$f \leftarrow$ target

$X_1, X_2, \ldots$

$p(x|y)$

$\hookrightarrow$ density for X_t, conditional on $X_{t-1} = y$

if we find some $p(x|y)$ s/t

f is stationary wrt to $p(x|y)$

then regardless of how we sample

X_1 $\quad P_t \longrightarrow f$ as t gets large

the question here:

how do we find such a transition kernel

$\Rightarrow$ partially answered using the metropolis hasting algorithm

① generate a proposal $h(x|y)$

② $a(x|y)$

$$a(x|y) = \min\left(1, \frac{f(x)\,h(y|x)}{f(y)\,h(x|y)}\right)$$

Random Walk Metropolis- Hastings

① $X_t = y$

$\Delta y \sim MVN(\vec{0}, \Sigma)$

proposal $y + \Delta y = x$

$$h(x|y) = f_{0,\Sigma}(x-y)$$
$$= f_{0,\Sigma}(y-x) = h(y|x)$$

$$a(x|y) = \min\left(1, \frac{f'(x)\,\cancel{h(y|x)}}{f(y)\,\cancel{h(x|y)}}\right)$$

$$= \min\left(1, \frac{f'(x)}{f(y)}\right)$$

<u>Hamiltonian Monte Carlo</u>

$h(x|y)$ that always has $a(x|y)$ of 100%.

that also gets far away

$X_t \in \mathbb{R}^d$

$X_t = x$

$\rho \in \mathbb{R}^d$ momentum vector

$\rho \sim MVN(0, \Sigma)$ $\quad \rho \perp\!\!\!\perp X_t$

$$H(x, \rho) = -\log(p_{x,\rho}(x, \rho))$$

$$= -\log(p_{\rho|x}(\rho|x)\,p(x))$$

$T(\rho)$

$$= -\log(p_\rho(\rho)) \quad \text{kinetic}$$

$$-\log(f(x))$$

$V(x)$ potential energy

$x(s)$ $\rho(s)$ up until K

s/t $H(x(s), \rho(s)) = c$

$$0 = \frac{\partial H}{\partial s} = \frac{\partial H}{\partial x}\frac{\partial x}{\partial s} + \frac{\partial H}{\partial \rho}\frac{\partial \rho}{\partial s}$$

$$= \frac{\partial V}{\partial x}\frac{\partial x}{\partial s} + \frac{\partial T}{\partial \rho}\frac{\partial \rho}{\partial s}$$

$$\frac{\partial x}{\partial s} = \frac{\partial T}{\partial \rho} \quad \& \quad -\frac{\partial V}{\partial x} = \frac{\partial \rho}{\partial s}$$

$$x(s) = x(0) + \int_0^s \frac{\partial T}{\partial \rho(u)}\, du$$

$$p(s) = p(0) - \int_0^s \frac{\partial V}{\partial x(u)}\, du$$

$$\frac{\partial T}{\partial p} = \underbrace{\Sigma^{-1} p}$$

$$(X, p) \xrightarrow[\text{until } K]{\text{evolve system}} (Y, p_N)$$

$$h(y|x) = \exp(-T(p))$$

$$h(x|y) = \exp(-T(p_N))$$

$$f(x) = \exp(-V(x))$$

$$f(y) = \exp(-V(y))$$

$$a(y|x) = \min\left(1, \frac{f(y)\, h(x|y)}{f(x)\, h(y|x)}\right)$$

$T(p))$

$$-(V(y) + T(p_N))$$

$$= \frac{\exp(-\underbrace{V(y) - T(p_N)}))}{\exp(-V(x) - T(p))}$$

$$= \exp(H(x, p) - H(y, p_N))$$

$$= 1$$

Need to do: solve differential equations numerically.

$\varepsilon > 0$ relatively step-size

leap frog integrator

(x_0, p_0)

N steps of size ε for X

$$N\varepsilon = K$$

$2N$ steps of size ε for p

$$p_{1/2} = p_0 - \frac{\varepsilon}{2} \frac{\partial V}{\partial x}(x_0)$$

$$x_1 = x_0 + \varepsilon \cdot \frac{\partial T}{\partial p}(p_{1/2})$$

$$= x_0 + \varepsilon \cdot \Sigma^{-1} p_{1/2}$$

$$p_1 = p_{1/2} - \frac{\varepsilon}{2} \frac{\partial V}{\partial x}(x_1)$$

$$p_{3/2} = p_1 - \frac{\varepsilon}{2} \frac{\partial V}{\partial x}(x_1)$$

$$x_2 = x_1 + \varepsilon \Sigma^{-1} p_{3/2}$$

$$p_2 = \ldots$$

$$(x_N, p_N)$$

$$a(x_N | x_0) = \min\left(1, \exp\left(H(x_0, p_0) - H(x_N, p_N)\right)\right)$$