

HMC with Normalizing Flows

**Sam Foreman,^{a,*} Taku Izubuchi,^{b,c} Luchang Jin,^d Xiao-Yong Jin,^a James C. Osborn^a
and Akio Tomiya^b**

^a*Argonne National Laboratory,
Lemont, IL 60439*

^b*RIKEN,
2-1 Hirosawa, Wako, Saitama, 351-0198, Japan*

^c*Brookhaven National Laboratory,
Upton, NY 11973*

^d*Dept. of Physics, University of Connecticut,
Storrs, CT 06269*

*E-mail: foremans@anl.gov, izubuchi@bnl.gov, luchang.jin@uconn.edu,
xjin@anl.gov, osborn@alcf.anl.gov*

We propose using Normalizing Flows as a trainable kernel within the molecular dynamics update of Hamiltonian Monte Carlo (HMC). By learning (invertible) transformations that simplify our dynamics, we can outperform traditional methods at generating independent configurations. We show that, using a carefully constructed network architecture, our approach can be easily scaled to large lattice volumes with minimal retraining effort.

*The 38th International Symposium on Lattice Field Theory
26-30 July 2021
Zoom / Gather @ MIT, Cambridge MA, USA*

*Speaker

1. Introduction

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. $q(\cdot) \simeq p(\cdot)$ for a suitably-chosen flow f .

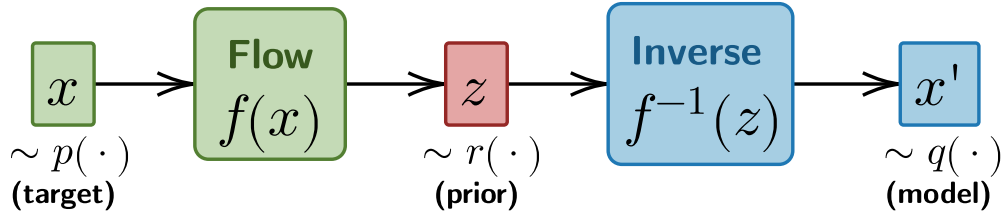


Figure 1: Using a flow to generate data x' . Image adapted from []

References

- [1]