



Contribution ID: 11

Type: **not specified**

NETS: A non-equilibrium transport sampler

Tuesday, October 22, 2024 11:50 AM (40 minutes)

We propose an algorithm, termed the Non-Equilibrium Transport Sampler (NETS), to sample from unnormalized probability distributions. NETS can be viewed as a variant of annealed importance sampling (AIS) based on Jarzynski's equality, in which the stochastic differential equation used to perform the non-equilibrium sampling is augmented with an additional learned drift term that lowers the impact of the unbiasing weights used in AIS. We show that this drift is the minimizer of a variety of objective functions, which can all be estimated in an unbiased fashion without backpropagating through solutions of the stochastic differential equations governing the sampling. We also prove that some these objectives control the Kullback-Leibler divergence of the estimated distribution from its target. NETS is shown to be unbiased and, in addition, has a tunable diffusion coefficient which can be adjusted post-training to maximize the effective sample size. We demonstrate the efficacy of the method on standard benchmarks, high-dimensional Gaussian mixture distributions, and a model from statistical lattice field theory, for which it surpasses the performances of related work and existing baselines.

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