

HMC with Normalizing Flows

Sam Foreman¹, Taku Izubuchi², Luchang Jin³, Xiao-Yong Jin¹, James C. Osborn¹, Akio Tomiya³

¹Argonne National Laboratory ²RIKEN-BNL ³University of Connecticut

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

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

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 .

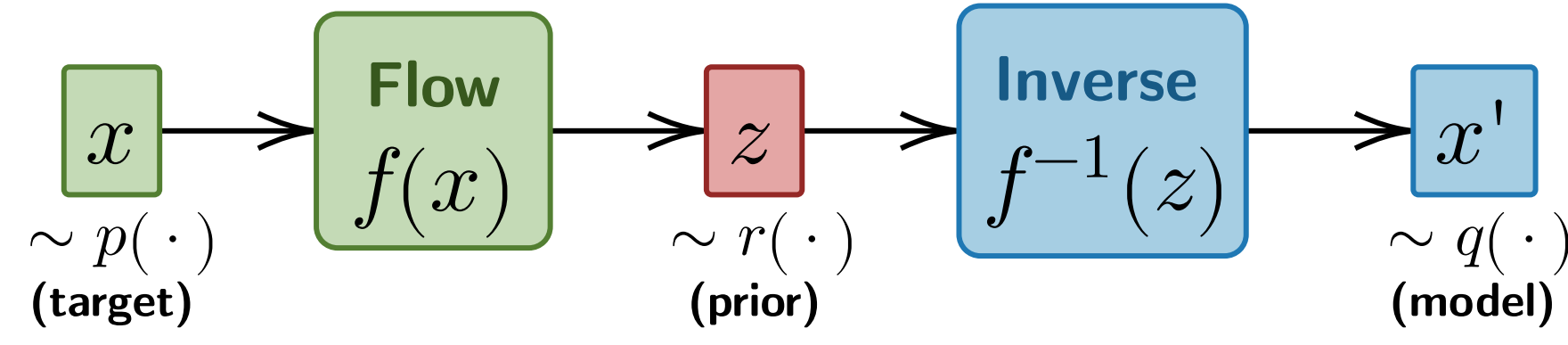


Figure 1. Using a Flow to generate data x' . Image adapted from [5]

We can construct a normalizing flow by composing multiple invertible functions f_i so that $x \equiv [f_1 \circ f_2 \circ \dots \circ f_K](z)$. 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

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

$$f^{-1}(x'_1, x'_2) = \left((x'_1 - t(x'_2)) e^{-s(x'_2)}, x'_2 \right) \quad \text{with} \quad \log J(x') = \sum_k -[s(x'_2)]_k \quad (3)$$

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 $p = q$.

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

Hamiltonian Monte Carlo (HMC)

1. Introduce $v \sim \mathcal{N}(0, \mathbb{I}_n) \in \mathbb{R}^n$ and write the joint distribution:

$$p(x, v) = p(x)p(v) \propto e^{-S(x)} e^{-\frac{1}{2}v^T v} = e^{-H(x, v)}. \quad (5)$$

2. Evolve the joint system $\xi \equiv (\dot{x}, \dot{v})$ using Hamilton's equations along $H = \text{const.}$

3. Accept or reject the proposal configuration using the Metropolis-Hastings test.

Leapfrog Integrator:

1. $\tilde{v} \leftarrow v - \frac{\varepsilon}{2} \partial_x S(x)$
2. $x' \leftarrow x + \varepsilon \tilde{v}$
3. $v' \leftarrow \tilde{v} - \frac{\varepsilon}{2} \partial_x S(x')$

Metropolis-Hastings:

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

Trivializing Map

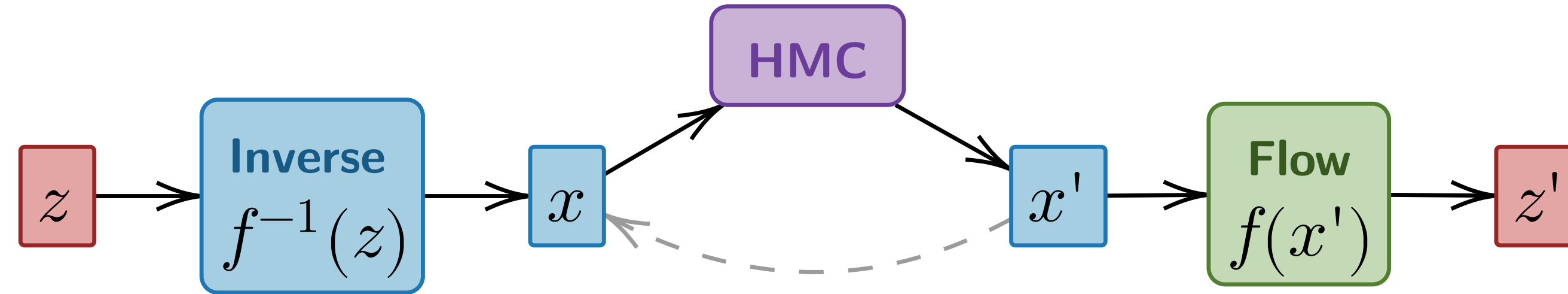


Figure 2. Normalizing Flow with inner HMC block.

Our goal is to evaluate expectation values of the form

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int dx \mathcal{O}(x) e^{-S(x)}. \quad (6)$$

. Using a normalizing flow, we can perform a change of variables $x = f(z)$ so Eq. 6 becomes

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int dz |\det[J(z)]| \mathcal{O}(f(z)) e^{-S(f(z))}, \quad \text{where} \quad J(z) = \frac{\partial f(z)}{\partial z} \quad (7)$$

$$= \frac{1}{\mathcal{Z}} \int dz \mathcal{O}(f(z)) e^{-S(f(z)) + \log |\det[J(z)]|}. \quad (8)$$

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

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}^*} \int dz \mathcal{O}(f(z)) \quad \text{where} \quad \frac{1}{\mathcal{Z}^*} = \frac{1}{\mathcal{Z}} \exp(-\text{const}). \quad (9)$$

HMC with Normalizing Flows

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

$$H(z, \pi) = \frac{1}{2} \pi^2 + S(f(z)) - \log |\det J(f(z))| \quad (10)$$

and the associated equations of motion as

$$\dot{z} = \frac{\partial H}{\partial \pi} = \pi \quad (11)$$

$$\dot{\pi} = -J(z) S'(f(z)) + \text{tr} \left[J^{-1} \frac{d}{dz} J \right] \quad (12)$$

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

$$\tilde{H}(x, \rho) = \frac{1}{2} \rho^\dagger \rho + S(x) - \log |\det J|. \quad (13)$$

As shown in Fig. 2, we can use $f^{-1} : z \rightarrow x$ to perform HMC updates on the transformed variables x , and $f : x \rightarrow z$ to recover the physical target distribution.

Acknowledgements

This research used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357. This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.

2D U(1) Gauge Theory

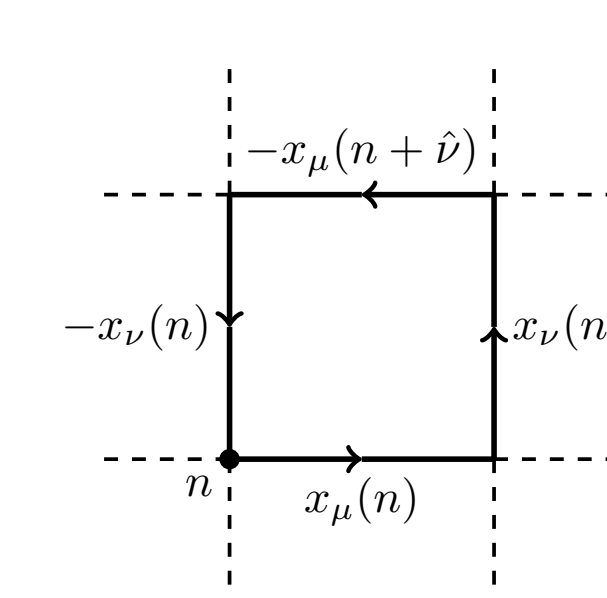


Figure 3. Plaquette

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

$$p(x) \propto e^{-S(x)}, \quad \text{where} \quad S(x) \equiv \sum_P 1 - \cos x_P \quad \text{and} \quad (14)$$

$$x_P = x_\mu(n) + x_\nu(n + \hat{\mu}) - x_\mu(n + \hat{\nu}) - x_\nu(n) \quad (15)$$

as shown in Figure. 3. For a given lattice configuration, we can define the *topological charge* $Q \in \mathbb{Z}$ as

$$Q = \frac{1}{2\pi} \sum_P \arg(x_P), \quad \text{where} \quad \arg(x_P) \in [-\pi, \pi]. \quad (16)$$

We are interested in how this quantity evolves over a finite length Markov Chain, in particular we can define the *tunneling rate*, dQ as

$$dQ = \sqrt{(Q_{i+1} - Q_i)^2} \quad (17)$$

where the difference is between subsequent states in the chain.

Results

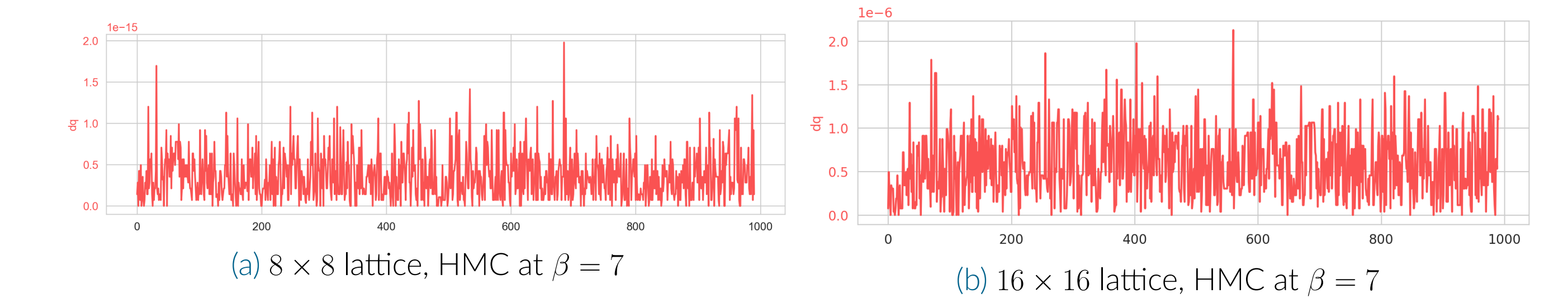


Figure 4. Tunneling rate vs MC trajectory for HMC, demonstrating *topological freezing* resulting in large integrated autocorrelation times.

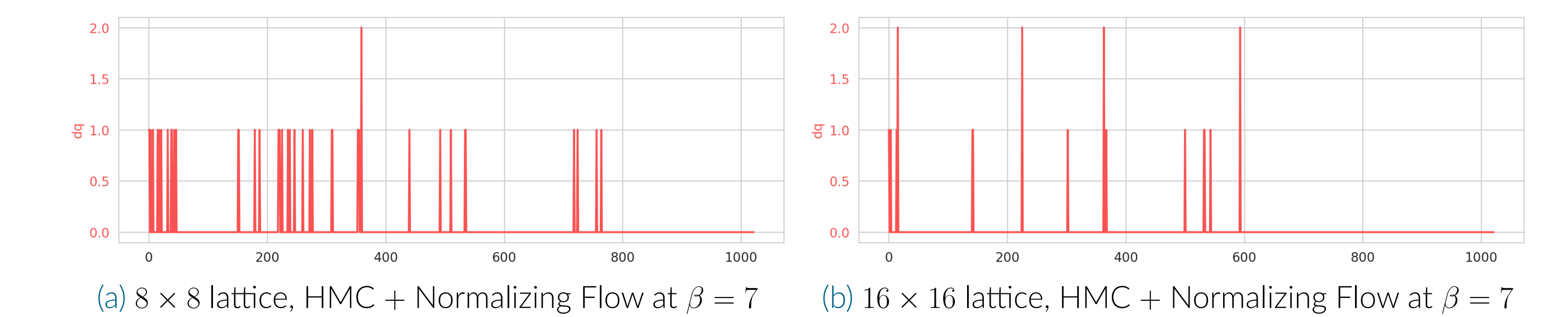


Figure 5. Tunneling rate vs MC trajectory for HMC with trained Normalizing Flow, demonstrating an improved tunneling rate compared to HMC.

References

- [1] Michael S. Albergo, Denis Boyda, Daniel C. Hackett, Gurtej Kanwar, Kyle Cranmer, Sébastien Racanière, Danilo Jimenez Rezende, and Phiala E. Shanahan. Introduction to normalizing flows for lattice field theory, 2021.
- [2] Luigi Del Debbio, Joe Marsh Rossney, and Michael Wilson. Efficient modelling of trivializing maps for lattice ϕ^4 theory using normalizing flows: A first look at scalability, 2021.
- [3] Martin Lüscher. Trivializing maps, the wilson flow and the hmc algorithm. *Communications in Mathematical Physics*, 293(3):899–919, Nov 2009.
- [4] Martin Lüscher. Trivializing maps, the wilson flow and the hmc algorithm. *Communications in Mathematical Physics*, 293(3):899–919, Nov 2009.
- [5] Lilian Weng. Flow-based deep generative models. *lilianweng.github.io/lil-log*, 2018.