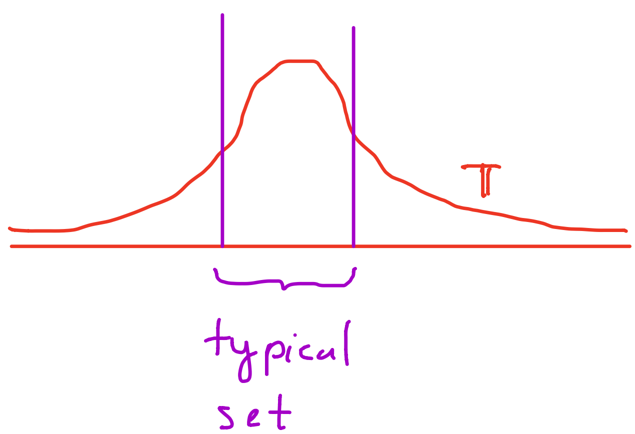
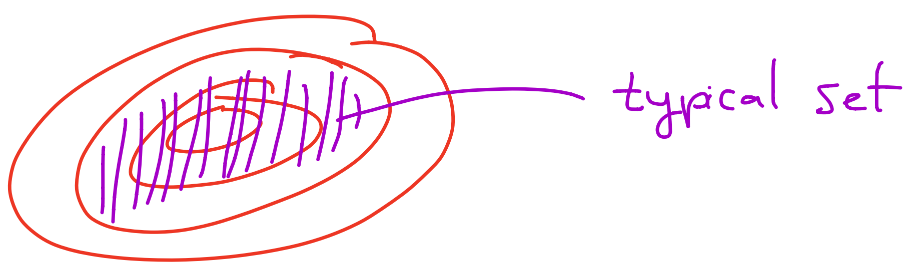
Hamiltonian Monte Carlo

Suppose we have a target π that contains a "typical set"



that is "very" curved e.g.



<u>Rmk</u>: A R.W. sampler on the boundary will reject with 50% prob.

Rmk: Can we correct to stay with the typical set?

One way of doing this Hamiltonian MC

Target: π **Parameter of interest:** z

Recall on the lattice

$$\pi(z) \propto \exp\{-\underbrace{E}_{\text{Energy}}(\underbrace{z}_{\text{state}})\}$$

We can extend this metaphor to include momentum

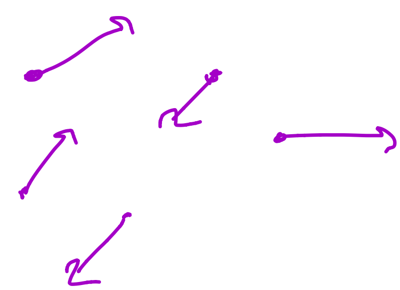
$$\pi(p,z) \propto \exp\{-H(\underbrace{p}_{\text{momentum}},z)\}$$

Hamiltonian

energy

$\pi(q)$ "state space"

$\pi(p, q)$ "phase space"



Notice

$$\pi(p, q) = \pi(p|q)\,\pi(q)$$

So

$$H(p, q) = K(p, q) + V(q)$$

$$V(q) = -\log \pi(q) \quad \text{Potential Energy}$$

$K(p, q) = -\log \pi(p \mid q)$ kinetic energy

Usually we take

$$K(p, q) = \frac{1}{2} p^T M^{-1}(q) p + \log |M(q)|$$

mass matrix

We refer to this as the Riemanian - Gaussian kinetics

For fixed M

$K(p) = \frac{1}{2} p^T M p$ (Euclidean - Gaussian kinetics)

We can then use Hamiltonian Dynamics

$$\frac{dz}{dt} = \frac{dH}{dp} = \frac{\partial K}{\partial p}$$

$$\frac{\partial p}{\partial t} = -\frac{\partial H}{\partial z} = -\frac{\partial K}{\partial z} - \frac{\partial U}{\partial z}$$

Ex: For the Euclidean-Gaussian kinetics

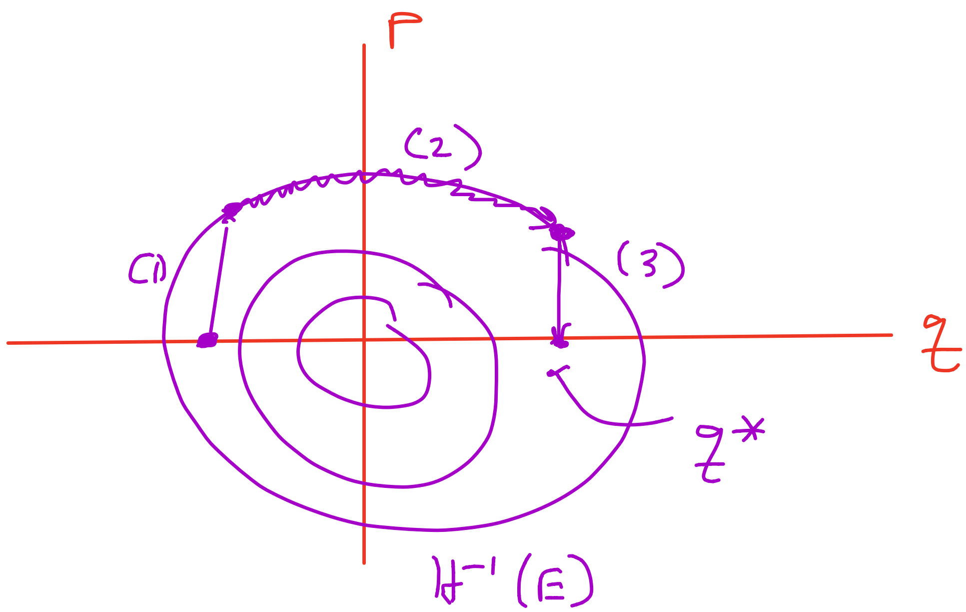
$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial z}\left(-\log \pi(z)\right)$$

$$= \frac{\partial}{\partial z} \log \pi(z)$$ "Score function"

force

$$\frac{\partial z}{\partial t} = \frac{\partial K}{\partial p} = M^{-1} p$$ speed

A Hamiltonian MC proposal has three steps



1. Sample $p^{(t)}$ based on $N(0,m)$

   Compute $H(p^{(t)}, q^{(t)}) = E$

2. Let the dynamics run deterministically on E level set.

3. Project onto Q space.

Random walk on the energy

levels

<u>Rmk</u>: Step (2) requires a "symplectic" integrator.

For Euclidean Gaussian kinetics

take a step size ε and a number of steps $L = \lfloor T/\varepsilon \rfloor$

Choosing ε small enough we have

$$q(t+\varepsilon) \simeq q(t) + \varepsilon \frac{\partial K}{\partial p}(p(t))$$

$$p(t+\varepsilon) \simeq p(t) - \varepsilon \frac{\partial V}{\partial q}(q(t))$$

<u>Euler Method</u>: (ε, L, p, q)

$q_1 \leftarrow q$; $p_1 \leftarrow p$

for: $t = 1, \ldots, L$ do:

for $t = 1, \dots, L$ **do**

$$p_{t+1} \leftarrow p_t - \varepsilon \frac{\partial U}{\partial q}(q_t)$$

$$q_{t+1} \leftarrow q_t + \varepsilon \frac{\partial K}{\partial p}(p_t)$$

return (p_L, q_L)

LeapFrog (ε, L, p, q)

$q_1 \leftarrow q$; $p_1 \leftarrow p$

for: $t = 1, \dots, L$ **do**

$$p_{t+1/2} \leftarrow p_t - \frac{\varepsilon}{2} \frac{\partial U}{\partial q}(q_t)$$

$$q_{t+1} \leftarrow q_t + \varepsilon \frac{\partial K}{\partial p}(p_{t+1})$$

$$p_{t+1} \leftarrow p_{t+1/2} - \frac{\varepsilon}{2} \frac{\partial V}{\partial q}(q_{t+1/2})$$

return: (p_L, q_L)

HMC Step: (Euc-Gaussian Kinetics)

1. Sample $p^{(t)} \sim N(0, m)$

2. $(p^*, q^*) = \text{LeapFrog}(\varepsilon, L, p^{(t)}, q^{(t)})$

3. Can show that

$$\log R(q^{(t)}, q^*) = -H(p^*, q^*) + H(p^{(t)}, q^{(t)})$$

4. $$q^{(t)} = \begin{cases} q^* & \min(1, R(q^{(t)}, q^*)) \\ q^{(t)} & \text{o.w.} \end{cases}$$