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Neural Quasiprobabilistic Likelihood Ratio Estimation with Negatively Weighted Data

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The likelihood ratio (LR) plays an important role in statistics and many domains of science. The Neyman-Pearson lemma states that it is the most powerful test statistic for simple statistical hypothesis testing problems [1] or binary classification problems. Likelihood ratios are also key to Monte Carlo importance sampling techniques [2]. Unfortunately, in many areas of study the probability densities comprising the likelihood ratio are defined by implicit models, and so are intractable to compute explicitly [3].

Neural based LR estimation using probabilistic classification has therefore had a significant impact in these domains, providing a scalable method for determining an intractable LR from simulated datasets via the so-called ratio trick [4, 5]. These approaches typically adhere to the standard Kolmogorov axioms of probability theory [6]. In particular, they assume the first axiom: the probability of an event is a non-negative real number. However, there are settings in which synthetically generated data (e.g. Monte Carlo sampling) $\{(x_i, w_i)\}_{i=1}^{N}$ contains weights that are negative $w_i < 0$ [7, 8]. These negative weights are a symptom of a class of distribution known as quasiprobabilities, which do not adhere to the first Kolmogorov axiom. Consequently, the probabilistic-like distribution has a negative density [9]; $q(x) < 0$ for some x.

In high energy physics, negative weights/densities are a commonly observed feature of Monte Carlo simulated proton-proton (pp) collision datasets [10-13]. Whether it be due to quantum interference between Standard Model and new physics processes, or algorithms that match/merge matrix element calculations of beyond leading order Quantum Chromodynamic processes with parton showers, Monte Carlo simulation codes often introduce negatively weighted data.

This work will present a general approach to extending the neural based LR trick to quasiprobabilistic distributions. It will demonstrate that a new loss function, combined with signed probability measures (Hahn-Jordan decomposition), can be used to decompose the likelihoods into signed mixture models. A quasiprobabilistic analog of the Likelihood Ratio is then constructed using a ratio of signed mixture models. The technique is demonstrated using di-Higgs production via gluon-gluon fusion in *pp* collisions at the Large Hadron Collider [14].

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