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GeN S: the new generation of sampling algorithms

The task of learning non-trivial probability densities is a crucial problem in machine learning with an uncountable number of applications in, among others, computer vision, sound synthesis, text generation, and natural sciences. The subfield of machine learning that leverages deep learning to learn complicated probability distributions and samples from them is known as Generative AI. Recently, the relevance of this problem has been extensively studied in several domains where deep generative models have been proposed to sample non-trivial Boltzmann-like densities in, for instance, lattice quantum field theory and statistical mechanics. Learning the underlying density, namely a normalized Boltzmann distribution, greatly improves the sampling task and opens the possibility of estimating physical observables, such as the partition function and related thermodynamic observables, which are notoriously hard to be estimated using standard sampling methods. I refer to this novel approaches as GEnerative Neural Samplers, or, “Gen S” for short: the new generation of sampling algorithms.

In my talk, I’ll start by describing some key general concepts such as the path integral formalism of quantum field theory and so-called Generative Neural Samplers with Exact Probability (GNSEP), namely, generative models having the desirable feature of allowing for an exact form of the probability density, thereby enabling exact likelihood inference. I will then discuss in more detail two examples of GNSEP, e.g., normalizing flows and variational autoregressive models, and present two Gen S algorithms, namely neural-enhanced sampling approaches, known as NeuralMCMC (NMCMC) and Neural Importance Sampling (NIS). Application of the NIS approach for estimating thermodynamic observables in the context of statistical mechanics and scalar lattice field theory will be presented. I’ll conclude the talk by summarizing the results and briefly discussing the challenges and the current limitations of these methods.

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