Hamiltonian MCMC-2

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3. Hamiltonian & Hamilton's equations

We define the quantity,

$$p_\sigma \equiv \frac{\partial \mathcal{L}}{\partial \dot{q}} \qquad \text{—— (8)}$$

as the generalized (/ canonical / conjugate) momentum.

And introduce the Hamiltonian,

$$H(p,q) = \sum_\sigma p_\sigma \dot{q}_\sigma - \mathcal{L}(\dot{q}, q, t) \qquad \text{—— (9)}$$

which satisfies the following coupled 1st order PDE called Hamilton's equations.

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

$$\frac{\partial H(p,q)}{\partial q} = -\dot{p} \qquad \text{—— (10)}$$

[SHM example : $x'' + x = 0$; $x' = v$; $v' = -x$]

Rewind:

Let's pause for a second and review the Lagrangian formalism.

We can think of the Euler-Lagrange equations of motion as a re-statement of Newton's

2^{nd} law of motion. More concretely,

$$\vec{F}(q) = m a = m \frac{d\vec{v}}{dt} = \frac{d\vec{p}}{dt}$$

Identifying,

$$\vec{F} = -\frac{\partial V}{\partial q} + \frac{\partial T}{\partial q}$$

$$\frac{d\vec{p}}{dt} = \frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}}\right) - \frac{d}{dt}\left(\frac{\partial V}{\partial \dot{q}}\right)$$

$$\Rightarrow \boxed{\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0}$$

Aside: Why can we write conservative forces as gradient of a scalar potential?

$$W = \int_c \vec{F} \cdot d\vec{r} = \vec{\nabla} \times \vec{F} = 0$$
(Stokes' theorem)

Using the properties of vector calculus, for a scalar field Φ,

$$\vec{\nabla} \times (\vec{\nabla} \Phi) = 0$$

Thus, for every conservative force, we can write,

$$\boxed{\vec{F} = -\nabla \Phi}$$

Back to Hamilton's equations

→ Eq. (2.3) , Eq. (2.6)

→ Characteristics

$\Bigg\}$ Neal review

. It's the Hamiltonian dynamics that allow us to construct a MCMC algorithm. As long as we're able to construct a Hamiltonian-like object by including a symmetric kinetic energy term:

$$K(p) = p^T M^{-1} p / 2$$

$$M_{ij} = \sigma_{ij} \rightarrow \text{positive, semi-definite covariance matrix.}$$

entries may be tuned to normalize scales of different parameters.

History of MCMC techniques leading upto HMCMC can be found in 1706.01520.

Hybrid MCMC was introduced in 1987 by Duane et. al. for numerical simulation of lattice QCD.

One of the popular implementations today is PyMC3, co-developed by T. Wiecki, one of the graduates of Frank lab.