HMC with Normalizing Flows

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Normalizing Flows

For a random variable z with a given distribution $z \sim \pi(z)$, and an invertible function $x = f(z)$ with $z = f^{-1}(x)$, we can write

$$p(x) = \pi(z)\left|\det \frac{dz}{dx}\right| = \pi(f^{-1}(x))\left|\det \frac{\partial f^{-1}}{\partial x}\right| \tag{1}$$

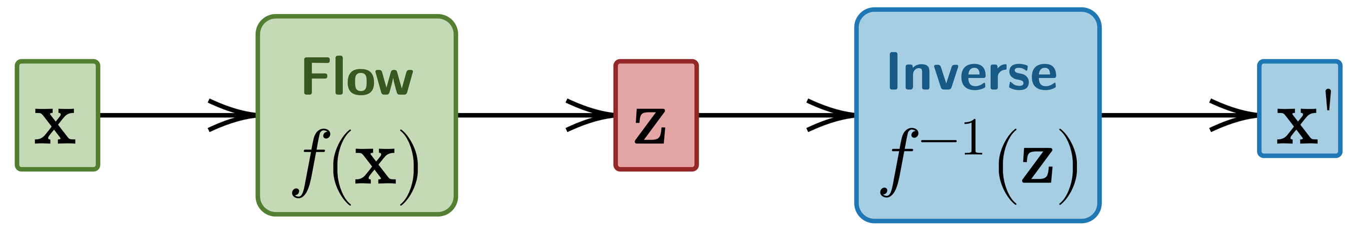

Figure 1. Using a Flow to generate data x'. Image adapted from [3]

We can construct a *normalizing flow* by applying a collection of invertible functions $f_1, f_2, \ldots, f_K$ sequentially, as shown in 2.

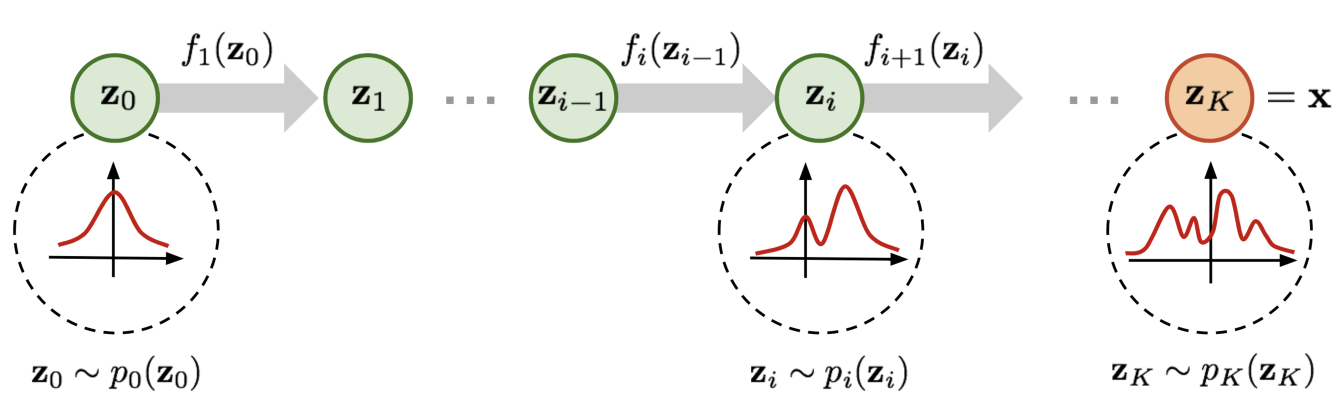

Figure 2. Illustration of a normalizing flow model which maps the initial distribution $p_0(z_0)$ to the final distribution $p_K(z_k)$. Figure from [3]

Hamiltonian Monte Carlo (HMC)

Goal

Sample from (difficult) target distribution $p(x) \propto e^{-S(x)}$. To do this, we construct a chain $x_0 \to x_1 \to, \ldots, \to x_N$ such that $x_N \sim p(x)$ as $N \to \infty$.

Method

1. Introduce $v \sim \mathcal{N}(0, \mathbb{I}_n) \in \mathbb{R}^n$ and write the joint distribution:
$$p(x, v) = p(x)p(v) \propto e^{-S(x)}e^{-\frac{1}{2}v^T v} = e^{-H(x,v)} \tag{2}$$
2. Evolve the joint system $\dot{x} = \frac{\partial H}{\partial v}$, $\dot{v} = -\frac{\partial H}{\partial x}$ using the *leapfrog integrator* along $H = \text{const}$, i.e. $\xi \equiv (x, v) \to (x', v') = \xi'$
3. Accept or reject the proposal configuration ξ' using the Metropolis-Hastings test.

Leapfrog Integrator

1. Half-step (v): $\tilde{v} = v - \frac{\varepsilon}{2}\partial_x S(x)$
2. Full-step (x): $x' = x + \varepsilon\tilde{v}$
3. Half-step (v): $v' = \tilde{v} - \frac{\varepsilon}{2}\partial_x S(x')$

Metropolis-Hastings

$$x_{i+1} = \begin{cases} x' & \text{w/ probability} \quad A(\xi'|\xi) \\ x & \text{w/ probability} \quad \min\left\{1, \frac{p(\xi')}{p(\xi)}\left|\frac{\partial \xi'}{\partial \xi^T}\right|\right\} \end{cases}$$

HMC with Normalizing Flow

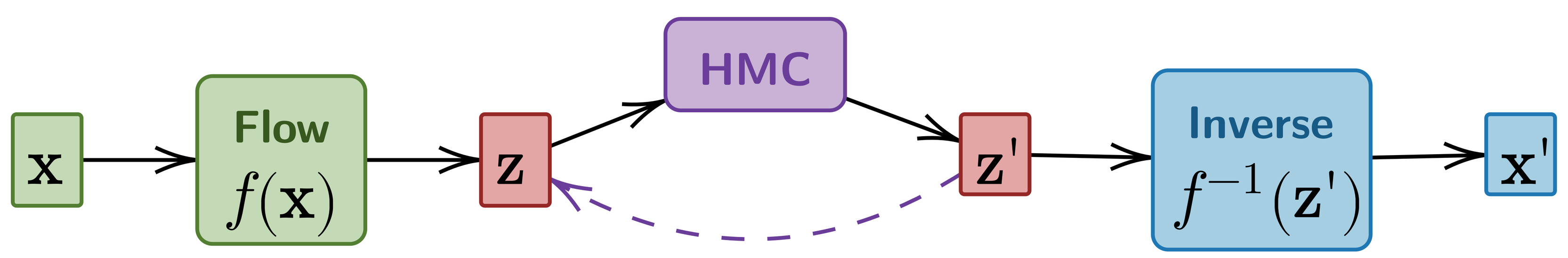

Figure 3. Normalizing Flow with inner HMC block.

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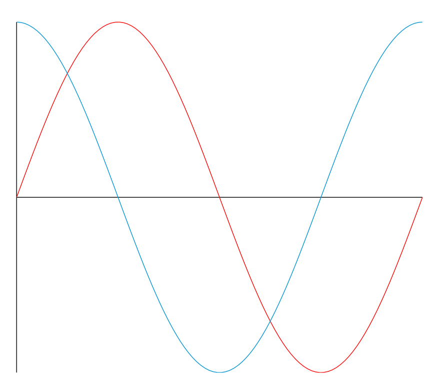

Figure 4. Another figure caption.

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Bar	2.17	1,392	β
Baz	3.14	83,742	δ
Qux	7.59	974	γ

Table 1. A table caption.

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References

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