Hamiltonian MCMC-1

Friday, March 8, 2019 10:48 AM

Classical Mechanics / Dynamics

[For HMCMC, variational Bayes ...]

0. Constrained motion, generalized coordinates
1. Lagrangian & Euler-Lagrange equations of motion.
2. Hamilton's principle
3. The Hamiltonian & Hamilton's equations

If time permits:

4. Forces of constraint & Lagrange multipliers

—— x ——

0. Generalized coordinates

· Goal: treat the motion of a particle with a set of independent coordinates that take into account the forces of constraint.

Consider N particles acting under k forces. We can describe their motion as,

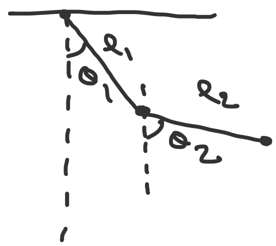
$$f_j(x_1, x_2, \ldots, x_n, t) = c_j \quad \text{—— (1)}$$

where

$n = 3N$ s.t. $(m, m+1, m+2)$ are the coordinates of the m^{th} particle and, $j \in \{1, \ldots, k\}$

These k relations are also called holonomic constraints.

For example,



$l_1, l_2 \to$ holonomic constraints

$\theta_1, \theta_2 \to$ 2 degrees of freedom

Thus, for a system of N particles with k holonomic constraints, we define n-k independent coordinates (also called generalized)

$$q_1, q_2, \ldots, q_{n-k}$$

that completely specify the configuration of the system.

These are related to the Cartesian coordinates through a linear map,

$$\begin{aligned} x_1 &= x_1(q_1, \ldots, q_{n-k}, t) \\ &\vdots \\ x_n &= x_n(q_1, \ldots, q_{n-k}, t) \end{aligned} \quad \text{—— (2)}$$

Alternatively, we can summarize it using differentials,

$$dx_i = \sum_{r=1}^{n-k} \frac{\partial x_i}{\partial q_r} dq_r + \frac{\partial x_i}{\partial t} dt \quad \forall\, i \in \{1, \ldots, n\} \quad \text{—— (3)}$$

Write matrix form:

$$\begin{pmatrix} dx_1 \\ \vdots \\ dx_n \end{pmatrix} = \begin{pmatrix} & \vdots & \\ & \vdots & n \times n-k \end{pmatrix} \begin{pmatrix} dq_1 \\ \vdots \\ dq_{n-k} \end{pmatrix}$$

1. Lagrangian & E-L equations of motion

We define the Lagrangian as,

$$\mathcal{L}(\dot{q}(t), q(t), t) = T(\dot{q}, q) - V(q) \qquad (4)$$

where we've assumed that only conservative forces act on the system, i.e.:

$$V(x_1, \dots, x_n) = V(q_1, \dots, q_{n-k}, t)$$

Very loosely, this implies

$$F = -\frac{\partial V}{\partial x}$$

or

$$Q_r = -\frac{\partial}{\partial q_r} V(q_1, \dots, q_{n-k}, t)$$

generalized force

We also require,

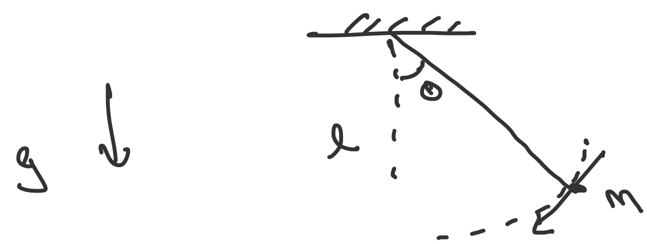
$$\frac{\partial V}{\partial \dot{q}_r} = 0$$

We postulate (without proof, but only for the moment) that for a system acting under conservative forces, the equations of motion are given by,

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_r} - \frac{\partial \mathcal{L}}{\partial q_r} = 0, \quad r = 1, \dots, n-k \qquad (5)$$

Note: This is huge!! In this formalism, We can solve the equations of motion for any system as long as we can identify all the forces acting on it.

Example:



$(x, y) \rightarrow \theta$ under a conservative force like gravity

$$T = \frac{1}{2} m (l\dot{\theta})^2$$

$$V = -mgl\cos\theta + K$$

gauge it away

$$\therefore \quad \mathcal{L} = \frac{1}{2} m (l\dot{\theta})^2 + mgl\cos\theta$$

Calculating the E-L equations of motion using Eq. (5),

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{\theta}} - \frac{\partial \mathcal{L}}{\partial \theta} = \frac{d}{dt}\left(ml^2\dot{\theta}\right) - mgl\sin\theta$$

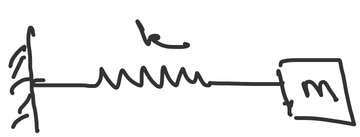
$$\Rightarrow \quad \ddot{\theta} + \frac{g}{l}\sin\theta = 0$$

For small angles,

$$\sin\theta \simeq \theta$$

$$\Rightarrow \quad \ddot{\theta} + \frac{g}{l}\theta = 0 \quad ; \quad \boxed{\omega^2 = \frac{g}{l}}$$

We can do the same exercise for a spring-mass system.



Read this work:

2. Hamilton's principle

was given using QM by Feynman

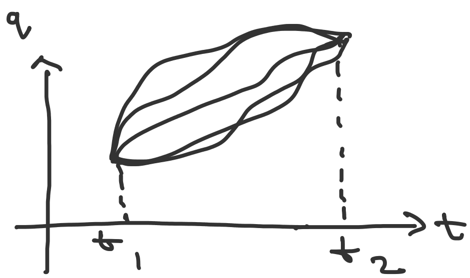
or the principle of stationary action:

"Of all the possible paths between two fixed endpoints, a particle takes the path that 'extremizes' (minimizes in most cases) the action."

We define the action as:

$$S = \int_{t_1}^{t_2} dt \; L(\dot{q}, q, t) \quad \text{———} \quad (6)$$

(Technically, S is a functional since it it's function valued)



Formally, the Hamilton's principle is given by,

$$\delta S = 0 \quad \text{———} \quad (7)$$

for paths between fixed endpoints x_1 & x_2,

$$\delta q(t_1) = \delta q(t_2) = 0$$

Now, for finding the stationary value of the action (or the equation of motion), we use calculus of variations (a.k.a the variational method). We consider two infinitesimally different paths with common endpoints. Let

$y(t) \rightarrow$ 'true' path

Then we can write the neighboring path as,

$$Y(t) = y(t) + \epsilon\,\eta(t) \quad \&$$

↳ infinitesimal

with the corresponding action,

$$S[Y(t)] = \int_{t_1}^{t_2} \mathcal{L}(Y(t), \dot{Y}(t), t)\, dt$$

$$\eta(t_1) = \eta(t_2) = 0$$

$\Rightarrow$ ** 1.) Since ϵ is small, we can Taylor expand about $\epsilon = 0$,

$$\therefore S[Y(t)] = \int_{t_1}^{t_2} \mathcal{L}(y(t), \dot{y}(t))\, dt$$

$$+ \epsilon \int_{t_1}^{t_2} \left[\frac{\partial \mathcal{L}}{\partial y} \eta(t) + \frac{\partial \mathcal{L}}{\partial \dot{y}} \dot{\eta}(t) \right] dt$$

$$+ O(\epsilon^2)$$

Using Hamilton's principle in Eq. (7),

$$\frac{d}{d\epsilon} S[Y(t)] = 0$$

[which gives us an extremum, but usually the context of the problem tells us if it's a minima or a maxima. Eg: distance between 2 points]

Thus, we obtain,

$$\int_{t_1}^{t_2} \left[\frac{\partial \mathcal{L}}{\partial y} \eta(t) + \underbrace{\frac{\partial \mathcal{L}}{\partial \dot{y}} \frac{d}{dt} \eta(t)}_{} \right] dt = 0$$

$\Rightarrow$ ** 2.) Using integration by parts for the second term above,

$$\therefore \quad \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{y}}\,\eta(t)\right) = \left(\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{y}}\right)\eta(t) + \frac{\partial \mathcal{L}}{\partial \dot{y}}\,\frac{d}{dt}\eta(t)$$

$$\therefore \quad \frac{\partial \mathcal{L}}{\partial \dot{y}}\,\frac{d}{dt}\eta(t) = \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{y}}\,\eta(t)\right) - \left(\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{y}}\right)\eta(t)$$

Resubstituting,

$$\int_{t_1}^{t_2}\left[\frac{\partial \mathcal{L}}{\partial y} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{y}}\right]\eta(t)\,dt$$

(Boundary term $\eta(t_1) = \eta(t_2) = 0$)

$$+ \cancelto{0}{\frac{\partial \mathcal{L}}{\partial \dot{y}}\,\eta(t)\Big|_{t_1}^{t_2}} = 0$$

If we want the equation to hold for arbitrary $\eta(t)$, its coefficient should vanish $\forall\, x \in [x_1, x_2]$,

$$\therefore \quad \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{y}} - \frac{\partial \mathcal{L}}{\partial y} = 0$$

Q.E.D.