Contribution ID: **5** Type: **Talk**

The quest for the lost mode: Overcoming Mode-Collapse in Flow-Based Sampling for Lattice Field Theories

Friday, 22 December 2023 11:15 (30 minutes)

Normalizing flows allow for independent sampling. For this reason, it is hoped that they can avoid the tunneling problem of local-update MCMC algorithms for multi-modal distributions. In this work, we first point out that the tunneling problem is also present for normalizing flows but is shifted from the sampling to the algorithm's training phase. Specifically, normalizing flows often suffer from mode-collapse for which the training process assigns vanishingly low probability mass to relevant modes of the physical distribution. This may result in a significant bias when the flow is used as a sampler in a Markov-Chain or with Importance Sampling. We propose a metric to quantify the degree of mode-collapse and derive a bound on the resulting bias. Furthermore, we propose various mitigation strategies in particular in the context of estimating thermodynamic observables, such as the free energy

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Session Classification: Machine learning for Lattice Field Theory