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Machine Learned Thermodynamics of Physical Systems Across Critical Phases

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In recent years, there has been a growing interest in the application of normalizing flows for sampling in lattice field theory. Successful achievements have been made in various domains, including scalar field theories, U(1) and SU(N) pure gauge theories, as well as fermionic gauge theories. Furthermore, recent developments have shown promising results for full Lattice QCD. Although these flow-based sampling methods remain challenging to scale for desired systems, they possess desirable properties that make them an attractive tool, despite their current limitations.
In particular, the combination of normalizing flows with importance sampling has demonstrated accurate measurement of thermodynamic observables. These quantities are typically difficult to estimate using standard sampling algorithms such as HMC. However, it is worth noting that normalizing flows are typically trained through self-sampling in this specific context, which introduces the risk of assigning extremely low probability mass to certain modes of the theory. This issue may lead to substantially biased estimators of physical observables, due to mode-collapse during the training phase of the algorithm.
In this work, we first introduce a framework that allows for the derivation of asymptotically unbiased estimators for thermodynamic observables. Secondly, we investigate the mode-mismatch phenomenon, both theoretically and numerically. We provide a detailed analysis of the mode-seeking nature of the standard self-sampling-based training procedure and compare it with alternative training objectives. Finally, we present numerical and theoretical results, including a derived bound on the bias of the estimator for physical observables. This proposal offers a natural metric to quantify the extent of mode-collapse in the sampler.

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