Diffusion Normalizing Flow

Anonymous Author(s)
Affiliation
Address
email

Abstract

We present a novel generative modeling method called diffusion normalizing flow based on stochastic differential equations (SDEs). The algorithm consists of two neural SDEs: a forward SDE that gradually adds noise to the data to transform the data into Gaussian random noise, and a backward SDE that gradually removes the noise to sample from the data distribution. By jointly training the two neural SDEs to minimize a common cost function that quantifies the difference between the two, the backward SDE converges to a diffusion process the starts with a Gaussian distribution and ends with the desired data distribution. Our method is closely related to normalizing flow and diffusion probabilistic models, and can be viewed as a combination of the two. Compared with normalizing flow, diffusion normalizing flow is able to learn distributions with sharp boundaries. Compared with diffusion probabilistic models, diffusion normalizing flow requires fewer discretization steps and thus has better sampling efficiency. Our algorithm demonstrates competitive performance in both high-dimension data density estimation and image generation tasks.

1 Introduction

Generative model is a class of machine learning models used to estimate data distributions and sometimes generate new samples from the distributions [8, 31, 16, 33, 7]. Many generative models learn the data distributions by transforming a latent variable $\mathbf{z}$ with a tractable prior distribution to the data space [8, 31, 28]. To generate new samples, one can sample from the latent space and then follow the transformation to the data space. There exist a large class of generative models where the latent space and the data space are of the same dimension. The latent variable and the data are coupled through trajectories in the same space. These trajectories serve two purposes: in the forward direction $\mathbf{x} \to \mathbf{z}$, the trajectories infer the posterior distribution in the latent space associated with a given data sample $\mathbf{x}$, and in the backward direction $\mathbf{z} \to \mathbf{x}$, it generates new samples by simulating the trajectories starting from the latent space. This type of generative models can be roughly divided into two categories, depending on whether these trajectories are deterministic or stochastic.

When deterministic trajectories are used, these generative models are known as flow-based models. The latent space and the data space are connected through an invertible map, which could either be realized by the composition of multiple invertible maps [31, 8, 20] or a differential equation [4, 14]. In these models, the probability density at each data point can be evaluated explicitly using the change of variable theorem, and thus training can be carried out by minimizing the negative log-likelihood (NLL) directly. One limitation of the flow-based model is that the invertible map used in it parameterized by neural networks imposes topological constraints on the transformation from $\mathbf{z}$ to $\mathbf{x}$. Such limitation affects the performance significantly when the prior distribution on $\mathbf{z}$ is a simple unimodal distribution such as Gaussian while the target data distribution is a well-separated multi-modal distribution, i.e., its support has multiple isolated components. In [6], it is shown there are some fundamental issues to use well-conditioned invertible functions to approximate such complicated data distributions.

Submitted to 35th Conference on Neural Information Processing Systems (NeurIPS 2021). Do not distribute.

When stochastic trajectories are used, the generative models are often known as the diffusion model [34]. In a diffusion model, a prespecified stochastic forward process gradually adds noise into the data to transform the data samples to simple random variables. A separate backward process is trained to revert this process to gradually removing the noise from the data to recover the original data distributions. When the forward process is modeled by a stochastic differential equations (SDE), the optimal backward SDE [1] can be retrieved by learning the score function [35, 36, 17, 2]. When the noise is added to the data sufficiently slow in the forward process, the backward diffusion can often revert the forward one reasonably well and is able to generate high fidelity samples. However, this also means that the trajectories have to be sufficiently long, which leads to slow training and sampling. In addition, since the forward process is fixed, the way noise is added is independent of the data distribution. This feature can make the model miss some complex details in the data distribution, as we will explain later.

In this work, we present a new generative modeling algorithm which resembles both the flow-based models and the diffusion models. It extends the normalizing flow method by gradually adding noise to the sampling trajectories to make them stochastic. It extends the diffusion model by making the forward process from $\mathbf{z}$ to $\mathbf{x}$ trainable. Our algorithm is thus termed *Diffusion Normalizing Flow (DiffFlow)*. The comparisons and relations among DiffFlow, normalizing flow, and diffusion models are shown in Figure 1. When the noise in DiffFlow shrinks to zero, it reduces to a standard normalizing flow. When the forward process is fixed to some specific type of diffusions, DiffFlow reduces to a diffusion model. In DiffFlow, the forward and backward diffusion processes are trained

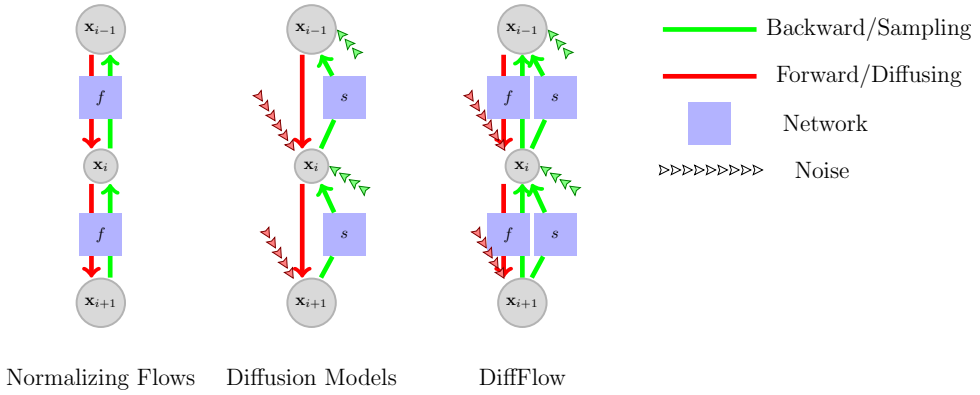


Figure 1: The schematic diagram for normalizing flows, diffusion models, and DiffFlow. In normalizing flow, both the forward and the backward processes are deterministic. They are the inverse of each other and thus collapse to a single process. The diffusion model has a fixed forward process and trainable backward process, both are stochastic. In DiffFlow, both the forward and the backward processes are trainable and stochastic.

simultaneously by minimizing the distance between the forward and the backward process in terms of the Kullback-Leibler (KL) divergence of the induced probability measures [38]. This cost turns out to be equivalent to (see Section 3 for a derivation) the (amortized) negative evidence lower bound (ELBO) widely used in variational inference [21]. One advantages to use the KL divergence directly is that it can be estimated with no bias using sampled trajectories of the diffusion processes. The KL divergence in the trajectory space also bounds the KL divergence of the marginals, providing an alternative method to bound the likelihood (see Section 3 for details). We have made the following contributions.

1. We propose a novel density estimation model termed diffusion normalizing flow (DiffFlow) that extends both the flow-based models and the diffusion models. The added stochasticity in DiffFlow boosts the expressive power of the normalizing flow and results in better performance in terms of sampling quality and likelihood. Compared with diffusion models, DiffFlow is able to learn a forward diffusion process to add noise to the data adaptively and more efficiently. This avoids adding noise to regions where noise is not so desirable. The learnable forward process also shorten the trajectory length, making the sampling much faster than standard diffusion models (We observe a 20 times speed up over diffusion models without decreasing sampling quality much).

2. We develop a stochastic adjoint algorithm to train the DiffFlow model. This algorithm evaluates the objective function and its gradient sequentially along the trajectory. It avoids storing all the

intermediate values in the computational graph, making it possible to train DiffFlow for high dimensional problems.

3. We apply the DiffFlow model to several generative modeling tasks with both synthetic and real datasets, and verify the performance of DiffFlow and advantages over other methods.

2 Background

Below we provide a brief introduction to normalizing flows and diffusion models. In both of these models, we use $\tau = \{\mathbf{x}(t), 0 \leq t \leq T\}$ to denote trajectories from the latent space to the data space in the continuous-time setting, and $\tau = \{\mathbf{x}_0, \mathbf{x}_1, \cdots, \mathbf{x}_N\}$ in the discrete-time setting.

Normalizing Flows The trajectory in normalizing flows is modeled by a differential equation

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, t, \theta), \tag{1}$$

parameterized by θ. This differential equation starts from random $\mathbf{x}(0) = \mathbf{z}$ and ends at $\mathbf{x}(T) = \mathbf{x}$. Denote by the $p(\mathbf{x}(t))$ the probability distribution of $\mathbf{x}(t)$, then under mild assumptions, it evolves following [4]

$$\frac{\partial \log p(\mathbf{x}(t))}{\partial t} = -\text{tr}(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}). \tag{2}$$

Using this relation (1) (2) one can compute the likelihood of the model at any data point $\mathbf{x}$.

In the discrete-time setting, the map from $\mathbf{z}$ to $\mathbf{x}$ in normalizing flows is a composition of a collection of bijective functions as $F = F_N \circ F_{N-1} \cdots F_2 \circ F_1$. The trajectory $\tau = \{\mathbf{x}_0, \mathbf{x}_1, \cdots, \mathbf{x}_N\}$ satisfies

$$\mathbf{x}_i = F_i(\mathbf{x}_{i-1}, \theta), \quad \mathbf{x}_{i-1} = F_i^{-1}(\mathbf{x}_i, \theta). \tag{3}$$

Similar to Equation (2), based on the rule for change of variable, the log-likelihood of any data samples $\mathbf{x}_0 = \mathbf{x}$ can be evaluated as

$$\log p(\mathbf{x}_0) = \log p(\mathbf{x}_N) - \sum_{i=1}^{N} \log |\text{det}(\frac{\partial F_i^{-1}(\mathbf{x}_i)}{\partial \mathbf{x}_i})|. \tag{4}$$

Since the exact likelihood is accessible in normalizing flows, these models can be trained by minimizing the negative log-likelihood directly.

Diffusion Models The trajectories in diffusion models are modeled by stochastic differential equations. More explicitly, the forward process is of the form

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}, \tag{5}$$

where the *drift* term $\mathbf{f} : \mathbb{R}^d \to \mathbb{R}^d$ is a vector-valued function, and the *diffusion* coefficient $g : \mathbb{R} \to \mathbb{R}$ is a scalar function (in fact, g is often chosen to be a constant). Here $\mathbf{w}$ denotes the standard Brownian motion. The forward process is normally a simple linear diffusion process [34, 16]. The forward trajectory τ can be sampled using (5) initialized with the data distribution. Denote by p_F the resulting probability distribution over the trajectories.

The backward diffusion from $\mathbf{z}$ to $\mathbf{x}$ is of the form

$$d\mathbf{x} = [\mathbf{f}(\mathbf{x}, t) - g^2(t)\mathbf{s}(\mathbf{x}, t, \theta)]dt + g(t)d\mathbf{w}. \tag{6}$$

It is well-known that when $\mathbf{s}$ coincides with the score function $\nabla \log p_F$, and $\mathbf{x}(T)$ in the forward and backward processes share the same distribution, the distribution p_B induced by the backward process (6) is equal to p_F. To train the score network $\mathbf{s}(\mathbf{x}, t, \theta)$, one can use the KL divergence between p_F and p_B as an objective function to reduce the difference between p_F and p_B. When the difference is sufficiently small, p_F and p_B should have similar distribution over $\mathbf{x}(0)$, and one can then use the backward diffusion (6) to sample from the data distribution.

In the discrete setting, the trajectory distributions can be more explicitly written as

$$p_F(\tau) = p_F(\mathbf{x}_0) \prod_{i=1}^{N} p_F(\mathbf{x}_i|\mathbf{x}_{i-1}), \quad p_B(\tau) = p_B(\mathbf{x}_T) \prod_{i=1}^{N} p_B(\mathbf{x}_{i-1}|\mathbf{x}_i). \tag{7}$$

The KL divergence between p_F and p_B can be decomposed according to this expression (7). Most diffusion models use this decomposition, and meanwhile take advantage the simple structure of the forward process (5), to evaluate the objective function in training [35, 36, 37].

3 Diffusion normalizing flow

We next present our diffusion normalizing flow models. Similar to diffusion models, the DiffFlow models also has a forward process

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t, \theta)dt + g(t)d\mathbf{w}, \tag{8}$$

and a backward process

$$d\mathbf{x} = [\mathbf{f}(\mathbf{x}, t, \theta) - g^2(t)\mathbf{s}(\mathbf{x}, t, \theta)]dt + g(t)d\mathbf{w}. \tag{9}$$

The major difference is that the drift term $\mathbf{f}$ is also learnable in DiffFlow instead of a fixed linear function in diffusion models. The forward process is initialized with the data samples at $t = 0$ and the backward process is initialized with a given noise distribution at $t = T$. Our goal is to ensure the distribution of the backward process at time $t = 0$ is close to the real data distribution. That is, we would like the difference between $p_B(\mathbf{x}(0))$ and $p_F(\mathbf{x}(0))$ to be small.

To this end, we use the KL divergence between $p_B(\tau)$ and $p_F(\tau)$ over the trajectory space as the training objective function. Since

$$KL(p_F(\mathbf{x}(t))|p_B(\mathbf{x}(t))) \leq KL(p_F(\tau)|p_B(\tau)) \tag{10}$$

for any $0 \leq t \leq T$, small difference between $p_B(\tau)$ and $p_F(\tau)$ implies small difference between $p_B(\mathbf{x}(0))$ and $p_F(\mathbf{x}(0))$ in terms of KL divergence.

3.1 Implementation

In real implementation, we discretize the forward process (8) and the backward process (9) as

$$\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{f}_i(\mathbf{x}_i)\Delta t_i + g_i \delta_i^F \sqrt{\Delta t_i} \tag{11}$$

$$\mathbf{x}_i = \mathbf{x}_{i+1} - [\mathbf{f}_{i+1}(\mathbf{x}_{i+1}) - g_{i+1}^2 \mathbf{s}_{i+1}(\mathbf{x}_{i+1})]\Delta t_i + g_{i+1}\delta_i^B \sqrt{\Delta t_i}, \tag{12}$$

where $\delta_i^F, \delta_i^B \sim \mathcal{N}(0, \mathbf{I})$ are unit Gaussian noise, $\{t_i\}_{i=0}^N$ are the discretization time points, and $\Delta t_i = t_{i+1} - t_i$ is the step size at the i-th step. Here we have dropped the dependence on the parameter θ to simplify the notation. With this discretization, the KL divergence between trajectory distributions becomes

$$KL(p_F(\tau)|p_B(\tau)) = \underbrace{\mathbb{E}_{\tau\sim p_F}[\log p_F(\mathbf{x}_0)]}_{L_0} + \underbrace{\mathbb{E}_{\tau\sim p_F}[-\log p_B(\mathbf{x}_N)]}_{L_N} + \sum_{i=1}^{N-1} \underbrace{\mathbb{E}_{\tau\sim p_F}[\log \frac{p_F(\mathbf{x}_i|\mathbf{x}_{i-1})}{p_B(\mathbf{x}_{i-1}|\mathbf{x}_i)}]}_{L_i}. \tag{13}$$

The term L_0 in (13) is a constant determined by entropy of the dataset as

$$\mathop{\mathbb{E}}_{\tau\sim p_F}[\log p_F(\mathbf{x}_0)] = \mathop{\mathbb{E}}_{\mathbf{x}_0\sim p_F}[\log p_F(\mathbf{x}_0)] =: -H(p_F(x(0))). \tag{14}$$

The term L_N is easy to calculate since $p_B(x_N)$ is a simple distribution, typically standard Gaussian distribution.

To evaluate $L_{1:N-1}$, we estimate it over sampled trajectory from the forward process p_F. For a given trajectory τ sampled from $p_F(\tau)$, we need to calculate $p_B(\tau)$ along the same trajectory. To this end, we chose δ_i^B such that the same trajectory can be reconstructed from the backward process. Thus, δ_i^B satisfies

$$\delta_i^B(\tau) = \frac{1}{g_{i+1}\sqrt{\Delta t}}\left[\mathbf{x}_i - \mathbf{x}_{i+1} + [\mathbf{f}_{i+1}(\mathbf{x}_{i+1}) - g_{i+1}^2 \mathbf{s}_{i+1}(\mathbf{x}_{i+1})]\Delta t\right]. \tag{15}$$

Since δ_i^B is a Gaussian noise, the log-likelihood term $p_B(\mathbf{x}_i|\mathbf{x}_{i+1})$ is equal to $\frac{1}{2}(\delta_i^B(\tau))^2$ (after dropping some constant). In view of the fact that the expectation of $\sum_i \frac{1}{2}(\delta_i^F(\tau))^2$ remains a constant, minimizing Equation (13) is equivalent to minimizing the following loss (see the supplemental material for the full derivation):

$$L := \mathbb{E}_{\tau\sim p_F}[-\log p_B(\mathbf{x}_N) + \sum_i \frac{1}{2}(\delta_i^B(\tau))^2] = \mathbb{E}_{\delta^F;\mathbf{x}_0\sim p_0}[-\log p_B(\mathbf{x}_N) + \sum_i \frac{1}{2}(\delta_i^B(\tau))^2], \tag{16}$$

where the last equality is based on a reparameterization trick [21]. We can minimize the loss in Equation (16) with Monto Carlo gradient estimation as in Algorithm 1.

Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim$ Real data distribution
  $\delta^F_{1:N} \sim \mathcal{N}(0, \mathbf{I})$
  Discrete timestamps: $t^N_{i=0}$
  Sample: $\tau = \{\mathbf{x}_i\}^N_{i=0}$ based on $\delta^F_{1:N}$
  Gradient descent step $\nabla_\theta[-\log p_B(\mathbf{x}_N) + \sum_i \frac{1}{2}(\delta^B_i(\tau))^2]$
until converged

Algorithm 2 Stochastic Adjoint Algorithm for DiffFlow

Input: Forward trajectory $\{\mathbf{x}_i\}^N_{i=0}$
$\frac{\partial L}{\partial \mathbf{x}_N} = \frac{1}{2}\frac{\partial(\delta^B_N(\tau))^2}{\partial \mathbf{x}_N} - \frac{\partial \log p_B(\mathbf{x}_N)}{\mathbf{x}_N}$
$\frac{\partial L}{\partial \theta} = 0$
for $i = N, N-1, \cdots, 1$ **do**
  $\frac{\partial L}{\partial \mathbf{x}_{i-1}} = (\frac{\partial L}{\partial \mathbf{x}_i} + \frac{1}{2}\frac{\partial(\delta^B_i(\tau))^2}{\partial \mathbf{x}_i})\frac{\partial \mathbf{x}_i}{\partial \mathbf{x}_{i-1}} + \frac{1}{2}\frac{\partial(\delta^B_i(\tau))^2}{\partial \mathbf{x}_{i-1}}$
  $\frac{\partial L}{\partial \theta} += \frac{1}{2}\frac{\partial(\delta^B_i(\tau))^2}{\partial \theta} + (\frac{\partial L}{\partial \mathbf{x}_i} + \frac{1}{2}\frac{\partial(\delta^B_i(\tau))^2}{\partial \mathbf{x}_i})\frac{\partial \mathbf{x}_i}{\partial \theta}$
end for

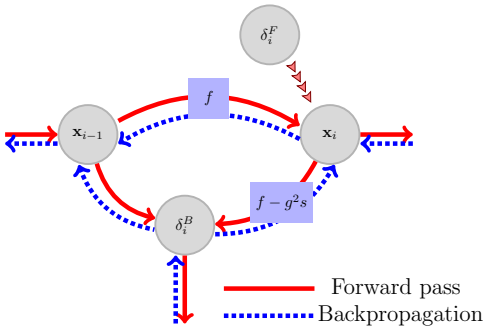


Figure 2: Gradient Flowchart.

3.2 Stochastic Adjoint method

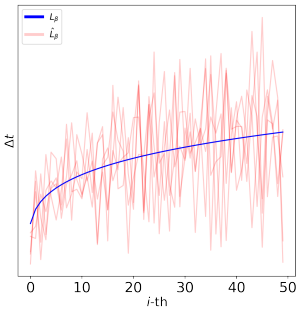
One challenge in training DiffFlow is the memory consumption. When a naive backpropagation strategy is used, the memory consumption explodes quickly. Indeed, differentiating through the operations of the froward pass requires unrolling networks N times and caching all network intermediate values for every step, which prevents this naive implementation of DiffFlow from being applied in high dimensional applications. Inspired by the adjoint method in Neural ODE [4], we propose a stochastic adjoint algorithm that allows training the DiffFlow model with a constant memory consumption. With cached intermediate state $\mathbf{x}_i$, we are able to reproduce the whole process, including δ^F_i, δ^B_i as well as f_i, s_i exactly for any numerical discretization. We summarize the method in Algorithm 2 and Figure 2. We include the Python implementation in the supplemental material.

3.3 Time discretization

We are interested in training DiffFlow with $N \leq 100$. Now we discuss the time discretization. We first use fixed $t_i = (\frac{i}{N})^\beta T$ across batches. With this time discretization, we denote loss function by L_β.

The next choice of time choice is sample different t_i across batches. $t_i = [\alpha_i(\frac{i-1}{N-1})^\beta + (1-\alpha_i)(\frac{i}{N-1})^\beta]T$ for $i \in \{1, \cdots, N-1\}$ and $\alpha_i \sim \text{Uniform}[0, 1)$. We denote the loss function as $\hat{L}_\beta$ Equation (13) with such flexible time discretization. We show the Δt_i of L_β and sampled Δt_i from $\hat{L}_\beta$ with $\beta = 0.9$. With such parametrization, DiffFlow has large Δt when close to noise and higher resolution when close to $\mathbf{x}_0$. The choice of polynomial function was arbitrary, other functions with similar sharps may work as well.

Figure 3: Δt_i of L_β and $\hat{L}_\beta$



3.4 Learnable forward process

Forward process not only is responsible for driving data into prior space, but also provides enough supervised information to learning backward process. Thanks to bijective property, NFs can reconstruct data exactly but there is no guarantee that it can reach the standard Gaussian. At the another extreme, Denoising diffusion probabilistic models (DDPM) [17] adopt a data-invariant forward diffusing schema and guarantees $\mathbf{x}_N$ is Gaussian. DDPM can even reach Gaussian in one step with $N = 1$, which output noise disregarding data samples. However, backward process will be difficult to learn if data is destroyed in one step. Therefore, DDPM adds noise slowly and needs one thousand steps for diffusion.

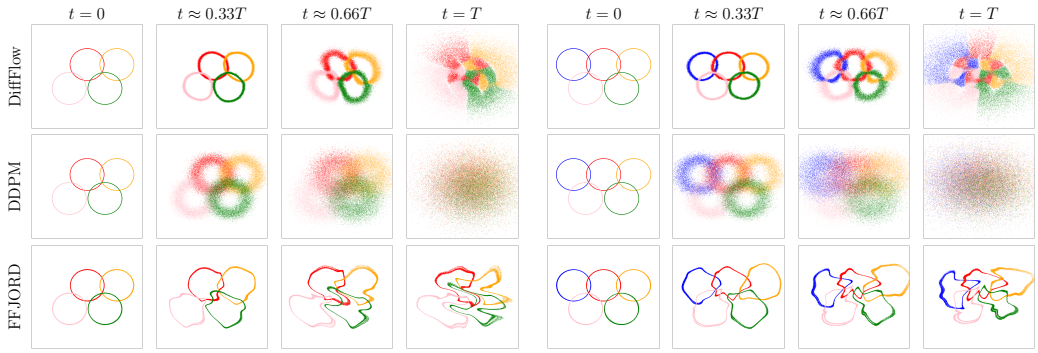


Figure 4: Illustration of forward trajectories of DiffFlow, DDPM and FFJORD. Each row shows two trajectories of transforming data distributions, four rings and olympics rings, to a base distribution. Different modes on densities are in different colors. Though FFJORD adjusts forward process based on data, its bijective property prevents the approach to expanding density support in whole space. DDPM can transofrm data distributions into Gaussian distribution but a data-invariant way can loss the details of densities, e.g. the densities on ring cross regions. DiffFlow not only transform data into base distribution, but also keep the typological information of the original datasets. Points from the same ring are transformed into continental plates instead of being distributed randomly.

The forward module of DiffFlow is a combination of normalizing flow and diffusion model. We share the comparision in fitting toy 2D datasets in Figure 4. We are especially interested in data with well-seperated modes and sharp density boundaries. Those properties are believed to appear in various datasets. As stated by manifold hypothesis [32], real-world data lie on low-dimensional manifold [26] embedded in a high-dimensional space. To construct the distributions in Figure 4, we rotate the 1-d Gaussian distribution $\mathcal{N}(1, 0.001^2)$ around the center to form a ring and copy the rings.

As a bijective model, FFJORD [14] struggles to diffuse the concentrated density mass into a Gaussian distribution. DiffFlow overcomes expressivity limitations of the bijective constraint by adding noise. As added noise shrinks to zero, the DiffFlow has no stochasticity and degrades to flow-based model. Based on this fact, we present the following theorem with proof in Appendix A.

Theorem 1. *As diffusion coefficients $g_i \to 0$, DiffFlow becomes a bijective model and reduces to Normalizing Flow. Minimizing the objective function in Equation* (13) *is equivalent to minimize the negative log-likelihood as in Equation* (4)*.*

DDPM [17] uses a fixed nosing transformation. Thanks to the data-invariant approach and $p(\mathbf{x}_T|\mathbf{x}_0) = p(\mathbf{x}_T)$, points are diffused in the same way even though they appear in different modes or different datasets. We also observe that sharp details are destroyed quickly in DDPM diffusion, such as the intersection regions between rings. However, with the help of learnable transformation, DiffFlow diffuses in a much efficient way. The data-dependent approach shows different diffusion strategies on different modes and different datasets. Meanwhile, similar to NFs, it keeps some typological information for learning backward process. We include more details about the toy sample in Section 4.

4 Experiments

We evaluate the performance of DiffFlow in sample quality and likelihood on test data. To evaluate the likelihood, we adopt the marginals distribution equivalent SDEs

$$d\mathbf{x} = [\mathbf{f}(\mathbf{x}, t, \theta) - \frac{1+\lambda^2}{2} g^2(t)\mathbf{s}(\mathbf{x}, t, \theta)]dt + \lambda g(t) d\mathbf{w}, \tag{17}$$

with $\lambda \geq 0$ (Proof see Appendix G). When $\lambda = 0$, it reduces to probability ODE [37]. The ODE provides an efficient way to evaluate the density and negative log-likelihood.

4.1 Synthetic 2D examples

We compare performance of DiffFlow and existing diffusion models and NFs on estimating the density of the 2 dimensional data. We compare the forward trajectories of DiffFlow, DDPM [17] and

FFJORD [14][1] in Figure 4 and its sampling performance in Figure 5. To make a fair comparison, we build models with comparable network size, around 90k learnable parameters. We include more training and model details in Appendix D.

All three algorithm has good performance on datasets whose underlying distribution has smooth density, such as 2 spirals. However, when we shrink the support of samples or add complex parttens, performance varies. we observe that FFJORD leaks many samples out of the main modes and datasets with complex details and sharp density exacerbate the disadvantage.

DDPM has higher sample quality but blurs density details , such as intersections between rings, areas around leaves of Fractal tree, and boxes in Sierpiński Carpet. The performance is within expectation given that details are easy to be destroyed and ignored with the data-invariant noising schema. On the less sharper dataset, such as 2 Spirals and Checkerboard, its samples align with data almost perfectly.

DiffFlow produces the best samples (according to a human observer). We owe the performance to the flexible noising forward process. As illustrated in Figure 4, DiffFlow provides more clues and retains detailed parttens longer for learning its reverse process. We also report a comprehensive comparison of the negative likelihood and more analysis in Appendix D. DiffFlow has a much lower negative likelihood, especially on sharp datasets.

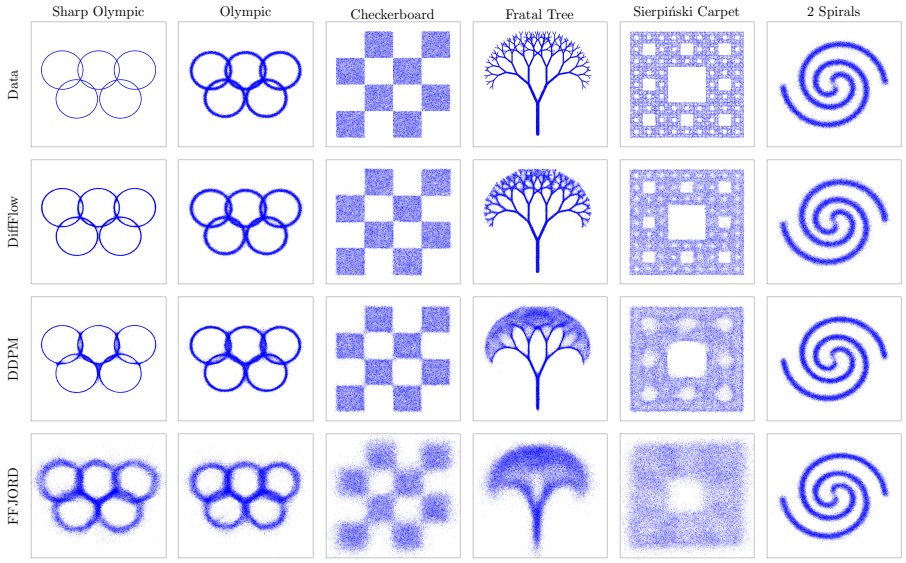


Figure 5: Samples from DiffFlow, DDPM and FFJORD on 2-D datasets. All three models have reasonable performance on datasets that have smooth underlying distributions. But only DiffFlow is capable to capture complex patterns and provides sharp samples when dealing with more challenging datasets.

4.2 Density estimation on real data

We perform density estimation on five tabular datasets [29]. We employ the probability flow to evaluate the negative log-likelihood. We surprisingly find our algorithm show better performance in most datasets than approaches trained by directly minimizing negative log-likelihood, including NFs and autoregressive models. DiffFlow outperforms FFJORD by a wide margin on all datasets except HEPMASS. Compared with autoregressive models, it excels NAF [18] on all but GAS. Those models require $\mathcal{O}(d)$ computations to sample from. Meanwhile, DiffFlow is quite effective to achieve such performance with no more than 5 layers. We include more details in Appendix E

4.3 Image generation

In this section, we report the quantitative comparison and qualitative performance of our method and existing methods on common image datasets, MNIST [24] and CIFAR-10 [23]. We use the same unconstrained U-net style model as used successfully by [17] for drift and score network. We reduce the network size to half of the original DDPM network so that the total number of trainable parameters

[1] Implementation of FFJORD and DDPM are based on official codebases.

Dataset	POWER	GAS	HEPMASS	MINIBOONE	BSDS300
RealNVP [8]	-0.17	-8.33	18.71	13.55	-153.28
FFJORD [14]	-0.46	-8.59	**14.92**	10.43	-157.40
DiffFlow (ODE)	**-1.04**	-10.45	15.04	**8.06**	**-157.80**
MADE [11]	3.08	-3.56	20.98	15.59	-148.85
MAF [29]	-0.24	-10.08	17.70	11.75	-155.69
TAN [27]	-0.48	-11.19	15.12	11.01	-157.03
NAF [18]	-0.62	**-11.96**	15.09	8.86	-157.73

Table 1: Average negative log-likelihood (in nats) on tabular datasets [29] for density estimation (lower is better).

Table 2: NLL on MNIST

Model	NLL (↓)
RealNVP [8]	1.06
Glow [20]	1.05
FFJORD [14]	0.99
ResFlow [5]	0.97
DiffFlow	0.93

Figure 6: MNIST Samples

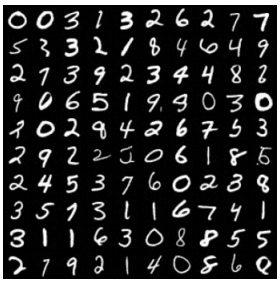
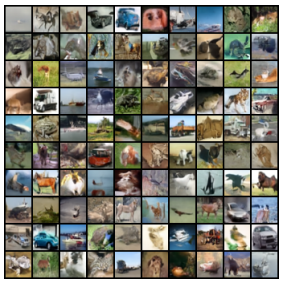


Figure 7: CIFAR10 Samples



of DiffFlow and DDPM are comparable. We use small $N = 10$ at the beginning of training and slowly increase to large N as training proceeds. The schedule of N reduces the training time greatly compared with use large N all the time. We use const $g_i = 1$ and $T = 0.05$ for MNIST and CIFAR10, and $N = 30$ for sampling MNIST data and $N = 100$ for sampling CIFAR10. As it is reported by Jolicoeur-Martineau et al. [19], adding noise at the last step will significantly decreasing sampling quality, we use one single denoising step at the end of sampling with Tweedie's formula [10].

We report negative log-likelihood (NLL) in bits per dimension or negative ELBO if NLL is unavailable. We also report the popular sample metric, Fenchel Inception Distance (FID) [15]. On MNIST, we achieve the state-of-the-art performance on NLL as in Table 2 and we show the uncurated samples from DiffFlow in Figure 6 and Figure 7. DiffFlow achieves the state-of-the-art NLL performance as shown in Table 3. Besides, we also show sampling quality of various number of sampling steps N in Table 4 [2]. We found DiffFlow retains better sampling quality when decreasing N. Full details on architectures used, training setup details and more samples can be found in Appendix F.

Table 3: NLLs and FIDs on CIFAR-10.

Model	NLL(↓)	FID (↓)
RealNVP [8]	3.49	-
Glow [20]	3.35	46.90
Flow++ [16]	3.29	-
FFJORD [14]	3.40	-
ResFlow [5]	3.28	46.37
DDPM (L) [17]	≤ 3.70	13.51
DDPM (L_{simple}) [17]	≤ 3.75	**3.17**
DDPM (L_{simple})(ODE) [17]	3.36	3.27
DiffFlow (L_β)	≤ 3.71	16.04
DiffFlow ($\hat{L}_\beta$)	≤ 3.67	16.14
DiffFlow ($\hat{L}_\beta$, ODE)	**3.04**	16.37

Table 4: FIDs with various N

N	DiffFlow	DDPM
5	28.51	370.23
10	22.66	365.12
20	19.05	135.44
50	17.72	34.56
100	16.14	10.04

[2]The performance of DDPM is evaluated based on the officially released checkpoint.

5 Related work

Normalizing flows [8, 31] have recently received lots of attention since its exact density evaluation and ability to model high dimensional data [20, 9]. However, the bijective requirement poses limitations on modeling complex data empirically and theoretically [38, 6]. Some works attempt to relax bijective, discretely index flows [9] use domain partitioning with locally invertible functions. Continuously indexed flows [6] extend discretely indexing to a continuously indexing approach. As pointed out in Stochastic Normalizing Flows (SNF) [38], stochasticity can effectively improve the expressive power of the flow-based model in low dimension applications. The architecture used in SNF, which requires known underlying energy models, presents challenges when learning density from data samples since SNF is designed for sampling from unnormalized probability distribution instead of density estimation. Besides, with ideal networks and the infinite amount of data, SNF has no promise to finding models with aligned forward and backward distribution as DiffFlow.

When it comes to stochastic trajectories, minimizing the distance between trajectory distributions has been explored in existing works. Denoising diffusion model [34] uses a fixed linear forward diffusion schema and reparameterizes the KL divergence such that minimizing loss is possible without computing whole trajectories. Diffusion models essentially corrupt real data iteratively and learn to remove the noise when sampling. Recently, Diffusion models have shown the capability to model high-dimensional data distribution, such as images [17, 36], shapes [3], text-to-speech [22]. Lately, the Score-based model [37] provides a unified framework for score-matching methods and diffusion models based on stochastic calculus. The diffusion processes and sampling processes can be viewed as forwarding SDE and reverse-time SDE. Since the usage of linear forward SDE, forward marginal distributions have a closed-form and suitable for training score functions on large-scale datasets. Also due to the reliance on fixed linear, it takes thousands of steps to diffuse data and generate samples. DiffFlow considers general SDEs and noising and sampling are more efficient.

Existing Neural SDE approaches suffer from poor scaling properties. Backpropagating through solver [12] has a linear memory complexity with the number of steps. The pathwise approach [13] scales poorly in computation complexity. Our stochastic adjoint approach shares a similar spirit with SDE adjoint sensitivity [25]. The choice of caching noise requires high resolution and prevents the approach from scaling to high dimension applications. By caching the trajectory states, DiffFlow can use a coarser discretization and deploy on much larger dimension problems and challenging density estimation problems. The additional memory footprint is ignorable compared with network memory consumption in DiffFlow.

6 Conclusions

We proposed a novel algorithm, the diffusion normalizing flow (DiffFlow), for generative modeling and density estimation. The proposed method extends both the normalizing flow models and the diffusion models. Our DiffFlow algorithm has two trainable diffusion processes modeled by neural SDEs, one forward and one backward. These two SDEs are trained jointly by minimizing the KL divergence between them. Compared with most normalizing flow models, the added noise in DiffFlow relaxes the bijectivity condition in deterministic flow-based models and improves their expressive power. Compared with diffusion models, DiffFlow learns a more flexible forward diffusion that is able to transform data into noise more effectively and adaptively. In our experiments, we observed that DiffFlow is able to model distributions with complex details that are not captured by representative normalizing flow models and diffusion models, including FFJORD, DDPM. For CIFAR10 dataset, our DiffFlow method has worse performance than DDPM in terms of FID score. We believe our DiffFlow algorithm can be improved further by using different neural network architectures, different time discretizing method, and different choice of time interval. We plan to explore these options in the near future.

Our algorithm is able to learn the distribution of high dimensional data and then generate new samples from it. Like many other generative modeling algorithms, it may be potentially used to generate misleading data such as fake images or videos.

References

[1] Anderson, B. D. Reverse-time diffusion equation models. *Stochastic Processes and their Applications*, 12 (3):313–326, 1982.

[2] Bordes, F., Honari, S., and Vincent, P. Learning to generate samples from noise through infusion training. *arXiv preprint arXiv:1703.06975*, 2017.

[3] Cai, R., Yang, G., Averbuch-Elor, H., Hao, Z., Belongie, S., Snavely, N., and Hariharan, B. Learning gradient fields for shape generation. In *Proceedings of the European Conference on Computer Vision (ECCV)*, 2020.

[4] Chen, R. T., Rubanova, Y., Bettencourt, J., and Duvenaud, D. Neural ordinary differential equations. *arXiv preprint arXiv:1806.07366*, 2018.

[5] Chen, R. T. Q., Behrmann, J., Duvenaud, D., and Jacobsen, J. Residual flows for invertible generative modeling. In *Advances in Neural Information Processing Systems*, 2019.

[6] Cornish, R., Caterini, A., Deligiannidis, G., and Doucet, A. Relaxing bijectivity constraints with continuously indexed normalising flows. In *International Conference on Machine Learning*, pp. 2133–2143. PMLR, 2020.

[7] Deng, Y., Bakhtin, A., Ott, M., Szlam, A., and Ranzato, M. Residual energy-based models for text generation. *arXiv preprint arXiv:2004.11714*, 2020.

[8] Dinh, L., Sohl-Dickstein, J., and Bengio, S. Density estimation using real nvp. *arXiv preprint arXiv:1605.08803*, 2016.

[9] Dinh, L., Sohl-Dickstein, J., Larochelle, H., and Pascanu, R. A rad approach to deep mixture models. *arXiv preprint arXiv:1903.07714*, 2019.

[10] Efron, B. Tweedie's formula and selection bias. *Journal of the American Statistical Association*, 106(496): 1602–1614, 2011.

[11] Germain, M., Gregor, K., Murray, I., and Larochelle, H. Made: Masked autoencoder for distribution estimation. In *International Conference on Machine Learning*, pp. 881–889. PMLR, 2015.

[12] Giles, M. and Glasserman, P. Smoking adjoints: Fast monte carlo greeks. *Risk*, 19(1):88–92, 2006.

[13] Gobet, E. and Munos, R. Sensitivity analysis using itô–malliavin calculus and martingales, and application to stochastic optimal control. *SIAM Journal on control and optimization*, 43(5):1676–1713, 2005.

[14] Grathwohl, W., Chen, R. T., Bettencourt, J., Sutskever, I., and Duvenaud, D. Ffjord: Free-form continuous dynamics for scalable reversible generative models. *arXiv preprint arXiv:1810.01367*, 2018.

[15] Heusel, M., Ramsauer, H., Unterthiner, T., Nessler, B., and Hochreiter, S. Gans trained by a two time-scale update rule converge to a local nash equilibrium. *arXiv preprint arXiv:1706.08500*, 2017.

[16] Ho, J., Chen, X., Srinivas, A., Duan, Y., and Abbeel, P. Flow++: Improving flow-based generative models with variational dequantization and architecture design. In *International Conference on Machine Learning*, pp. 2722–2730. PMLR, 2019.

[17] Ho, J., Jain, A., and Abbeel, P. Denoising diffusion probabilistic models. *arXiv preprint arXiv:2006.11239*, 2020.

[18] Huang, C.-W., Krueger, D., Lacoste, A., and Courville, A. Neural autoregressive flows. In *International Conference on Machine Learning*, pp. 2078–2087. PMLR, 2018.

[19] Jolicoeur-Martineau, A., Piché-Taillefer, R., Combes, R. T. d., and Mitliagkas, I. Adversarial score matching and improved sampling for image generation. *arXiv preprint arXiv:2009.05475*, 2020.

[20] Kingma, D. P. and Dhariwal, P. Glow: Generative flow with invertible 1x1 convolutions. *arXiv preprint arXiv:1807.03039*, 2018.

[21] Kingma, D. P. and Welling, M. Auto-encoding variational bayes. *arXiv preprint arXiv:1312.6114*, 2013.

[22] Kong, Z., Ping, W., Huang, J., Zhao, K., and Catanzaro, B. Diffwave: A versatile diffusion model for audio synthesis. *arXiv preprint arXiv:2009.09761*, 2020.

[23] Krizhevsky, A., Hinton, G., et al. Learning multiple layers of features from tiny images. 2009.

[24] LeCun, Y. The mnist database of handwritten digits. *http://yann. lecun. com/exdb/mnist/*, 1998.

[25] Li, X., Wong, T.-K. L., Chen, R. T., and Duvenaud, D. Scalable gradients for stochastic differential equations. In *International Conference on Artificial Intelligence and Statistics*, pp. 3870–3882. PMLR, 2020.

[26] Narayanan, H. and Mitter, S. Sample complexity of testing the manifold hypothesis. In *Proceedings of the 23rd International Conference on Neural Information Processing Systems-Volume 2*, pp. 1786–1794, 2010.

[27] Oliva, J., Dubey, A., Zaheer, M., Poczos, B., Salakhutdinov, R., Xing, E., and Schneider, J. Transformation autoregressive networks. In *International Conference on Machine Learning*, pp. 3898–3907. PMLR, 2018.

[28] Oord, A. v. d., Dieleman, S., Zen, H., Simonyan, K., Vinyals, O., Graves, A., Kalchbrenner, N., Senior, A., and Kavukcuoglu, K. Wavenet: A generative model for raw audio. *arXiv preprint arXiv:1609.03499*, 2016.

[29] Papamakarios, G., Pavlakou, T., and Murray, I. Masked autoregressive flow for density estimation. *arXiv preprint arXiv:1705.07057*, 2017.

[30] Paszke, A., Gross, S., Massa, F., Lerer, A., Bradbury, J., Chanan, G., Killeen, T., Lin, Z., Gimelshein, N., Antiga, L., et al. Pytorch: An imperative style, high-performance deep learning library. *arXiv preprint arXiv:1912.01703*, 2019.

[31] Rezende, D. and Mohamed, S. Variational inference with normalizing flows. In *International Conference on Machine Learning*, pp. 1530–1538. PMLR, 2015.

[32] Roweis, S. T. and Saul, L. K. Nonlinear dimensionality reduction by locally linear embedding. *science*, 290(5500):2323–2326, 2000.

[33] Salimans, T., Karpathy, A., Chen, X., and Kingma, D. P. Pixelcnn++: Improving the pixelcnn with discretized logistic mixture likelihood and other modifications. *arXiv preprint arXiv:1701.05517*, 2017.

[34] Sohl-Dickstein, J., Weiss, E., Maheswaranathan, N., and Ganguli, S. Deep unsupervised learning using nonequilibrium thermodynamics. In *International Conference on Machine Learning*, pp. 2256–2265. PMLR, 2015.

[35] Song, Y. and Ermon, S. Generative modeling by estimating gradients of the data distribution. In *Advances in Neural Information Processing Systems*, pp. 11895–11907, 2019.

[36] Song, Y. and Ermon, S. Improved techniques for training score-based generative models. *arXiv preprint arXiv:2006.09011*, 2020.

[37] Song, Y., Sohl-Dickstein, J., Kingma, D., Kumar, A., Ermon, S., and Poole, B. Score-based generative modeling through stochastic differential equations. In *International Conference on Learning Representations*, 2021. URL `https://openreview.net/forum?id=PxTIG12RRHS`.

[38] Wu, H., Köhler, J., and Noe, F. Stochastic normalizing flows. In Larochelle, H., Ranzato, M., Hadsell, R., Balcan, M. F., and Lin, H. (eds.), *Advances in Neural Information Processing Systems*, volume 33, pp. 5933–5944. Curran Associates, Inc., 2020.

Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] See conclusion.
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] See conclusion.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes]
   (b) Did you include complete proofs of all theoretical results? [Yes] Proofs are in supplementary materials.
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] See supplementary materials and we will release out-of-box code in the future.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] Partial details are in supplementary materials.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] .
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] See supplementary materials.
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes]
   (b) Did you mention the license of the assets? [Yes]
   (c) Did you include any new assets either in the supplemental material or as a URL? [N/A]
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [Yes]
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A]
5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]