is equivalent to: Cromer's algorithm

$$v_1 = v + \Delta t\, a(q)$$
$$q_1 = q + \Delta t\, v_1$$

(the order of the algorithm is)

Similarly $T_{1b} = e^{\delta t\, T} e^{\delta t\, V}$

what are $T_{1b}\, q$, $T_{1b}\, v$?

what is the resulting algorithm?

To create second-order algorithm (the Hamilton has second-order error in Δt $\sim \Delta t^2$)

$$T_{2a} = T_{1a}\left(\tfrac{1}{2}\Delta t\right) T_{1b}\left(\tfrac{1}{2}\Delta t\right)$$

$$= e^{\frac{\Delta t}{2}V} e^{\frac{\Delta t}{2}T} e^{\frac{\Delta t}{2}T} e^{\frac{\Delta t}{2}V}$$

$$= e^{\frac{\Delta t}{2}V} e^{\Delta t T} e^{\frac{\Delta t}{2}V}$$

2a :

$$v_1 = v + \tfrac{1}{2}\Delta t\, a(q)$$

$$q_1 = q + \Delta t\, v_1$$

$$v_2 = v_1 + \tfrac{1}{2}\Delta t\, a(q_1)$$

equivalent

$$\begin{pmatrix} q(\Delta t) \\ v(\Delta t) \end{pmatrix} = e^{\frac{\Delta t}{2}V} e^{\Delta t T} e^{\frac{\Delta t}{2}V} \begin{pmatrix} q \\ v \end{pmatrix}$$

$$= e^{\frac{\Delta t}{2}V} e^{\Delta t T} \begin{pmatrix} q \\ v + \Delta t\, a(q) \end{pmatrix}$$

$$= e^{\frac{\Delta t}{2}V} \begin{pmatrix} q + \Delta t\, v \\ v + \Delta t\, a(q + \Delta t v) \end{pmatrix}$$

$$= \begin{pmatrix} q + \Delta t\left(v + \frac{\Delta t}{2} a(q)\right) \\ v + \frac{\Delta t}{2} a(q) + \Delta t\, a\left(q + \Delta t\left(v + \frac{\Delta t}{2} a\right)\right) \end{pmatrix}$$

$$T_{2b} = e^{\frac{\Delta t}{2}T} e^{\Delta t V} e^{\frac{\Delta t}{2}T}$$

You derive the corresponding algorithm.

Late assignment : 2 by Friday
1 by next wednesday.

Prove that 2a + 2b are second-order algorithm

Since T_{2a} + T_{2b} are Left-right symmetric

$$T_2(-\Delta t)\,T(\Delta t) = 1$$

time - symmetric

$$\cancel{e^{-\frac{\Delta t}{2}V}}\;\cancel{e^{-\Delta t T}}\;\cancel{e^{-\frac{1}{2}\Delta t V}}\;\cancel{e^{\frac{1}{2}\Delta t V}}\;\cancel{e^{\Delta t T}}\;\cancel{e^{\frac{1}{2}\Delta t V}} = 1$$

therefore :

$$T_2(\Delta t) = e^{\Delta t \underbrace{(T+V) + \Delta t^3 E_3 +}_{} \Delta t^5 E_5 + \cdots}$$

must be at least second-order in Δt

otherwise cannot be $T_2(-\Delta t)\,T(\Delta t) = 1$