Suppose that π is our target of interest on $\mathbb{R}^p$

Define the map $T: \mathbb{R}^p \to \mathbb{R}^p$ s.t. $T^{-1} = T$.

Ex: $T(x_1, \dots, x_p) = (x_2, x_1, x_3, \dots, x_p)$

Algo: Given $X_n = x$ do

(1) Compute $y = T(x)$

(2) Set

$$X_{n+1} = \begin{cases} y & \text{wp} \quad \alpha(x,y) \\ x & \text{wp} \quad 1-\alpha(x,y) \end{cases}$$

$$\alpha(x,y) = \min\left[1, \frac{\pi(y)}{\pi(x)\,|\det(\nabla T(y))|}\right]$$

Proposition: If $X_0 \sim \pi$ then $X_1 \sim \pi$.

Pf: We look to show that the chain is π reversible

$$T_1 \equiv \int_A \pi(x) P(x,B)\,dx = \int_B \pi(x) P(x,A)\,dx \equiv T_2$$

for all $A, B \in \mathcal{F}$. when $P(x,A) = \mathbb{P}(X_1 \in A \mid X_0 = x)$

[Why is this sufficient?

W.t.s. $P(X_1 \in A) = \int_A \pi(x)\,dx$ if $X_0 \sim \pi$

But also notice that

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

So if we can show

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

then choose A to finish. $\lrcorner$

Now notice

$$\mathbb{P}(x, A) = \alpha(x, T(x))\,\mathbb{1}_A(T(x)) + (1 - \alpha(x,y))\,\mathbb{1}_A(x)$$

$$T_1 = \int_A \pi(x)\,\alpha(x, T(x))\,\mathbb{1}_B(T(x))\,dx + \int \pi(x)\,(1-\alpha(x,y))\,\mathbb{1}_B(x)\,dx$$

$$//$$

$$T_2 = \int_B \pi(x)\,\alpha(x, T(x))\,\mathbb{1}_A(T(x))\,dx + \int \pi(x)\,(1-\alpha(x,y))\,\mathbb{1}_A(x)\,dx$$

With a multivariate change of variables we see

$$T(x) = y \implies x = T^{-1}(y) = T(y) \implies dx = |\det(\nabla T(y))|\,dy$$

which yields

$$\int_A \pi(x)\,\alpha(x, T(x))\,\mathbb{1}_B(T(x))\,dx$$

$$= \int_{\mathbb{R}^p} \pi(T(y))\, \alpha(T(y), y)\, |\det \nabla T(y)|\, 1_A(T(y))\, 1_B(y)\, dy$$

therefore $T_1 = T_2$ iff

$$\pi(x)\alpha(x, T(y)) = \pi(T(x))\, \alpha(T(x), y)\, |\det \nabla T(x)|, \quad \forall x \in \mathbb{R}^p.$$

But as

$$\pi(x)\alpha(x, T(x)) = \min\left[\pi(x), \frac{\pi(T(x))}{|\det(\nabla T(T(x)))|}\right]$$

$$= \min\left[\pi(x), \pi(T(x))\, |\det(\nabla T(x))|\right]$$

and $\pi(T(x))\, |\det(\nabla T(x))|\, \alpha(T(x), x)$

$$= \pi(T(x))\, |\det(\nabla T(x))| \min\left(1, \frac{\pi(x)}{\pi(T(x))\, |\det(\nabla T(x))|}\right)$$

Therefore ______ is satisfied by our choice of $\alpha(x, y)$.

Parallel Tempering

Suppose we can write

$$\pi(x_1, \dots, x_K) = \prod_{i=1}^{K} \pi_i(x_i), \quad \pi_i(x) \propto e^{-U(x)/t}$$

for $1 = t_1 < t_2 < \cdots < t_K$

Suppose $T(x_1, \dots, x_K) = (x_2, x_1, \dots, x_K)$

$$\Longrightarrow \nabla T(x_1, \dots, x_K) = \begin{pmatrix} \square & \square & & \\ & & \square & \\ & & \square & \\ & & & \ddots \end{pmatrix}$$

$$\det \nabla T(x_1, \dots, x_n) = \pm 1$$

$$\alpha(x, T(x)) = \min\left\{1, \frac{\pi(T(x))}{\pi(x)} \cdot \frac{1}{|\det \nabla T(x)|}\right\}$$

$$= \min\left\{1, \frac{\pi(x_2, x_1, \dots, x_K)}{\pi(x_1, x_2, \dots, x_n)}\right\}$$

$$= \min\left\{1, \frac{\pi_1(x_1)\pi_1(x_2)}{\pi_1(x_1)\pi_2(x_2)}\right\}$$

Hamitonian Monte Carlo

$$\pi(x) \propto \exp(-U(x)) \qquad U : \mathbb{R}^d \mapsto \mathbb{R} \qquad U \in C^2$$

Introduce a new variable $p \in \mathbb{R}$ momentum

which gives

$$\pi(p, x) \propto \exp\left\{-\frac{1}{2} p^T C^{-1} p - U(x)\right\}$$

when C is a p.s.d. matrix

$\pi(x) = \int \pi(p,x)\,dp$ and we try to instead

sample from $\overline{\pi}$.

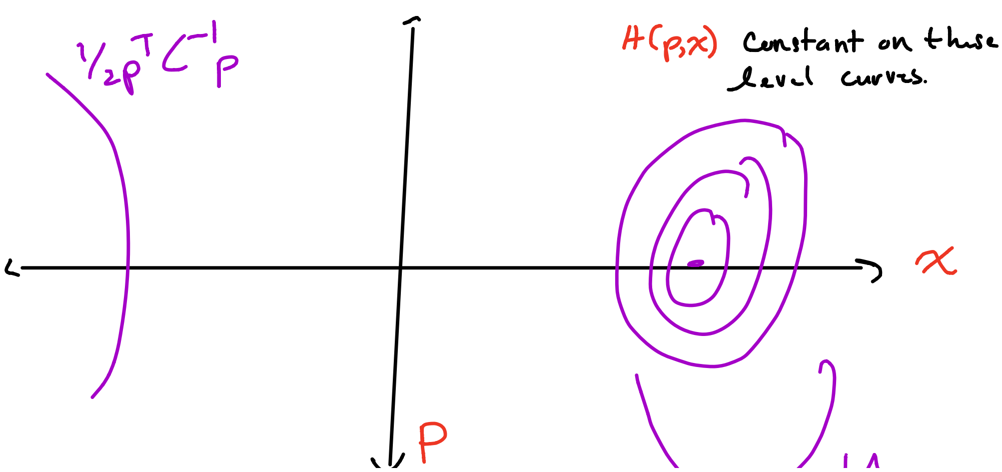
Define the <u>hamiltonian</u> $H(p,x) = \frac{1}{2} p^T C^{-1} p + U(x)$

Want to find the curve in which $H(p,x)$ is constant.

Consider the O.D.E. with initial conditions (p_0, x_0)

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

<u>Note</u>: $\dfrac{d}{dt} H(p_t, x_t) = \dfrac{\partial}{\partial p} H(p_t, x_t) \dfrac{dp_t}{dt} + \dfrac{\partial H}{\partial x}(p_t, x_t) \dfrac{dx_t}{dt} = 0$



Set $y=\begin{pmatrix}p\\ x\end{pmatrix}$ then the Hamiltonian flow can be written as

$$\frac{dy_t}{dt} = \underbrace{\begin{bmatrix}0 & -I\\ I & 0\end{bmatrix}}_{J^T}\underbrace{\begin{pmatrix}\partial/\partial p\, H(p_t,x_t)\\ \partial/\partial t\, H(p_t,x_t)\end{pmatrix}}_{\nabla H(y_t)}$$

$$\frac{dy_t}{dt} = J^T \nabla H(y_t)$$

Set $H_t : (p_0, x_0) \longmapsto (p_t, x_t)$

H_t satisfies

$$\nabla H_t(y)\, J\, \nabla H_t^T(y) = J \quad \forall y$$

$$\Longrightarrow \quad \det \nabla H_t(y) = \pm 1$$

With this we can set up a similar alg. as before.

<u>Algo:</u> Given $x_k = x$:

1. Draw $\bar{p} \sim N(0,C)$
2. Propose $(\bar{\bar{p}}, y) = H_t(\bar{p}, x)$

Set $\quad X_{n+1} = \begin{cases} y & \text{w.p. } \alpha \\ x & \text{w.p. } 1-\alpha \end{cases} \qquad \alpha = \min\left\{1,\ e^{-H(\bar{p},y)+H(\bar{p},x)}\right\}$