# HMC with Normalizing Flows

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## Normalizing Flows

For a random variable $z$ with a given distribution $z \sim r(z)$, and an invertible function $x = f(z)$ with $z = f^{-1}(x)$, we can use the change of variables formula to write

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

Where $r(z)$ is the (simple) prior density, and our goal is to generate independent samples from the (difficult) target distribution $p(x)$. This can be done using *normalizing flows* to construct a model density $q(x)$ that approximates the target distribution, i.e. $q(\cdot) \approx p(\cdot)$ for a suitably-chosen flow $f$.

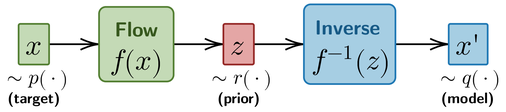



Figure 1. Using a Flow to generate data $x'$. Image adapted from [5]

We can construct a normalizing flow by composing multiple invertible functions $f_i$ so that $x \equiv [f_1 \circ f_2 \circ \cdots \circ f_K](z)$. In practice, the functions $f_i$ are usually implemented as *coupling layers*, which update an "active" subset of the variables, conditioned on the complimentary "frozen" variables.

### Affine Coupling Layers

A particularly useful template function for constructing our normalizing flow is the affine coupling layer which is defined as

$$f(x_1, x_2) = \left(e^{s(x_2)}x_1 + t(x_2),\ x_2\right), \qquad \text{with} \quad \log J(x) = \sum_k [s(x_2)]_k \tag{2}$$

$$f^{-1}(x_1', x_2') = \left((x_1' - t(x_2'))e^{-s(x_2')},\ x_2'\right) \quad \text{with} \quad \log J(x') = \sum_k -[s(x_2')]_k \tag{3}$$

where $s(x_2)$ and $t(x_2)$ are of the same dimensionality as $x_1$ and the functions act elementwise on the inputs.

In order to effectively draw samples from the correct target distribution $p(\cdot)$, our goal is to minimize the error introduced by approximating $q(\cdot) \approx p(\cdot)$. To do so, we use the (reverse) Kullback-Leibler (KL) divergence from Eq. 4, which is minimized when $p = q$.

$$D_{\mathrm{KL}}(q||p) \equiv \int dy\, q(y)[\log q(y) - \log p(y)] \approx \frac{1}{N}\sum_{i=1}^{N}[\log q(y_i) - \log p(y_i)] \quad \text{where} \quad y_i \sim q. \tag{4}$$

## 2D U(1) Gauge Theory

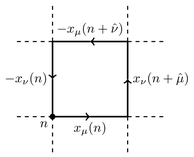



Figure 2. Plaquette

Let $U_\mu(n) = e^{ix_\mu(n)} \in U(1)$, with $x_\mu(n) \in [-\pi, \pi]$ denote the *link variables*, where $x_\mu(n)$ is a link at the site $n$ oriented in the direction $\hat{\mu}$.

We can write our target distribution, $p(x)$, in terms of the Wilson action $S(x)$ as

$$p(x) \propto e^{-S(x)}, \quad \text{where} \quad S(x) \equiv \sum_P 1 - \cos x_P \quad \text{and} \tag{5}$$

$$x_P = x_\mu(n) + x_\nu(n+\hat{\mu}) - x_\mu(n+\hat{\nu}) - x_\nu(n) \tag{6}$$

as shown in Figure. 2. For a given lattice configuration, we can define the *topological charge* $Q \in \mathbb{Z}$ as

$$Q = \frac{1}{2\pi}\sum_P \arg(x_P), \quad \text{where} \quad \arg(x_P) \in [-\pi, \pi] \tag{7}$$

## Trivializing Map

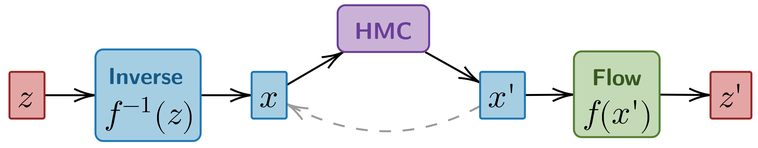



Figure 3. Normalizing Flow with inner HMC block.

Our goal is to evaluate expectation values of the form

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}}\int dx\, \mathcal{O}(x) e^{-S(x)}. \tag{8}$$

. Using a normalizing flow, we can perform a change of variables $x = f(z)$ so Eq. 8 becomes

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}}\int dz\, |\det[J(z)]|\, \mathcal{O}(f(z))\, e^{-S(f(z))}, \quad \text{where} \quad J(z) = \frac{\partial f(z)}{\partial z} \tag{9}$$

$$= \frac{1}{\mathcal{Z}}\int dz \mathcal{O}(f(z)) e^{-S(f(z)) + \log|\det[J(z)]|}. \tag{10}$$

The Jacobian matrix $J(z)$ must satisfy

1. Injective (1-to-1) between domains of integration
2. Continuously differentiable (*or*, differentiable with continuous inverse).

The function $f$ is a *trivializing map* when $S(f(z)) - \log|\det J(z)| = \text{const.}$, and our expectation value simplifies to

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}^*}\int dz\, \mathcal{O}(f(z)) \quad \text{where} \quad \frac{1}{\mathcal{Z}^*} = \frac{1}{\mathcal{Z}}\exp(-\text{const}). \tag{11}$$

## HMC with Normalizing Flows

We can implement the trivializing map defined above using a normalizing flow model. For conjugate momenta $\pi$, we can write the Hamiltonian

$$H(z, \pi) = \frac{1}{2}\pi^2 + S(f(z)) - \log|\det J(f(z))| \tag{12}$$

and the associated equations of motion as

$$\dot{z} = \frac{\partial H}{\partial \pi} = \pi \tag{13}$$

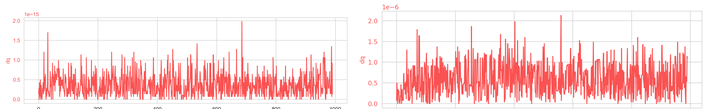
$$\dot{\pi} = -J(z)S'(f(z)) + \mathrm{tr}\left[J^{-1}\frac{d}{dz}J\right] \tag{14}$$

If we introduce a change of variables $\pi = J(z)\rho = J(f^{-1}(x))\rho$ and $z = f^{-1}(x)$, the determinant of the Jacobian matrix reduces to 1 and we obtain the modified Hamiltonian

$$\tilde{H}(x, \rho) = \frac{1}{2}\rho^\dagger\rho + S(x) - \log|\det J|. \tag{15}$$

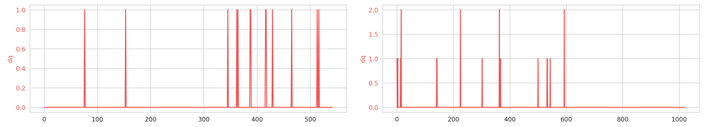
As shown in Fig. 3, we can use $f^{-1} : z \to x$ to perform HMC updates on the transformed variables $x$, and $f : x \to z$ to recover the physical target distribution.

## Results




(a) $8 \times 8$ lattice, HMC (b) $16 \times 16$ lattice, HMC

Figure 4. Topological charge vs MC trajectory for HMC, demonstrating *topological freezing* resulting in large integrated autocorrelation times.




(a) $8 \times 8$ lattice, HMC with Normalizing Flow (b) $16 \times 16$ lattice, HMC with Normalizing Flow

Figure 5. Topological charge vs MC trajectory for ftHMC demonstrating an improvement in the topological tunneling, indicating an improvement against HMC.

## References

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