Machine Learning in Natural Sciences: from Quantum Physics to Nanoscience and Structural Biology

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Machine learning of thermodynamic observables in lattice quantum field theory

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The application of Machine Learning techniques in many field of theoretical physics has been very successful in the last years, leading to great improvement over existing standard methods.

In this work, we demonstrate how deploying deep generative machine learning models for estimating thermodynamic observables in lattice field theory

is a promising route for addressing many drawbacks typical of Markov Chain Monte Carlo (MCMC) methods. More specifically, we show that generative models can be used to estimate the absolute value of the free energy, which is in contrast to existing MCMC-based methods which are limited to only estimate free energy differences. Moreover, we combine this with two efficient sampling techniques namely neural importance sampling (NIS) and neural HMC-estimation (NHMC) and leverage on the fact that some kind of deep generative models give access to a good approximation of the true Boltzmann distribution. We demonstrate the effectiveness of the proposed method for two-dimensional ϕ^4 theory and compare it to MCMC-based methods in detailed numerical experiments.

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