HMC

Given $\pi(x) = \frac{e^{-U(x)}}{Z}$ $\quad U(\cdot)$ smooth

Idea: Define $H(p,x) = \frac{1}{2} p^T \underbrace{C^{-1}}_{\text{psd}} p + U(x)$

Algo: Given $x^{(i)}$:

- $p \sim N(0, C)$
- $(p', c') = S_L(p, x^{(i)})$
- Set $x^{(i+1)} = \begin{cases} x' & \min[1, \exp(H(p,x) - H(p',x'))] \\ x^{(i)} & \text{o.w.} \end{cases}$

where $S : \mathbb{R}^{2d} \longmapsto \mathbb{R}^{2d}$ is the leapfrog map where

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

$$S_L = \underbrace{S \circ \cdots \circ S}_{L\text{-times}}$$

We sometimes replace $\nabla U(x)$ for computational speedup.

Ex: $\pi(x) \propto \exp\left(\sum_{i=1}^{n} U_i(x)\right)$

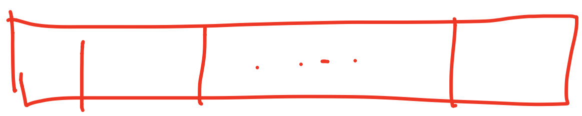
If $\mathbb{E}[\hat{\pi}(x)] = \pi(x)$ then we can do mcmc based on $\hat{\pi}$. pseudo-mcmc

Still unsure what to do with $\mathbb{E}(\hat{u}(x)) = u(x)$

* get $(\hat{u}^{(i)})_{i=1}^{J}$ s.t. $\mathbb{E}[\hat{u}^{(j)}(x)] = u(x)$

then $\hat{\pi}^{(j)}(x) \propto \exp(-\hat{u}^{(j)}(x))$ and then combine these estimated posteriors

Useful when we think about splitting our the dataset.



<u>Two Properties</u>

1. S_L is simplectic $\nabla S(p,x) J \nabla S(p,x)^T = J$

   $J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$

2. $S_L^{-1}(p,x) = F \circ S_L \circ F(p,x) = F \circ S_L(-p,x)$

   $= (-S_{L,1}(-p,x), S_{L,2}(p,x))$

<u>Rmk</u>: These properties still hold when $U' \in C^2$ replaces U

Langevin MCMC

Define $T(x) = x - \varepsilon \nabla U(x)$

Then for $X^{(i)} = x$

$$\bar{x} = T^L(x) + z$$

$$x^{(i+1)} = \begin{cases} \bar{x} & \text{w.p.} \\ x^{(i)} & \text{w.p.} \end{cases}$$

Similiar to the Hamiltonian MCMC

→ Controlled convergence to the mode

→ A little worse

Prop: In the HMC sampler given, if $X_0 \sim \pi$ then $X_1 \sim \pi$

Proof: $\mathbb{P}(X_1 \in A) = \int \pi(x) \mathbb{P}(X_1 \in A \mid X_0 = x)\, dx$

$$= \int \pi(x) \int q_c(p)\, \mathbb{P}(X_1 \in A \mid X_0 = x, P = p)\, dp\, dx$$

$$= \int \pi(x) \int q_c(p) \Big[\min(1, e(H(p,x) - H(S_L(p,x)))\, \mathbb{1}_A(S_L(p,x))$$

$$+ (1 - \min(*))\, \mathbb{1}_A(x) \Big]\, dx\, dp$$

$$= \int_A \pi(x)\, dx + \frac{1}{Z} \iint \min\left[e^{-H(p,x)}, e^{-H(S_L(p,x))} \right] \mathbb{1}_A(S_L(p,x))\, dx\, p\, x$$

(WTS)

$$-\frac{1}{Z}\iint \min\left(e^{-H(p,x)}, e^{-H(S_L(p,x))}\right) \mathbb{1}_A(x)\,dx\,dp$$

Looking at this last term we do the change of variable given by

$(p',x') \longmapsto S_L(p,x)$ or $S_L^{-1}(p',x') = (p,x)$

S_L simplectic $\Longrightarrow |\det \nabla S_L^{-1}(p,x)| = 1$

$$\Longrightarrow \iint \min\left(e^{-H(S_L^{-1}(p',x'))}, e^{-H(p',x')}\right) \mathbb{1}_A(x')\,dx'\,dp'$$

$\Longrightarrow H(S_L^{-1}(p',x')) = H(S_L(-p',x'))$ by symmetry of $H(\cdot,x)$

Plugging back in gives

$$= \iint_A \min\left(e^{-H(S_L(-p,x))}, e^{-H(p,x)}\right) dp\,dx$$

$p \longmapsto -p$ gives

$$\iint_A \min\left(e^{-H(S_L(p,x))}, e^{-H(p,x)}\right) dp\,dx$$

Therefore these terms cancel and we get

$$\mathbb{P}(X_1 \in A) = \int_A \pi(x_0)\, dx_0 = \mathbb{P}(x_0 \in A).$$

$\blacksquare$

Rmk: Proof didn't rely on $U(\cdot)$ so we can have some flexibility in choice of $U(\cdot)$.