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Calibrating Bayesian Generative Machine Learning for Bayesiamplification

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Generative models are on a fast track to becoming a mainstay in particle physics simulation chains, seeing active work towards adoption by nearly every large experiment and collaboration. However, the question of estimating the uncertainties and statistical expressiveness of samples produced by generative ML models is still far from settled.

Recently, combinations of generative and Bayesian machine learning have been introduced in particle physics for both fast detector simulation and inference tasks. These neural networks aim to quantify the uncertainty on the generated distribution originating from limited training statistics. The interpretation of a distribution-wide uncertainty however remains ill-defined. We show a clear scheme for quantifying the calibration of Bayesian generative machine learning models. For a Continuous Normalizing Flow applied to a low-dimensional toy example, we evaluate the calibration of Bayesian uncertainties from either a mean-field Gaussian weight posterior, or Monte Carlo sampling network weights, to gauge their behaviour on unsteady distribution edges. Well calibrated uncertainties can then be used to roughly estimate the number of uncorrelated truth samples that are equivalent to the generated sample and clearly indicate data amplification for smooth features of the distribution.

Track

Uncertainties

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