Formatting Instructions For NeurIPS 2023

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Abstract

The abstract paragraph should be indented ½ inch (3 picas) on both the left- and right-hand margins. Use 10 point type, with a vertical spacing (leading) of 11 points. The word **Abstract** must be centered, bold, and in point size 12. Two line spaces precede the abstract. The abstract must be limited to one paragraph.

1 Submission of papers to NeurIPS 2023

2 Introduction

3 Diffusion Models

In this section we quckly review the basics of diffusion models. We focus on the stochastic differential equation formulation first presented by **(author?)** [5].

Let $p(\boldsymbol{y})_{\text{data}}$ denote the data distribution. The goal of a diffusion model is to learn a mapping from a simple distribution $p(\boldsymbol{z})$ to the data distribution $p(\boldsymbol{y})_{\text{data}}$.

This is achived by reversing a diffusion process. In particular, we construct a stochastic differential equation $\boldsymbol{y}(t)$ from $t \in [0, T]$ such that $\boldsymbol{y}(0) \sim p(\boldsymbol{y})_{\text{data}}$ and $\boldsymbol{y}(1) \sim p(\boldsymbol{y}(T))$ is a simple distribution we can sample from and whose evolution is given by

$$d\boldsymbol{y}(t) = \boldsymbol{f}(\boldsymbol{y}(t), t)dt + \boldsymbol{g}(t)d\boldsymbol{w}(t), \tag{1}$$

where $\boldsymbol{w}(t)$ is a standard Brownian motion and $\boldsymbol{f} : \mathbb{R}^d \times [0, T] \to \mathbb{R}^d$ and $\boldsymbol{g} : [0, T] \to \mathbb{R}$ are called the drift coefficient and the diffusion coefficient, respectively.

It is possible to reverse this SDE and sample from $p(\boldsymbol{y})_{\text{data}}$ by first sampling $\boldsymbol{y}(1) \sim p(\boldsymbol{y}(T))$ and then evolving the system backwards in time. This is done by solving the reverse SDE (Cite anderson 1982)

$$d\boldsymbol{y}(t) = [f(\boldsymbol{y}(t), t) - g(t)^2 \nabla_{\boldsymbol{y}(t)} \log p(\boldsymbol{y}(t))]dt + g(t)d\bar{\boldsymbol{w}}(t). \tag{2}$$

where $\bar{\boldsymbol{w}}(t)$ is a standard Brownian with reversed time. Thus because $\boldsymbol{f}$ and g are known, and we construct the SDE so that $p(\boldsymbol{y}(T))$ is simple, as long as we know the score $\nabla_{\boldsymbol{y}(t)} \log p(\boldsymbol{y}(t))$ we can sample from $p(\boldsymbol{y})_{\text{data}}$.

Estimating the Score

An important result by **(author?)** [6] is that it is possible to estimate the score $\nabla_{\boldsymbol{y}(t)} \log p(\boldsymbol{y}(t))$ by computing

$$\boldsymbol{s}^* = \text{argmin}_{\boldsymbol{s} \in \mathcal{S}} \mathbb{E}_t \mathbb{E}_{p(\boldsymbol{y}(0))_{\text{data}}} \mathbb{E}_{p(\boldsymbol{y}(t)|\boldsymbol{y}(0))} \left[\left\| \nabla_{\boldsymbol{y}(t)} \log p(\boldsymbol{y}(t)|\boldsymbol{y}(0)) - \boldsymbol{s}(\boldsymbol{y}(t), t) \right\|^2 \right]. \tag{3}$$

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where $\mathcal{S} = \{\boldsymbol{s} : \mathbb{R}^d \times [0, T] \to \mathbb{R}^d\}$ is the set of all possible score functions indexed by time t, and $\mathbb{E}_t$ denotes the expectaion over uniformly sampled $t \in [0, T]$.

Conditional Diffusion Models

Although it is most common to train diffusion models unconditionally as explained above, one can also train diffusion models conditionally on some input $\boldsymbol{x}$.

To do so we make the following modifications to the above formulation.

1. We construct one separate SDE per value of $\boldsymbol{x}$. Each SDE shares the same drift and diffusion coefficients but the initial distribution $p_{\boldsymbol{x}}(\boldsymbol{y}(0))$ is given by $p(\boldsymbol{y}|\boldsymbol{x})_{\text{data}}$.
2. The reverse SDE is now given by
$$d\boldsymbol{y}(t) = [f(\boldsymbol{y}(t), t) - g(t)^2 \nabla_{\boldsymbol{y}(t)} \log p_{\boldsymbol{x}}(\boldsymbol{y}(t))]dt + g(t)d\bar{\boldsymbol{w}}(t). \tag{4}$$
where $\nabla_{\boldsymbol{y}(t)} \log p_{\boldsymbol{x}}(\boldsymbol{y}(t))$ is the score of the conditional distribution $p_{\boldsymbol{x}}(\boldsymbol{y}(t))$. Importantly, because we choose the diffusion and drift coefficients so that at $t = T$ the distribution is the same for all values of $\boldsymbol{x}$, we can still sample from the data distribution in the same way as before.
3. The final change is that the score function is now estimated by
$$\boldsymbol{s}^* = \text{argmin}_{\boldsymbol{s} \in \mathcal{S}} \mathbb{E}_t \mathbb{E}_{p(\boldsymbol{y}(0), \boldsymbol{x})_{\text{data}}} \mathbb{E}_{p(\boldsymbol{y}(t)|\boldsymbol{y}(0))} \left[\left\| \nabla_{\boldsymbol{y}(t)} \log p(\boldsymbol{y}(t)|\boldsymbol{y}(0)) - \boldsymbol{s}(\boldsymbol{y}(t), \boldsymbol{x}, t) \right\|^2 \right].$$
with the changes being that now $\mathcal{S} = \{\boldsymbol{s} : \mathbb{R}^d \times \mathbb{R}^m \times [0, T] \to \mathbb{R}^d\}$ is the set of all possible score functions but now allowing for the score to depend on the input $\boldsymbol{x}$, and the expectation is taken over the joint distribution $p(\boldsymbol{y}(0), \boldsymbol{x})_{\text{data}}$. We emphasize that the score of the conditional distribution $p(\boldsymbol{y}(t)|\boldsymbol{y}(0))$ is still the same because once we condition on $\boldsymbol{y}(0)$ the distribution is the same for all values of $\boldsymbol{x}$.

This formulation of conditional diffusion models is different than controllable generation as presented in [5]. There, a conditional diffusion model is constructed by noting that
$$\nabla_{\boldsymbol{y}(t)} p(\boldsymbol{y}(t)|\boldsymbol{x}) = \nabla_{\boldsymbol{y}(t)} p(\boldsymbol{y}(t)) + \nabla_{\boldsymbol{y}(t)} p(\boldsymbol{x}|\boldsymbol{y}(t))$$
and hence if we obtain the first term from an unconditional diffusion model, and the second term by differentiating through another trained model $p(\boldsymbol{x}|\boldsymbol{y}(t))$, we can obtain the score of the conditional distribution. In our case this is not feasible because in general the dimension of $\boldsymbol{y}$ will be much smaller than the dimension of $\boldsymbol{x}$.

4 Gradient Boosted Trees

Gradient Boosted Trees (GBT) [2] are a popular non-parametric machine learning model for function approximation. The objective is to find a function $F : \mathbb{R}^d \to \mathbb{R}$ that minimizes
$$L(F) = \mathbb{E}_{\boldsymbol{x},y} \left[l(y, F(\boldsymbol{x})) \right], \tag{5}$$
where $l : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ is a loss function, and the expectation is taken over the joint distribution of the input $\boldsymbol{x}$ and the target y. It does this by imposing the requirement that F is as a scaled sum of M decision trees $f_m : \mathbb{R}^d \to \mathbb{R}$, i.e.
$$F(\boldsymbol{x}) = \sum_{m=1}^{M} \epsilon f_m(\boldsymbol{x}), \quad \epsilon \in (0, 1). \tag{6}$$
where ϵ is a learning rate or shrinkage parameter. In the most basic form of the algorithm each tree is constructed to approximate gradient descent on the loss function $L(F)$. In particular, if we let $F_i = \sum_{m=1}^{i} f_m$ denote the function after i iterations and then the i-th tree is constructed to approximately minimize the squared error
$$f_i = \text{argmin}_f \mathbb{E}_{\boldsymbol{x},y} \left(f(\boldsymbol{x}) - \left. \frac{\partial l(y, \hat{y})}{\partial \hat{y}} \right|_{\hat{y} = F_i(\boldsymbol{x})} \right)^2. \tag{7}$$

using empirical risk minimization and a greedy algorithm to construct the tree.

Various modifications to the basic algorithm have been proposed and implemented such as regularization, special ways of optimizing the tree, support for categorical functions, higher order optimization[1, 3, 4]. In this paper we focus on the implementation of GBTs in the LightGBM library [3] with the understanding that the same principles apply to any other GBT implementation.

5 Treeffuser/Treeffusion Models

For $\boldsymbol{x} \in \mathbb{R}^d$, $\boldsymbol{y} \in \mathbb{R}^m$ the objective of probabilistic predictions is to produce an estimate of the full conditional distribution $\mathbb{P}[\boldsymbol{y}|\boldsymbol{x}]$. This objective is different than in standard regression where the goal is usually to predict $\mathbb{E}[\boldsymbol{y}|\boldsymbol{x}]$.

The most common approach to solve this problem is via parametric models. This procedure assumes that the distribution $\mathbb{P}[\boldsymbol{y}|\boldsymbol{x}]$ can be well approximated by a parametric family of distributions

$$\mathbb{P}[\boldsymbol{y}|\boldsymbol{x}] = p[\boldsymbol{y}|\theta(\boldsymbol{x})],$$

where p is a well known distribution (e.g Gaussian) and $\theta(\boldsymbol{x})$ is a function that maps $\boldsymbol{x}$ to the parameters of the distribution p (e.g. the mean and covariance of a Gaussian). Optimization is then performed by finding the function $\theta(\boldsymbol{x})$ that minimizes a proper-scoring rule such as the negative log-likelihood.

References

References follow the acknowledgments in the camera-ready paper. Use unnumbered first-level heading for the references. Any choice of citation style is acceptable as long as you are consistent. It is permissible to reduce the font size to `small` (9 point) when listing the references. Note that the Reference section does not count towards the page limit.**(author?)** [5]

References

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