Hamiltonian Monte Carlo (HMC)

Just MH, we only need to be able to evaluate a function

$$\log P(x) = \underbrace{-E(x)}_{\text{potential energy}} + \text{const} \qquad x \in \mathbb{R}^d$$

we will also need to evaluate $\nabla E(x) \in \mathbb{R}^d$

(modern languages, we can often get derivative info at the same time as evaluating function for negligible extra cost.)

~~Pos~~ x called positions, we introduce <u>momentum</u> variable $p \in \mathbb{R}^d$

$(x, p) \in \mathbb{R}^{2d}$

for the momentum p, introduce a new distribution

$$Q(p) = \mathcal{N}(0, \underline{\underline{M}})$$

this should be: - easy to sample from

- have symmetry $Q(p) = Q(-p)$

$$\log Q(p) = -\underset{\substack{\uparrow \\ \text{kinetic energy}}}{K(p)} + \text{const}$$

$(x, p) \in \mathbb{R}^{2d}$

new distribution $\log R(x, p) = -\mathcal{H}(x, p) + \text{const}$

where $\mathcal{H}(x, p) = E(x) + K(p)$ "Hamiltonian" target dist $P(x) = \int dp \; R(x, p)$ is recovered by marginalising R w.r.t. p.

similarly $Q(p) = \int dx \; R(x, p)$

<u>also</u> target if $x, p \sim R$

then $x \mid p \sim P$

$\cancel{x}\, p \mid x \sim Q$

we will try to sample $x, p \sim R$ if we throw out p then we are left with $x \sim P$, as required.

equations of Hamiltonian dynamics

$$\frac{dx^k}{dt} = \frac{\partial H}{\partial p^k} \qquad \frac{dp^k}{dt} = -\frac{\partial H}{\partial x^k}$$

t is a new ~~fictit~~ made up time coordinate.

choose a fixed interval s

$\cancel{\Omega : (x, p)}$ $\qquad x(t), p(t)$

evolve E.O.M. forwards in time s, we get (deterministically)

$$x(t+s), \; p(t+s)$$

- Reversible $\quad x, p \xrightarrow{S} x', p'$

$$x', -p' \xrightarrow{S} x, p$$

- Volume - preserving (Liouville's theorem)

take points in some $\Delta x, \Delta p$ of phase space, evolve forwards in time S, $\Delta x', \Delta p'$.

$$\Delta x \Delta p = \Delta x' \Delta p'.$$

- Conserves $\mathcal{H}(x,p) = E(x) + K(p)$

$$\frac{d}{dt}\mathcal{H} = \frac{\partial \mathcal{H}}{\partial x}\frac{dx}{dt} + \frac{\partial \mathcal{H}}{\partial p}\frac{dp}{dt} = \overbrace{\frac{\partial \mathcal{H}}{\partial x}\frac{\partial \mathcal{H}}{\partial p} - \frac{\partial \mathcal{H}}{\partial p}\frac{\partial \mathcal{H}}{\partial x}}^{\text{used Hamilton's EOM.}} = 0.$$

It will be necessary to numerically integrate EOM.

$x(t)$, $p(t)$ inputs

$x(t+\Delta t)$, $p(t+\Delta t)$ outputs

Leapfrog takes a step forward in t, approximates Hamiltonian dynamics.

Recall $\log Q(p) = -K(p) + c$

$$K(p) = \tfrac{1}{2}\underline{p}^T \cdot \underline{\underline{M}} \cdot \underline{p}$$

M the mass matrix. (symmetric positive definite)

$$\frac{\partial K}{\partial p^k} = \underline{\underline{M}} \cdot \underline{p}$$

Leapfrog is Reversible + Vol. pres. exactly for any Δt.

but $\mathcal{H}$ is only approximately conserved

$$\mathcal{H}(x(t+\Delta t), p(t+\Delta t))$$
$$= \mathcal{H}(x(t), p(t)) + O(\Delta t^2).$$

2 ways to think about HMC.

1 : as a version of MH on space (x, p)

with a proposal $Q_{MH}(y \mid x) = Q(\hat{p})\, \delta^{(2d)}(z - \text{Hamilton}(x, \hat{p}))$

let $z = (x, p)$

2: as a version of blocked Gibbs sampler. (sweep)

we 2 blocks ~~(x, p)~~ (p, x)

$p_{i+1} \sim R(p \mid x_i)$ sweep step 1

$p_{i+1} \sim Q(p)$

$x_{i+1} \sim R(x \mid p_{i+1})$ sweep step 2

$x_{i+1} \sim P(x)$ accept/reject according MH rule

accept with prob $\alpha \approx 1$.