Approximations of the Inverse Cumulative Distribution Function using Transport Maps and Physics-informed Neural Networks

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1. Problem Statement

Inverse cumulative distribution functions (inverse CDFs), also known as quantile functions, typically lack closed-form analytical solutions for many important probability distributions, including the normal distribution. Approximating inverse CDFs is an inverse problem that plays a critical role in uncertainty quantification and statistical inference. Traditional approaches are often non-parametric, relying on numerical integration and interpolation to build approximate solutions. This paper presents two novel parametric methods that aim to provide more accurate approximations compared to non-parametric methods.

2. Methods:

We propose using a composite approximation function formed by combining a logit function with a neural network. We present two ways to train the neural network: Inverse Transport Map Learning (ITML) and Inverse Physics-informed Learning (IPIL). The ITML approach exploits the fact that when the reference distribution is chosen as a uniform distribution $U(0, 1)$, the associated transport map exactly represents the inverse CDF, enabling the approximation function to be constructed without numerical integration. The IPIL approach formulates the inverse CDF approximation as a differential equation solving problem and leverages physics-informed neural networks to obtain the solution. Although IPIL still requires numerical integration, it avoids the use of interpolation.

3. Experiments:

We conduct validation experiments on standard normal, Beta, Gamma distributions, and a non-normalized abstract distribution. Experimental results show that our proposed parametric methods achieve higher accuracy in inverse CDF approximation compared to existing non-parametric methods. The associated code and datasets are publicly available at: `https://github.com/wuwudawen/IP-Inverse-CDF`.

4. Related Work

The approximation methods proposed in this paper build upon two lines of research, transport maps and physics-informed neural networks. Below is a brief overview of these two areas.

Transport Maps Transport maps are used for sampling and estimating PDFs of unknown probability distributions by constructing a coupling between a reference and target distribution. Triangular maps (Knothe–Rosenblatt rearrangement) offer computational efficiency through their simplified Jacobian determinant calculation [1]. Applications include Bayesian inference [2] and optimized proposal distributions in MCMC [3]. Unlike MCMC, transport maps can directly estimate unknown PDFs without requiring kernel density estimation. In machine learning, normalizing flows represent a neural network-based implementation of transport maps used in generative AI [4].

Physics-informed Neural Networks Deep learning for solving differential equations emerged in the 1990s [5], with recent advances in Physics-informed Neural Networks (PINNs)[6]. PINNs' loss functions combine PDE residuals computed via automatic differentiation with supervised boundary condition errors. Their flexible architecture enables applications across physics and engineering problems[7]. Various PINN variants incorporate either machine learning techniques [8] or finite element methods [9] to improve accuracy. Theoretical studies have addressed existence theorems and stability problems [10].

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