Hamiltonian Monte Carlo

Goal: Sample from $\pi(x) \propto e^{-U(x)}$, $U : \mathbb{R}^d \mapsto \mathbb{R}$, $U \in C^2$

Idea: introduce the *hamiltonian* $H : \mathbb{R}^{2d} \mapsto \mathbb{R}$ where

$(p, x) \mapsto U(x) + \frac{1}{2} p^T C^{-1} p$ for some psd C

Then we consider a distribution $\overline{\pi}(p, x) \propto e^{-H(p,x)}$

which is easier to sample from and marginalizing

gives samples from π.

Consider the ODE

$$\begin{cases} \partial p / \partial t = -\dfrac{\partial H}{\partial x}(p_t, x_t) = -\nabla U(x_t) \\[2ex] \partial x / \partial t = \dfrac{\partial H}{\partial p}(p_t, x_t) = C^{-1} p_t \end{cases}$$

with initial condition $(p_0, x_0) \Rightarrow \{(p_t, x_t), t \geq 0\}$

$$\frac{d}{dt} H(p_t, x_t) = \frac{\partial H}{\partial p}(p_t, x_t) \frac{dp_t}{dt} + \frac{\partial H}{\partial x}(p_t, x_t) \frac{dx}{dt} = 0$$

$\Longrightarrow H(p_t, x_t) = H(p_0, x_0)$ i.e. constant hamiltonian

Ex: Find $U(x) = \frac{x^2}{\ }$, $p^T C^{-1} p = \frac{p^2}{\ }$

—　　$2a$　　b

$$H(x_t, p_t) \equiv cst \iff \frac{x^2}{2a} + \frac{p^2}{2b} \equiv cst$$

Given (p_0, x_0) and set $M_t : \mathbb{R}^{2p} \mapsto \mathbb{R}^{2p}$
$$(p_0, x_0) \longmapsto (p_t, x_t)$$

<u>Algorithm:</u> Given $X_n = x$

1. Draw $p_0 \sim N(0, c)$
2. Compute $(p', x') = M_t(p_0, x)$
3. Set $X_{n+1} = X'$

<u>Prop:</u> If $X_n \sim \pi$, $X_{n+1} \sim \pi$

<u>Proof:</u> If $X_n \sim \pi$ then $(X_n, p_0) \sim \bar{\pi}$

$(p', x') = M_t(p_0, x_n)$

Properties of M_t ensure that $(p', x') \sim \bar{\pi}$

which imply that $x' \sim \pi$.

So we can travel long distances along the hamiltonian <u>without</u> destroying the target dist.

Estimating the map M_t

Intractable in general.

Given $\varepsilon > 0$ consider $S = S_\varepsilon : \mathbb{R}^{2p} \longmapsto \mathbb{R}^{2p}$

s.t. $(p, x) \longmapsto (p', x')$

Define
$$\left.\begin{aligned} \bar{p} &= p - \frac{\varepsilon}{2} \nabla U(x) \\ x' &= x + \varepsilon C^{-1} \bar{p} \\ p' &= \bar{p} - \frac{\varepsilon}{2} \nabla U(x') \end{aligned}\right\} \text{Leap frog approximation}$$

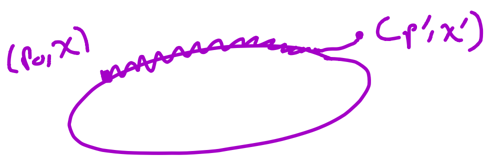
Consider $S_L \equiv S^L = \underbrace{S \circ S \circ \cdots \circ S}_{L\text{-times}} : \mathbb{R}^{2d} \longmapsto \mathbb{R}^{2d}$

Algorithm: Given $x_n = x$

1. $p_0 \sim N(0, C)$

2. Compute $(p', x') = S_L(p_0, x)$

3. $$x_{n+1} = \begin{cases} x' & \text{w.p. } \min\left[1, \exp\left(-H(p', x') + H(p_0, x)\right)\right] \\ x & \text{o.w.} \end{cases}$$



- Should be able to travel long distance

- MH step helps us self correct if the discretization is far off.

Prop: If $X_n \sim \pi$, $X_{n+1} \sim \pi$

Proof:

(*) Need to show $(S^L)^{-1} = F \circ S_L \circ F$, $F: (p,x) \to (-p, x)$

Justification: If true for $L=1$,

$$S_2^{-1} = S^{-1} \circ S^{-1} = F \circ S \circ \underbrace{F \circ F}_{I} \circ S \circ F = F \circ S^2 \circ F$$

By induction $S_L^{-1} = F \circ S^L \circ F$

Sufficient to show $S^{-1} = F \circ S \circ F$

$S: (p,x) \to (p', x')$

$$\begin{cases} \bar{p} = p - \frac{\varepsilon}{2} \nabla U(x) \\ x' = x + \varepsilon C^{-1} \bar{p} \\ p' = \bar{p} - \frac{\varepsilon}{2} \nabla U(x') \end{cases}$$

(p_n, x_n) (p', x')

$$\begin{cases} -\bar{p} = (-p') - \varepsilon/_2 \nabla u(x') \\ x = x' + \varepsilon C^{-1}(-\bar{p}) \\ -\tilde{p} = (-\bar{p}) - \frac{\varepsilon}{2} \nabla u(x) \end{cases}$$

A map $T: \mathbb{R}^{2d} \longrightarrow \mathbb{R}^{2d}$ is simplectic if $\nabla T(y)$

$\forall y \in \mathbb{R}^{2d}$ $\quad \nabla T(y) J \nabla T(y)^T = J \qquad J = \begin{bmatrix} 0_d & I_d \\ -I_d & 0 \end{bmatrix}$

$\Rightarrow \det |\nabla T(y)| = \pm 1$

(*) the map S_L is simplectic

If S_1, S_2 are simplectic $\quad S_1 \circ S_2$ is simplectic

b/c $\nabla S(y) = \nabla S_1(S_2(y)) \nabla S_2(y)$

$$\nabla S(y) J \nabla S(y)^T = \nabla S_1(S_2(y)) \nabla S_2(y) J \nabla S_2(y)^T \nabla S_1(S_2(y))^T$$
$$= \nabla S_1(S_2(y)) J \nabla S_1(S_2(y))^T = J$$

$S_1 : (p, x) \longmapsto \left(p - \frac{\varepsilon}{2} \nabla u(x), \; x + \varepsilon C^{-1} p - \frac{\varepsilon^2}{2} C^{-1} \nabla u(x) \right)$

$S_2 : (p, x) \longmapsto \left(p - \frac{\varepsilon}{2} \nabla u(x), \; x \right)$

$S = S_2 \circ S_1$

$$\nabla S_2(p,x) = \begin{bmatrix} I & 0 \\ -\frac{\varepsilon}{2}\nabla^{(2)}U(x) & I \end{bmatrix}$$

$$\nabla S_2(p,x) J = \begin{bmatrix} 0 & I \\ -I & -\frac{\varepsilon^2}{2}\nabla^{(2)}U(x) \end{bmatrix}$$

$$\nabla S_2(p,x) J \nabla S_2(p,x)^T = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} = J$$

Similar for S_1.

So together we get simplectic maps $S_1, S_2, S_2 \circ S_1$