

HMC with Normalizing Flows

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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.

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References

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