
DIFFUSION MODELS: A COMPREHENSIVE SURVEY OF METHODS AND APPLICATIONS

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ABSTRACT

Diffusion models are a class of deep generative models that have shown impressive results on various tasks with dense theoretical founding. Although diffusion models have achieved impressive quality and diversity of sample synthesis than other state-of-the-art models, they still suffer from costly sampling procedure and sub-optimal likelihood estimation. Recent studies have shown great enthusiasm on improving the performance of diffusion model. In this article, we present a first comprehensive review of existing variants of the diffusion models. Specifically, we provide a first taxonomy of diffusion models and categorize them variants to three types, namely sampling-acceleration enhancement, likelihood-maximization enhancement and data-generalization enhancement. We also introduce in detail other five generative models (i.e., variational autoencoders, generative adversarial networks, normalizing flow, autoregressive models, and energy-based models), and clarify the connections between diffusion models and these generative models. Then we make a thorough investigation into the applications of diffusion models, including computer vision, natural language processing, waveform signal processing, multi-modal modeling, molecular graph generation, time series modeling, and adversarial purification. Furthermore, we propose new perspectives pertaining to the development of this generative model.

1 Introduction

Diffusion models have emerged as the new state-of-the-art among the deep generative models. After surpassing GAN on image synthesis [1], diffusion model has also shown to be a promising algorithm on different tasks [2, 3], such as computer vision [4, 5, 6], natural language processing [7], waveform signal processing [8, 9], multi-modal modeling [10, 11, 12], molecular graph modeling [13, 14, 15, 16], time series modeling [17], and adversarial purification [18]. Furthermore, diffusion models have close connections with other research area, such as robust learning [19, 20, 21], representative learning [12, 22, 23, 24] and reinforcement learning [25]. However, original diffusion models still suffer from slow sampling procedure which usually requires thousands of steps of evaluations to draw a sample [26]. And it have struggled to achieve log-likelihoods competitive with other likelihood-based models, for example autoregressive models [27]. A number of efforts have been made, and recent studies improve the performance of diffusion models with practical consideration or analysing the model capacity from theoretical perspectives. Nevertheless, there is no literature focusing on a systematically review of the recent progresses on diffusion models in both algorithms and applications. To reflect the progresses on this fast-growing field, we conduct a first comprehensive review on the diffusion models. We envision that our work will elucidate design considerations and advanced methods for diffusion model, present its applications in different areas, and point out directions for future researches, a schema about our survey is illustrated in Fig.1.

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Diffusion probabilistic models were originally proposed as a latent variable generative model, inspired by the non-equilibrium thermodynamics. This class of models consist of two processes, first the forward process that progressively disturbs the data distribution by adding noise in multiple scales, and then the reverse process that learns to restore the data structure [26, 28]. From a perspective of this, diffusion model can be viewed as a very deep hierarchical VAE, which means the destroying and restoration process corresponds to the encoding and the decoding process in VAE, respectively. And thus many studies have focused on learning the encoding and decoding process, coupled with designing of the variational lower bound to improve the model performance. Alternatively, the processes of diffusion models can be viewed as discretization of stochastic differential equations(SDE) [29, 30], where the forward and reverse process corresponding the the forward SDE and reverse SDE. Therefore, analysis of the diffusion model through SDE provide dense theoretical results and model improvements, especially in sampling strategies. Motivated by these point of views, we propose to categorize the diffusion models into three categories: sampling-procedure enhancement (Section.3), likelihood-maximization enhancement (Section.4), and generalization-ability enhancement (Section.5). And in each categorize, we analysis the models in the discrete-time setting and continuous-time setting which are both abundant in empirical and theoretical results. After analyzing the three types of diffusion models, we introduce



Figure 1: Taxonomy of diffusion models variants, applications, and connections with other generative models.

other five commonly-used generative models (Section.6), namely variational autoencoders, generative adversarial

networks, normalizing flow, autoregressive models, and energy-based models. Due to the good properties of diffusion models, researchers begin to combine diffusion modeling with these traditional generative models. We provide specific introduction to these combinational works and clarify the improvement over the original generative models. Then we systematically introduce the applications of diffusion models on extensive tasks (Section.7), including computer vision, natural language processing, waveform signal processing, multi-modal modeling, molecular graph generation, time series modeling, and adversarial purification. For each task, we provide the definition of the problem and introduce the works that utilize diffusion models to handle the problem. In Section.8, we propose potential research directions in this rapidly growing field and conclude the survey in Section.9.

Main Contributions of This Survey

- **New Taxonomy.** We first propose a new and systematical taxonomy of both diffusion models and their applications. Specifically, We categorize the existing diffusion models into three categories: sampling-acceleration enhancement, likelihood-maximization enhancement, and data-generalization enhancement. Moreover, we categorize the applications of diffusion models into seven categories: computer vision, natural language processing, waveform signal processing, multi-modal learning, molecular graph generation, time series modeling, and adversarial purification.
- **Comprehensive Review.** We provide the first comprehensive overview of modern diffusion models and their applications. For each type of diffusion models, we demonstrate the main improvements, make the necessary comparisons, and summarize the corresponding papers. For each type of applications of diffusion models, we demonstrate the main problems to deal with, and illustrate how they address these problems.
- **Future Research Directions.** We propose open problems for future research and provide some suggestions about future development of diffusion models in both algorithms and applications.

2 Preliminaries of Diffusion Models

A central problem in generative modelling is the trade-off between the flexibility and the tractability of the models probability distributions. The essential idea of diffusion model, is to systematically perturb the structure in a data distribution through an forward diffusion process, and then recover the structure by learning a reverse diffusion process, resulting in a highly flexible and tractable generative model. A denoising diffusion probabilistic model (DDPM) [26] consists of two parameterized Markov chain, and uses variational inference to produce samples matching the original data after finite time. The forward chain perturbs the data distribution by gradually adding Gaussian noise with pre-designed schedule until the data distribution converges to a given prior, i.e. standard Gaussian distribution. The reverse chain starts with the given prior and uses a parameterized Gaussian transition kernel, learning to gradually restore the undisturbed data structure. Formally: Given a data distribution $\mathbf{x}_0 \sim q(\mathbf{x}_0)$, we define a forward noising process q which produces latents $\mathbf{x}_1, \mathbf{x}_2 \dots \mathbf{x}_T$, by adding Gaussian noise at time t with variance $\beta_t \in (0, 1)$ as follows:

$$q(\mathbf{x}_1, \dots, \mathbf{x}_T | \mathbf{x}_0) = \prod_{t=1}^T q(\mathbf{x}_t | \mathbf{x}_{t-1}) \quad (1)$$

$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1 - \beta_t} \mathbf{x}_{t-1}, \beta_t \mathbf{I}) \quad (2)$$

Here we use $q(\mathbf{x}_t)$ to denote the distributions of latent variables \mathbf{x}_t in forward process. As noted in [26], the noising process defined in Eq.2 allows us to sample an arbitrary step of the noised latents directly conditioned on the input \mathbf{x}_0 . With $\alpha_t = 1 - \beta_t$ and $\bar{\alpha}_t = \prod_{s=0}^t \alpha_s$, we can write the marginal as:

$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t} \mathbf{x}_0, (1 - \bar{\alpha}_t) \mathbf{I}) \quad (3)$$

$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon \quad (4)$$

When $\bar{\alpha}_T$ approximates 0, \mathbf{x}_T is practically indistinguishable from pure Gaussian noise: $p(\mathbf{x}_T) \approx \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$. The joint distribution $p_\theta(\mathbf{x}_{0:T})$ is called the *reverse process*, and when β_t is sufficiently small, $q(\mathbf{x}_{t-1} | \mathbf{x}_t)$ is approximately Gaussian. And thus we can parameterize this reverse process as follows, starting at $p(\mathbf{x}_T) = \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$:

$$p_\theta(\mathbf{x}_{0:T}) = p(\mathbf{x}_T) \prod_{t=1}^T p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t), \quad (5)$$

$$p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \mu_\theta(\mathbf{x}_t, t), \Sigma_\theta(\mathbf{x}_t, t)) \quad (6)$$

Table 1: Notions in Diffusion Models.

Notations	Descriptions
T	Total time steps of diffusion process
t	Time step t on the range of $[0, T]$
$\ \cdot\ $	L_2 norm
A	Linear transformation
b	Bias term
\mathcal{T}	Transformation in $SE(3)$
ϵ	Standard gaussian noise
z_t	Standard gaussian noise at time t
\mathcal{U}	Uniform distribution
\mathcal{N}	Normal distribution
β_t	Variance coefficient at time t
$\beta(t)$	Continuous-time limit of β_t
α_t	$1 - \beta_t$
$\bar{\alpha}_t$	Cumulative product of α_t
$\alpha(t)$	Continuous-time signal scale
$\sigma(t)$	Continuous-time noise scale
$R(t)$	Signal-to-Noise ratio
\mathbf{x}	Original data
\mathbf{x}_0	Unperturbed data in diffusion model
\mathbf{x}_t	Diffused data at time t
\mathbf{x}'	Intermediate data in diffusion process
$q(\mathbf{x}_t \mathbf{x}_s)$	Transition kernel in forward chain, from time s to time t
$q(\mathbf{x}_t)$	Marginal distribution of forward chain at time t
$p_\theta(\mathbf{x}_t \mathbf{x}_s)$	Transition kernel of reverse chain, from time s to time t , parameterized by θ
$p_\theta(\mathbf{x}_t)$	Marginal distribution in forward chain at time t
$q_{st}(\mathbf{x}_t \mathbf{x}_s)$	Transition kernel of forward SDE, from time s to time t
$q_t(\mathbf{x})$	Marginal distribution of diffusion SDE at time t
$p_t(\mathbf{x})$	Marginal distribution of data generated by plug-in reverse SDE at time t
$\nabla_x \log p_t(\mathbf{x})$	Score function at time t
$\mathbf{f}(\cdot, \cdot)$	Drift coefficient of SDE
$\mathbf{f}_i(\cdot)$	Drift coefficient at pre-fixed time t_i
$\mathbf{g}(\cdot)$	Diffusion coefficient of SDE
$\mathbf{g}_i(\cdot)$	Diffusion coefficient at pre-fixed time t_i
w	Standard Wiener process
\bar{w}	Reverse time Wiener process
$\mu_\theta(\mathbf{x}_t, t)$	Learnable mean of reversed process at time t
$\Sigma_\theta(\mathbf{x}_t, t)$	Learnable variance coefficient of reversed step at time t
$\epsilon_\theta(\mathbf{x}_t, t)$	Estimated noise function at time t
$s_\theta(\mathbf{x}_t, t)$	Estimated score function at time t
$\hat{\mathbf{x}}_\theta(\mathbf{x}_t; t)$	Estimation of \mathbf{x}_0 at time t
L_{VLB}	Variational Lower Bound
E_q	Scaled error
$\mathbf{P}_r(\cdot)$	Polynomial extrapolation of degree r

Here we use $p_\theta(\mathbf{x}_t)$ to denote the distributions of latent variables \mathbf{x}_t in reverse process, or $p(\mathbf{x}_t)$ for simplicity. Training is performed by optimizing the variational upper bound on negative log likelihood:

$$\mathbb{E}[-\log p_\theta(\mathbf{x}_0)] \leq \mathbb{E}_q \left[-\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \right] = \mathbb{E}_q \left[-\log p(\mathbf{x}_T) - \sum_{t \geq 1} \log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})} \right] = -L_{\text{VLB}} \quad (7)$$

Reparameterize the right side of Eq.7 [26], and we get the general objective:

$$\mathbb{E}_{t \sim \mathcal{U}(0,T), \mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \left[\lambda(t) \left\| \epsilon - \epsilon_\theta(\sqrt{\alpha_t}\mathbf{x}_0 + \sqrt{1-\alpha_t}\epsilon, t) \right\|^2 \right] \quad (8)$$

Here ϵ_θ is a neural network, which uses input \mathbf{x}_t and t to predict ϵ that can generate \mathbf{x}_t , resembling denoising score matching over multiple noise scales indexed by t [31]. $\lambda(t)$ is a positive weighting function. The objective function can be estimated by Monte-Carlo algorithm and trained with stochastic optimizers. In generation procedure, It first picks a sample \mathbf{x}_T from the standard Gaussian prior, and then sequentially draws sample \mathbf{x}_t using the reverse chain until we get a new data \mathbf{x}_0 .

The aforementioned diffusion probabilistic model can be viewed as a score-based generative model [29]. In the continuous-time setting, score-based generative model constructs a stochastic differential equation(SDE) to smoothly disturb a data distribution to a known prior distribution, and a corresponding reverse-time SDE to transform the prior distribution back into the data distribution. Formally the forward diffusion process is the solution of the following SDE:

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w} \quad (9)$$

Here \mathbf{w} is standard Wiener process, aka standard Brownian motion. \mathbf{x}_0 is the original data sample and \mathbf{x}_T is the perturbed data that approximate standard Gaussian distribution. The solution of the following reverse SDE has the same marginal densities as the forward SDE, but it evolves reverse in time [29]:

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t) - g(t)^2 \nabla_{\mathbf{x}} \log q_t(\mathbf{x})dt + g(t)d\bar{\mathbf{w}} \quad (10)$$

Here $\bar{\mathbf{w}}$ is a standard Wiener process where time flows backwards from T to 0 , and dt is an infinitesimal negative time step. Therefore, to reverse the diffusion process and generate data, the only information we need is the score function at each time step t : $\nabla_{\mathbf{x}} \log q_t(\mathbf{x})$. Here we use $q_t(\mathbf{x})$ to denote the distributions of latent variables \mathbf{x}_t in forward process. Borrowing techniques from score-matching [31], we can train a time-dependent score-based model $\mathbf{s}_\theta(\mathbf{x}_t, t)$ to estimate the score function by optimizing the denoising score-matching objective:

$$\mathbb{E}_{t, \mathbf{x}_0, \mathbf{x}_t} \left[\lambda(t) \left\| \mathbf{s}_\theta(\mathbf{x}_t, t) - \nabla_{\mathbf{x}_t} \log q_{0t}(\mathbf{x}_t | \mathbf{x}_0) \right\|^2 \right] \quad (11)$$

[29] demonstrates that the generation process in DDPM is a special discretization of the reverse SDE:

$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}dt + \sqrt{\beta(t)}d\mathbf{w} \quad (12)$$

where $\beta(\frac{i}{N}) = N\beta_i$ in Eq.2 as N goes to infinity. There are many other advanced discretization techniques capable of improving model performance. In next three sections (Section.3, 4, and 5), we will introduce three main enhancements on diffusion models with corresponding works in detail. In Tab.2, we list the three types of diffusion models with corresponding articles and years, under continuous and discrete settings.

3 Diffusion Models with Sampling-Acceleration Enhancement

Despite the great success of diffusion models in generating high-quality and diverse samples, they have time-consuming sampling procedure which usually requires thousands of time discretization steps of the learned diffusion process to reach the desired accuracy. In continuous-time setting, [29, 36] point out that the error of the generative model is mainly caused by two limitations, one is the fitting error from the mismatch between the learned score function $\mathbf{s}_\theta(\mathbf{x}_t, t)$ and oracle score function $\nabla_{\mathbf{x}} \log p_t(\mathbf{x})$, and another is the discretization error from discretization of SDE. Many studies have focused on designing proper solvers for the learned reverse SDE to reduce error in discretization, and thus we can reduce the sampling steps while preserve good sample quality. [29, 32, 34, 37, 35, 36]. [29] proposes to discretize the reverse-time SDE in the same way as the forward one. To discretize a forward SDE and a reverse SDE as Eq.9 and Eq.10 and suppose the following iteration rule is a discretization of the forward SDE:

$$\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{f}_i(\mathbf{x}_i) + \mathbf{g}_i \mathbf{z}_i, \quad i = 0, 1, \dots, N-1 \quad (13)$$

where $\mathbf{z}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$. \mathbf{f}_i and \mathbf{g}_i are determined by SDE and the discretization scheme. We can discretize the reverse-time SDE as follows:

$$\mathbf{x}_i = \mathbf{x}_{i+1} - \mathbf{f}_{i+1}(\mathbf{x}_{i+1}) + \mathbf{g}_{i+1} \mathbf{g}_{i+1}^t \mathbf{s}_{\theta^*}(\mathbf{x}_{i+1}, i+1) + \mathbf{g}_{i+1} \mathbf{z}_{i+1}, \quad (14)$$

Table 2: Three types of diffusion models are listed with corresponding articles and years, under continuous and discrete settings.

Category	Time Setting	Article	Year
Sampling Acceleration	Continuous	Song et al. [29]	2020
		Jolicœur et al. [32]	2021
		Karras et al. [33]	2022
		Lu et al. [34]	2022
		Chuang et al. [35]	2022
		Zhang et al. [36]	2022
		Liu et al. [37]	2022
		Dockhorn et al. [38]	2022
		Zhang et al. [39]	2022
		Watson et al. [40]	2022
	Discrete	Song et al. [41]	2020
		Nichol et al. [42]	2021
		Watson et al. [43]	2021
		Luhman et al. [44]	2021
		SanRoman et al. [45]	2021
		Zheng et al. [46]	2021
		Lyu et al. [47]	2021
		Watson et al. [40]	2022
		Salimans et al. [48]	2022
		Bao et al. [49]	2022
Likelihood Maximization	Continuous	Song et al. [50]	2021
		Huang et al. [30]	2021
		Lu et al. [51]	2022
		Kim et al. [52]	2022
		Franzese et al. [53]	2022
	Discrete	Ho et al. [26]	2020
		Nichol et al. [42]	2021
		Kingma et al. [54]	2021
		Bao et al. [49]	2022
Data Generalization	Continuous	Vahdat et al. [55]	2021
		Huang et al. [56]	2021
		Liu et al. [37]	2022
		Campbell et al. [57]	2022
		De et al. [58]	2022
	Discrete	Niu et al. [59]	2020
		Wehenkel et al. [60]	2021
		Austin et al. [61]	2021
		Xie et al. [62]	2022
		Gu et al. [63]	2022
		Xu et al. [64]	2022

using the trained score function $s_{\theta^*}(\mathbf{x}_i, i)$. This process can be apply to any diffusion model, and experiments show that this sampler performs slightly better DDPM. Moreover, at each time step, after the numerical SDE solver gives an estimate of the sample, a "corrector" will corrects the marginal distribution of the estimated sample using Markov Chain Monte Carlo method. Experiments show that it is more efficient adding a corrector to the SDE solver than using more steps.

[32] proposes an adaptive step-size SDE solver tailored to score-based generative models piece by piece. They combine a fast high-order SDE solver with a accurate low-order SDE solver. At the time step, the high- and low-order solvers generate new sample \mathbf{x}'_{high} and \mathbf{x}'_{low} from previous sample \mathbf{x}'_{prev} . If \mathbf{x}'_{high} and \mathbf{x}'_{low} is similar, the algorithm will accept the extrapolation \mathbf{x}' between \mathbf{x}'_{high} and \mathbf{x}'_{low} as the new sample at current step, and increases the step size. The dissimilarity between \mathbf{x}'_{high} and \mathbf{x}'_{low} is defined as:

$$E_q = \left\| \frac{\mathbf{x}'_{low} - \mathbf{x}'_{high}}{\delta(\mathbf{x}', \mathbf{x}'_{prev})} \right\|^2 \quad (15)$$

where $\delta(\mathbf{x}'_{low}, \mathbf{x}'_{prev}) = \max(\epsilon_{abs}, \epsilon_{rel} \max(|\mathbf{x}'_{low}|, |\mathbf{x}'_{prev}|))$ is the tolerance. Here $\epsilon_{abs}, \epsilon_{rel}$ are hyper-parameters. If $E_q \leq 1$, then \mathbf{x}'_{high} is similar to \mathbf{x}'_{low} and thus accurate. Therefore one can use the extrapolation as the new sample at this time step since it is a accurate sample drawn with large step size.

Inspired by the contraction theory of the stochastic difference equations, [35] shows that starting from a single forward diffusion with better initialization significantly reduces the number of sampling steps. At each generation step, they transform the generated sample using non-expansive linear mapping:

$$\tilde{\mathbf{x}}_{i-1} = f(\mathbf{x}_i, i) + g(\mathbf{x}_i, i)\mathbf{z}_i \quad (16)$$

$$\mathbf{x}_{i-1} = \mathbf{A}\tilde{\mathbf{x}}_{i-1} + \mathbf{b} \quad (17)$$

where $\mathbf{z}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ and A is non-expansive:

$$\|\mathbf{A}\mathbf{x} - \mathbf{A}\mathbf{y}\| \leq \|\mathbf{x} - \mathbf{y}\|, \quad \forall \mathbf{x}, \mathbf{y} \quad (18)$$

Using theory from stochastic contraction, they demonstrate there exists a shorter sampling path depending on the \mathbf{A} , and the estimation error of this shorter sampling path can be bounded by the that of the original estimation. And thus we can start the generation at earlier step to get better results.

As shown in [29], every diffusion model has a corresponding ODE which has a same marginal distribution as diffusion SDE:

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t) - \frac{1}{2}g(t)^2\nabla_{\mathbf{x}} \log q_t(\mathbf{x})dt \quad (19)$$

and thus we can design better ODE solver and generate data using the derived discretized ODE [34, 36, 37, 33]. [34] demonstrates exact formulation of the solution of diffusion ODEs. The formulation analytically computes the linear part of the solution and the non-linear part can be approximated by exponentially-weighted integration of the neural networks. Formally, they consider the following diffusion ODE which includes DDPM as a special case:

$$\frac{d\mathbf{x}_t}{dt} = f(t)\mathbf{x}_t - \frac{1}{2}g^2(t)\nabla_{\mathbf{x}} \log q_t(\mathbf{x}_t) \quad (20)$$

It has analytical solution:

$$\mathbf{x}_t = e^{\int_s^t f(\tau)d\tau} \mathbf{x}_s + \int_s^t \left(e^{\int_\tau^t f(r)dr} \frac{g^2(\tau)}{2\sigma_\tau} \epsilon_\theta(\mathbf{x}_\tau, \tau) \right) d\tau. \quad (21)$$

Here the learned score function $-\frac{\epsilon_\theta(\mathbf{x}_\tau, \tau)}{2\sigma_\tau}$ is used to replace the oracle score function. This formula can reduce the discretization error of the linear part. And one can reduce the fitting error by expand the score function to a high-order one, and this method is theoretically guaranteed. They propose to combine different order solvers to dynamically adjust the step size to further improve efficiency as [32].

[36] also leverages the semi-linear structures of learned diffusion process and derives similar solution for Eq.20. They propose to discretize the diffusion ODE using quadratic time step, as in [41]. And they also propose to use Exponential Integrator to approximately calculate the solution of ODE in the time step, and use polynomial extrapolation for better score estimation. After estimating the score function $\epsilon_\theta(\mathbf{x}_{t_i}, t_i)$ at time discretization $\{t_i\}_{i=0}^N$, we fit a polynomial $\mathbf{P}_r(t)$ of degree r with respect to the interpolation points $(t_i, \epsilon_\theta(\mathbf{x}_{t_i}, t_i))$:

$$\mathbf{P}_r(t) = \sum_{j=0}^r \left[\prod_{k \neq j} \frac{t - t_{i+k}}{t_{i+j} - t_{i+k}} \right] \epsilon_\theta(\mathbf{x}_{t_{i+j}}, t_{i+j}). \quad (22)$$

We then use $\mathbf{P}_r(t)$ to approximate $\epsilon_\theta(\mathbf{x}_\tau, \tau)$ over the interval $[t_{i-1}, t_i]$. Combining all ingredients, they can reduce the discretization error and fitting error, leading to fewer evaluation steps. [37] demonstrates that by solving the differential equations of DDPM on manifolds, we can design faster higher-order ODE. [33] illustrates that the tangent of the solution trajectory should point towards the denoised output by properly designing the noise schedule for reducing the discretization error.

In the discrete time setting, generation speed can be improved through reducing the fitting error [42, 43, 49, 44, 48, 41]. [42] observed that learning the variance in the reverse process allows sampling with an order of magnitude fewer steps. They artificially set the reverse variance in Eq.6 as:

$$\Sigma_\theta(\mathbf{x}_t, t) = \exp(v \cdot \log \beta_t + (1 - v) \cdot \log \tilde{\beta}_t) \quad (23)$$

where $\tilde{\beta}_t = \frac{1 - \bar{\alpha}_{t-1}}{1 - \bar{\alpha}_t} \cdot \beta_t$ and v is the parameter to be learned using VLB. This simple tuning can reduce the time steps for sampling. In [43], fast sampling can be achieved by selecting a optimal sub-trajectory which maximizes the training

VLB using dynamic programming algorithm. The key observation here is that we can decompose the VLB according to sub-trajectory. Given path of inference timesteps $0 = t'_0 < t'_1 < \dots < t'_{K-1} < t'_K = T$, one can derive a corresponding ELBO:

$$-L_{\text{VLB}} = \mathbf{E}_q \mathbf{D}_{KL}[q(\mathbf{x}_1 | \mathbf{x}_0) || p_\theta(\mathbf{x}_1)] + \sum_{i=1}^K L(t'_i, t'_{i-1}) \quad (24)$$

$$L(t, s) = \begin{cases} -\mathbf{E}_q \log p_\theta(\mathbf{x}_t | \mathbf{x}_0) & s = 0 \\ \mathbf{E}_q \mathbf{D}_{KL} q(\mathbf{x}_s | \mathbf{x}_t, \mathbf{x}_0) p_\theta(\mathbf{x}_s | \mathbf{x}_t) & s > 0 \end{cases} \quad (25)$$

And thus each $L(i, j)$ is remembered and one can apply dynamic programming to select a optimal trajectory with contiguous time steps for any pre-trained DDPM. Furthermore, [49] demonstrates that the optimal reverse variance and the corresponding optimal KL divergence of a DDPM have analytic forms w.r.t. its score function. Thus one can indeed choose a optimal sub-trajectory.

Other approaches either adopt early stopping to truncate the forward and reverse process [47, 46], or retrain student networks that can take shortcuts via knowledge distillation [44, 48], or generalize the forward process to non-markovian process[41].

4 Diffusion Models with Likelihood-Maximization Enhancement

Denoising Diffusion Probabilistic Model (DDPM) [26] does not have competitive log-likelihoods compared to other likelihood-based models [26, 54], and recently there are various methods to enhance the maximization of log-likelihoods. Due to the intractability of the direct computation of the log-likelihood, studies mainly focus on designing and analysing the variational lower bound. In the discrete time setting, studies have found that it is beneficial to learn the noise schedule in the forward process as well as the variance in each time step of the reverse process [42, 54, 49]. In [42], hand-crafted noise schedule and reverse variance estimation already achieve competitive log likelihoods. They propose the following noise schedule:

$$\bar{\alpha}_t = \frac{h(t)}{h(0)}, \quad h(t) = \cos \left(\frac{t/T + m}{1 + m} \cdot \frac{\pi}{2} \right)^2, \quad (26)$$

where $\bar{\alpha}_t$ is defined in Eq.4. One can use $\beta_t = 1 - \frac{\bar{\alpha}_t}{\bar{\alpha}_{t-1}}$ to calculate the forward variance in Eq.2. In this scheme, $\bar{\alpha}_t$ progresses smoothly, and prevents abrupt changes at noise level. Thus the reverse process can recover the data structure easily.

[54] shows that variational lower bound of data \mathbf{x} can be simplified to a short expression in terms of the signal-to-noise ratio $R(t)$ of the diffused data:

$$\mathcal{L}(\mathbf{x}_0) = \frac{T}{2} \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I}), i \sim U\{1, T\}} \left[\left(R\left(\frac{t-1}{T}\right) - R\left(\frac{t}{T}\right) \right) \|\mathbf{x}_0 - \hat{\mathbf{x}}_\theta(\mathbf{x}_t; t)\|_2^2 \right] \quad (27)$$

$$\approx -\frac{1}{2} \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \int_0^1 R'(t) \|\mathbf{x}_0 - \hat{\mathbf{x}}_\theta(\mathbf{x}_t; t)\|_2^2 dt \quad \text{as } T \rightarrow \infty \quad (28)$$

$$= -\frac{1}{2} \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I}), t \sim \mathcal{U}(0, 1)} \left[R'(t) \|\mathbf{x}_0 - \hat{\mathbf{x}}_\theta(\mathbf{x}_t; t)\|_2^2 \right]. \quad (29)$$

where \mathbf{x}_t denotes corrupted data \mathbf{x} after t steps, $\mathbf{x}_t = \alpha(t)\mathbf{x}_0 + \sigma^2(t)\epsilon$. The $R(t)$ is defined as the following:

$$R(t) = \frac{\alpha^2(t)}{\sigma^2(t)}. \quad (30)$$

Applying change-of-variable to the objective function in Eq.28 shows that, in the infinitely deep setting, the VLB is fully determined by the end point of noise schedule:

$$\mathcal{L}(\mathbf{x}) = \frac{1}{2} \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \int_{R_{\min}}^{R_{\max}} \|\mathbf{x} - \tilde{\mathbf{x}}_\theta(\mathbf{x}_v, v)\|_2^2 dv, \quad (31)$$

Thus, in the infinitely deep setting, the noise schedule between the endpoints does not affect the objective function. One can alternatively optimize the noise schedule between end points for other objectives, like variance reduction, and optimize the end points for VLB. [49] demonstrates a remarkable result that the optimal reverse variance for the VLB a DDPM have analytic forms w.r.t. its score function. Thus one can indeed approximately achieve the optimal VLB for DDPM in discrete setting.

In the continuous time setting, new data is generated by the plug-in reverse SDE with learned score function $\mathbf{s}_\theta(\mathbf{x}_t, t)$:

$$d\mathbf{x} = f(\mathbf{x}, t) - g(t)^2 \mathbf{s}_\theta(\mathbf{x}_t, t) dt + g(t) d\mathbf{w}. \quad (32)$$

Otherwise data can be generated by the learned diffusion ODE:

$$\frac{d\mathbf{x}_t}{dt} = f(t, \mathbf{x}_t) - \frac{1}{2} g^2(t) \mathbf{s}_\theta(\mathbf{x}_t, t). \quad (33)$$

Studies have focused on maximizing the likelihood of the solution of above SDE and ODE at time 0, denoted by p_0^{sde} and p_0^{ode} , respectively [50, 51, 30]. [50] demonstrates that with specific weighting scheme, the objective can be an upper bound of the negative log-likelihood of the generated sample, thus it enables approximate maximum likelihood training of score-based diffusion models:

$$\mathbf{D}_{KL}(q_0 \parallel p_0^{sde}) \leq \mathcal{L}(\theta; g(\cdot)^2) + \mathbf{D}_{KL}(q_T \parallel \pi), \quad (34)$$

where $\mathcal{L}(\theta; g(\cdot)^2)$ is the objective in Eq.11 with weighting function $\lambda(t) = g(t)^2$. Since $\mathbf{D}_{KL}(q_0 \parallel p_0^{sde}) = -\mathbb{E}_{q_0} \log(p_0^{sde}) + C$, the proposed weighting scheme can bound the negative log-likelihood of the generated sample. Concurrently, [30] and [50] both demonstrate that the negative log-likelihood of any given sample can be bounded as the following:

$$-\log p_0^{sde}(\mathbf{x}) \leq \mathcal{L}'(\mathbf{x}), \quad (35)$$

$$\mathcal{L}'(\mathbf{x}) = -\mathbb{E}_{\mathbf{x}_T} [\log p_0^{sde}(\mathbf{x}_T) \mid \mathbf{x}_0 = \mathbf{x}] + \int_0^T \mathbb{E}_{\mathbf{x}_s} \left[\frac{1}{2} \|g(s) \mathbf{s}_\theta(\mathbf{x}_s, s)\|^2 + \nabla \cdot (g(s)^2 - f(s, \mathbf{x}_s)) \mid \mathbf{x}_0 = \mathbf{x} \right] ds. \quad (36)$$

The second part of Eq.36 can be seen as the objective of implicit score matching method [65]. And thus matching the score function amounts to minimizing an upper bound of the negative log-likelihood of samples, which are generated by the reverse plug-in SDE.

On the other hand, [51] proves that we need to bound the first, second, and third-order score matching errors to maximize the likelihood of diffusion ODE. They demonstrate that matching the first order score is not enough to maximize the log-likelihood of generated data in the diffusion ODE:

$$\mathbf{D}_{KL}(q_0 \parallel p_0^{ode}) = \mathbf{D}_{KL}(q_T \parallel p_T^{ode}) + \mathcal{L}_{ode}(\theta), \quad (37)$$

where $\mathcal{L}_{ode}(\theta) = \mathcal{L}(\theta; g(\cdot)^2) + \mathcal{L}_{dif}(\theta)$ and:

$$\mathcal{L}_{dif}(\theta) := \frac{1}{2} \int_0^T g(t)^2 \mathbb{E}_{q_t(\mathbf{x}_t)} \left[(\mathbf{s}_\theta(\mathbf{x}_t, t) - \nabla_{\mathbf{x}} \log q_t(\mathbf{x}_t))^\top (\nabla_{\mathbf{x}} \log p_t^{ode}(\mathbf{x}_t) - \mathbf{s}_\theta(\mathbf{x}_t, t)) \right] dt. \quad (38)$$

Thus optimizing $\mathcal{L}(\theta; g(\cdot)^2)$ alone is not equivalent to maximize an upper bound of sample likelihood in diffusion ODE. Further more, they prove that, under mild conditions, one can minimize the upper bound of the likelihood by matching the first, second and third-order of score function. And efficient training algorithm is available.

5 Diffusion Models with Data-Generalization Enhancement

Diffusion models assume that data is supported on a Euclidean space, i.e. a manifold with flat geometry, and adding Gaussian noise would inevitably transform the data to continuous state spaces. Various studies have focused on addressing these limitations [60, 55, 63, 62, 61, 56, 37, 58, 59]. Diffusion models can be applied to various data types by first encoding the data to the latent space and then applying the diffusion model to the space, relying on the VAE framework. The key issue here is how to design loss function to jointly learn the VAE and the diffusion model, since the prior distribution of the latent variable should achieve both flexibility and tractability. [55] handles the problem in the continuous-time setting directly. It identifies that the score-matching loss is no longer applicable due to the intractability of the latent prior:

$$\nabla_{\mathbf{x}} \log p_t(\mathbf{x}) = \int p_{0t}(\mathbf{x}_t \mid \mathbf{x}_0) p_\theta(\mathbf{x}_0) d\mathbf{z} \quad (39)$$

where $p_\theta(\mathbf{x}_0)$ is the latent prior parameterized by a neural network. This issue is inevitable for objectives in score-based generative model, since they require the score function in the forward process to be available or prefixed. Using the ELBO in VAE as loss function, [55] derives its connection to score-matching objectives in score-based generative model,

allowing for efficient training and sampling. They prove that the cross entropy term in the ELBO can be transformed as follow:

$$\mathcal{H}(q(\mathbf{x}_0|\mathbf{x}), p(\mathbf{x}_0)) = \mathbb{E}_{t \sim \mathcal{U}[0,1]} \left[\frac{g(t)^2}{2} \mathbb{E}_{q_{0:t}(\mathbf{x}_t, \mathbf{x}_0|\mathbf{x})} [\|\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t|\mathbf{x}_0) - \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t)\|_2^2] \right] + C, \quad (40)$$

where $q(\mathbf{x}_0|\mathbf{x})$ and $p(\mathbf{x}_0)$ are marginal distribution of SDE (Eq.9) and \mathbf{x} is the original data. Using this formula and the fact that $\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t|\mathbf{x}_0)$ is tractable, one can parameterize $\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t)$ and optimize the ELBO. Alternatively, [60] circumvents the problem by designing the VLB of diffusion model combined with reconstruction loss of VAE. [63, 62, 61] generalize DDPM to discrete state case, where the data is binary or categorical. Here the noise is a random walk on all states or a random mask operation. The transition kernel can be written as follows:

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathbf{v}^\top(\mathbf{x}_t) \mathbf{Q}_t \mathbf{v}(\mathbf{x}_{t-1}), \quad (41)$$

where $\mathbf{v}(\mathbf{x})$ is a one-hot column vector, and \mathbf{Q}_t is the transition kernel of a lazy random walk and can be parameterized as follows:

$$\mathbf{Q}_t = \begin{bmatrix} \alpha_t + \beta_t & \beta_t & \cdots & \beta_t \\ \beta_t & \alpha_t + \beta_t & \cdots & \beta_t \\ \vdots & \vdots & \ddots & \vdots \\ \beta_t & \beta_t & \cdots & \alpha_t + \beta_t \end{bmatrix}. \quad (42)$$

Other methods include using absorbing state kernel or a discretized Gaussian kernel [61]. [57] provides the first continuous time framework for denoising diffusion models of discrete data, and derives new transition kernel and samplers. The unsolved problem here is that data in discrete space does not have score function, even in the continuous time setting. For further discussion, please refer to Section.8.

There are also generalization examples of other data structures, such as graphs and point clouds [59, 64]. To get an ordering-invariant graphs distribution, [59] designs a permutation-equivariant graph neural network to model the gradients of the data distribution. To get a rotation and translation-invariant distribution for point clouds data, [64] proves that Markov chains starting with an invariant prior and evolving with equivariant Markov kernels can induce an invariant marginal distribution. Formally, \mathcal{T} is a rotation or translation operation, if:

$$p(\mathbf{x}_T) = p(\mathcal{T}(\mathbf{x}_T)), \quad p(\mathbf{x}_{t-1}|\mathbf{x}_t) = p(\mathcal{T}(\mathbf{x}_{t-1})|\mathcal{T}(\mathbf{x}_t)), \quad (43)$$

then the marginal distribution is invariant, i.e., $p_0(\mathbf{x}) = p_0(\mathcal{T}(\mathbf{x}))$. They further build blocks for the equivariant Markov kernels. Recent theoretical and empirical founding is that diffusion model can be generalized to data on manifold, including graph as a special case [56, 37, 66]. Assuming mild conditions fit a large class of manifolds such as sphere and torus, [67] proves that we can extend diffusion models on manifold, and [37] proposes a pseudo numerical methods to solve differential equations on manifolds.

6 Connections with Other Generative Models

Generative models are a hot research area which have many applications. For example, they can be utilized to generate high-quality images [68], synthesize realistic speech and music [69], advance semi-supervised learning [70, 71], identify adversarial examples [72], conduct imitation learning [73], and make optimization in reinforcement learning [74]. In each subsection, we first introduce five other important classes of generative models, and analysis their advantages and limitations. Then we introduce how diffusion models are connected with them, and illustrate how these generative models are promoted by incorporating diffusion models. The algorithms that integrate diffusion models with other generative models are summarized in Tab.3.

6.1 Variational Autoencoder and Its Connections with Diffusion Models

Variational Autoencoders [83, 84, 85] expect to learn both an encoder and a decoder to map input data to values in a continuous latent space. They provide a formulation where the embedding can be interpreted as a latent variable in a probabilistic generative model, and a probabilistic decoder can be formulated by a parameterized likelihood function. To guarantee an effective inference, a variational bayes approach and this process is implemented by maximizing the evidence lower bound (ELBO). Provided that the parameterized likelihood function $p_\theta(\mathbf{x}|\mathbf{z})$ and the parameterized posterior approximation $q_\phi(\mathbf{z}|\mathbf{x})$ can be computed in a point-wise way, and are differentiable with their parameters, the ELBO can be maximized with gradient descent. It allows flexible choices of encoder and decoder models. Usually, they will be represented by exponential family distributions whose parameters are generated by multi-layer neural networks.

DDPM can be treated as a hierarchical Markovian VAE and with a prefixed encoder. The forward process denotes the encoder, and the reverse process denotes the decoder. Furthermore, DDPM shares the decoder across multiple

Table 3: Diffusion models are incorporated into different generative models.

Model	Article	Year
VAE	Luo et al. [75]	2022
	Hunag et al. [30]	2021
	Vadhat et al. [55]	2021
GAN	Wang et al. [76]	2022
	Xiao et al. [77]	2021
Normalizing Flow	Zhang et al.[78]	2021
	Gong et al. [79]	2021
Autoregressive Model	Hoogetboom et al.[27]	2021
	Rasul et al. [80]	2021
Energy-Based Model	Gao et al. [81]	2021
	Yu et al. [82]	2022

layers, and all the latent variables are of the same size as the sample data [75]. In the continuous-time setting, [30] demonstrates that the score-matching objective can be further approximated by the ELBO of a deep hierarchical VAE. In this way, optimizing a diffusion model can be viewed as training an infinite, deep, hierarchical VAE, which justifies the common belief that the diffusion models can be interpreted as the continuous limit of hierarchical VAEs. [55] also illustrates that the ELBO is a special score-matching objective by diffusing the latent space.

6.2 Generative Adversarial Network and Its Connections with Diffusion Models

Generative adversarial networks (GANs) [86, 87, 88] have received lots of attention because of their interesting adversarial ideas and promising architectures. GANs mainly consist of two models: a generator G and a discriminator D . These two models are typically constructed by neural networks but could be implemented with any form of differentiable system that maps input data from one space to another. The generator G tries to model the distribution of true examples, and generate new examples. The discriminator D is usually a binary classifier that is used to identify generated examples from true examples with maximally possible accuracy. The optimization of GANs can be viewed as a minimax optimization problem with value function $V(G, D)$ as the following:

$$\min_G \max_D V(G, D) = \mathbb{E}_{\mathbf{x} \sim p_{\text{data}}(\mathbf{x})} [\log D(\mathbf{x})] + \mathbb{E}_{\mathbf{z} \sim p_{\mathbf{z}}(\mathbf{z})} [\log(1 - D(G(\mathbf{z})))] \quad (44)$$

The optimization finishes at a saddle point that produces a minimum about the generator and a maximum about the discriminator. It means, the goal of GAN optimization is to achieve Nash equilibrium [89]. At that point, the generator can be considered that it has captured the accurate distribution of real examples.

One of the main practical issues of GAN is the instability in training process, which is mainly caused by the non-overlapping between the distribution of input data and that of the generated data. A practical solution is to inject noise to the discriminator input. Taking advantages of the flexible diffusion model, [76] proposes to inject noise to the discriminator with an adaptive noise schedule, determined by a diffusion model. Conversely, GAN can help with the sampling speed of diffusion model. [77] argues that slow sampling is caused by the Gaussian assumption in the denoising step, which is justified only for small step sizes. Thus they propose to model each denoising step using a conditional GAN, allowing larger step size.

6.3 Normalizing Flow and Its Connections with Diffusion Models

Normalizing flows [90, 91] are a kind of promising class of models, due to the exact density evaluation and ability to model high-dimensional data [92, 93]. Normalizing flow can transform simple probability distribution into extremely complex probability distribution, which can be used in generative model, reinforcement learning, variational inference and other fields. The tools needed to build it are Determinant, Jacobi Matrix and Change of Variable Theorem. The trajectory in normalizing flows is formulated by a differential equation. In the discrete-time setting, the mapping from input to output in normalizing flows is a composition of a sequence of bijective functions. Similar to the continuous setting, based on the rule for variable changing, the exact log-likelihood is accessible in normalizing flows. Unfortunately, the bijective requirement also has limitations on modeling complex data, both empirically and theoretically [94, 95]. Some works make an attempt to relax the bijective requirement [94, 93]. DiffFlow [78] presents a novel generative modeling algorithm, which combines the advantages of both flow-based models and the diffusion models. And thus it can not only acquire sharper boundary than normalizing flow, but also learn more general distribution with fewer discretization steps than diffusion probabilistic models.

6.4 Autoregressive Models and Its Connections with Diffusion Models

Autoregressive Models (ARMs) is to decompose the joint distribution of data into a product of conditional distributions [96, 97]. Recent techniques in deep learning have allowed tremendous progress on various modalities, such as images [98, 99], audio [69, 100], and text [101, 102, 103, 104, 105], where they are referred to as language models in text modeling. The possibility of ARMs can be retrieved through the call of a single neural network, the generation of samples from the model requires the same number of network calls as the data dimension. Although autoregressive models are very powerful density estimators, sampling is essentially a continuous process and may be very slow on high-dimensional data. Autoregressive Diffusion Models (ARDMs) [27] propose a different autoregressive models, which learns to generate arbitrary-order data. ARDMs extend order-agnostic autoregressive models and discrete diffusion models [106, 107, 7]. Different from ARMs, ARDMs have no need to conducts a causal masking on representations, and thus can be trained with an effective objective, which is similar to diffusion probabilistic models. And during test procedure, ARDMs are capable of parallel generation so that it is able to apply to arbitrary-budget generation tasks.

6.5 Energy-Based Models and Its Connections with Diffusion Models

Energy-Based Models (EBMs) [108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125] have recently received lots of attention. EBMs can be viewed as a kind of generative versions of discriminators [126, 127, 128, 123], while can be learned from unlabeled input data. Let $\mathbf{x} \sim p_{\text{data}}(\mathbf{x})$ denote a training example, and $p_{\theta}(\mathbf{x})$ denote a model’s probability density function that aims to approximates $p_{\text{data}}(\mathbf{x})$. An energy-based model (EBM) is defined as the following:

$$p_{\theta}(\mathbf{x}) = \frac{1}{Z_{\theta}} \exp(f_{\theta}(\mathbf{x})), \quad (45)$$

where $Z_{\theta} = \int \exp(f_{\theta}(\mathbf{x})) d\mathbf{x}$ is the partition function, which is analytically intractable for high-dimensional \mathbf{x} . For images, $f_{\theta}(\mathbf{x})$ is parameterized by a convolutional neural network with a scalar output.

Although EBMs have a number of desirable properties, two challenges remain for training EBMs on high-dimensional data. First, learning EBMs by maximizing the likelihood requires Markov Chain Monte Carlo (MCMC) method to generate samples from the model, which can be very expensive. Second, as demonstrated in [129], the energy potentials learned with non-convergent MCMC is not stable, in the sense that samples from long-run Markov chains can be significantly different from the observed samples, and thus it is difficult to evaluate the learned energy potentials. A recent study [81] presents a diffusion recovery likelihood method to tractably learn and samples from a sequence of EBMs in the reverse process of the diffusion model. Each EBM is trained with recovery likelihood, which aims to maximize the conditional probability of the data at a certain noise level, given their noisy versions at a higher noise level. EBMs maximize the recovery likelihood because it is more tractable than marginal likelihood, as sampling from the conditional distributions is much easier than sampling from the marginal distributions. This model can generate high quality samples, and long-run MCMC samples from the conditional distributions still resemble realistic images.

7 A Collection of Applications with Diffusion Models

Due to the flexibility and strength of diffusion models, they have recently been applied in many real-world applications. In this section, we categorize these applications into seven parts, including computer vision, natural language processing, waveform signal processing, multi-modal learning, molecular graph modeling, time series modeling, and adversarial purification. In each subsection, we first give the brief introduction to each task, and then introduce in detail how diffusion models are utilized to promote the performances. We summarize all the applications that utilize the diffusion models in Tab.4.

7.1 Computer Vision

7.1.1 Image Generation

Image Super Resolution and Inpainting. Image super resolution aims to restore high-resolution (HR) images from low-resolution (LR) images while image inpainting is to reconstruct missing or ruined regions of an image. Super-Resolution Diffusion (SRDiff) [4] is the first diffusion-based model for single image super-resolution, optimized with the variational bound on likelihood of the data. SRDiff is able to provide diverse and realistic super-resolution (SR) results through a gradual transformation of the Gaussian noise conditioned on an LR input with a Markov chain. Super-Resolution via Repeated Refinement (SR3) [130] adopts denoising diffusion probabilistic models [26, 28] to make conditional image generation, and conducts image super resolution through a stochastic iterative denoising process. LDM [131] proposes latent diffusion models, an effective method to advance both the training and sampling

Table 4: Summary of all the applications utilize the diffusion models.

Primary Category	Secondary Category	Article
Computer Vision	Image Super Resolution and Inpainting	[4],[130],[131],[132],[133],[134],[135],[136],[137],[138],[139]
	Semantic Segmentation	[5],[140]
	Anomaly Detection	[141],[142]
	Point Cloud Completion and Generation	[143],[144],[145],[146]
	Video Generation	[147],[148],[149],[150]
Natural Language Processing	Natural Language Processing	[7],[151],[152]
Waveform Signal Processing	Waveform Signal Processing	[8],[9]
Multi-Modal Learning	Text-to-Image Generation	[10],[153],[11],[154],[63],[155],[156]
	Text-to-Audio Generation	[157],[158],[159],[160],[161],[162],[163]
Molecular Graph Modeling	Molecular Graph Modeling	[13],[14],[16],[64],[164],[165],[166],[167]
Time Series Modeling	Time Series Imputation	[168],[169],[170]
	Time Series Forecasting	[171],[169]
Adversarial Purification	Adversarial Purification	[172],[173],[18],[174],[175],[176]

efficiency of denoising diffusion models without the loss of quality. To help diffusion models training using limited computational resources while maintaining both quality and flexibility, LDM also utilizes them in the latent space with pre-trained autoencoders. RePaint [132] designs an improved denoising strategy with resampling iterations for better conditioning the image. Instead of slowing down the diffusion process [177], RePaint goes forward and backward in diffusion process, producing semantically meaningful images. Palette [133] proposes a unified framework based on conditional diffusion models, and evaluates this framework on four challenging image generation tasks [178], such as colorization, inpainting, uncropping, and JPEG restoration. Cascaded Diffusion Models (CDM) [134] consists of cascaded multiple diffusion models which generate images of gradually increasing resolution. CDM is capable of generating high-quality images on the class-conditional ImageNet [179] generation benchmark dataset, without any supervision information from auxiliary image classifiers. Multi-Speed Diffusion (MSDiff) [135] produces a conditional multi-speed diffusive estimator (CMDE), an estimator of conditional score, which combines previous conditional score estimation methods [130, 168]. Additionally, there are also some works applying the diffusion models to medical image denoising and super resolution [136, 137, 138, 139].

Semantic Segmentation. Semantic segmentation is to cluster parts of an image together which belong to the same category. Pre-training can improve the label utilization of semantic segmentation models, and an alternative way to pre-train semantic segmentation models is generative modeling. A recent study [5] conducts an investigation into the representations learned by the state-of-the-art DDPM [26], and demonstrates that they have the ability to capture high-level semantical information that is valuable for downstream vision tasks. It develops a simple approach in the few-shot operating point that exploits these learned representations and significantly outperforms the alternatives including VDVAE [180] and ALAE [19]. Inspired by the success of diffusion models, scholars also investigate the effectiveness of representations learned by denoising autoencoders [181] for semantic segmentation. Decoder Denoising Pretraining (DDeP) [140] make an initialization of the encoder using supervised learning procedure, and pre-train only the decoder guided by the denoising objective.

Anomaly Detection. Anomaly detection is a critical and challenging problem in machine learning and computer vision [182]. Generative models have been shown to own a powerful mechanism for anomaly detection. They help modeling normal or healthy reference data which can subsequently be utilized as a baseline for scoring anomalies [183], including GAN, VAE, and diffusion models [141, 142]. AnoDDPM [141] presents a new anomaly detection method which utilizes DDPM to corrupt the input image and reconstruct a healthy approximation of the image. This method has superiority over adversarial training as it can better model smaller datasets with advanced sample quality and more stable training. DDPM-CD [142] proposes a new way to incorporate large numbers of unsupervised remote sensing images into the training process through DDPM. It conducts remote sensing change detection by utilizing a pre-trained DDPM and applying the multi-scale representations from the diffusion model decoder. It aims to train a light change detection classifier to detect precise changes effectively.

Point Cloud Completion and Generation. 3D point cloud is a critical form of 3D representation for capturing real-world 3D objects. Nevertheless, scanned point clouds in the real world are usually incomplete because of partial

observation and self occlusion. It is important to recover the complete shape by reasoning the missing parts for many downstream tasks, including 3D reconstruction, augmented reality (AR) and scene understanding [145]. A probabilistic model captures the uncertain, multi-modal nature of the generation or completion problem: it may sample and produce diverse shapes from scratch or partial observations [184]. PVD [143] integrates denoising diffusion models with the pointvoxel representation of 3D shapes. Inspired by the diffusion process in non-equilibrium thermodynamics, [144] treats the points in point clouds as particles in a thermodynamic system in connection with a heat bath, which makes diffusion from the original distribution to a noise distribution. Point Diffusion-Refinement (PDR) [145] utilizes a conditional DDPM to generate a coarse completion given the partial observation, and constructs a 1-to-1 point-wise mapping between the generated point cloud and the uniform ground truth. Then it optimizes the mean squared error loss to achieve uniform generation.

7.1.2 Video Generation

In the era of deep learning, high-quality video generation still remains challenging due to the spatio-temporal continuity and complexity of video frames [6, 185]. Recent studies resort to diffusion models for improve the quality of the generated videos. Flexible Diffusion Model (FDM) [147] proposes a new video generation framework based on DDPM that produces long-term video completions in different realistic scenarios. It introduces a generative model that can sample any arbitrary subset of video frames conditioned on any other subset during test time, and present an architecture designed for this purpose. Inspired by recent advances in neural video compression [186], Residual Video Diffusion (RVD) [149] presents an autoregressive, end-to-end optimized video diffusion model. It successively generates future frames by correcting a deterministic next-frame prediction with a stochastic residual, which is generated by an inverse diffusion process. Video Diffusion Model (VDM) [148] introduces a conditional sampling method for spatio-temporal video extension. It outperforms previous proposed methods and generates long, higher resolution videos.

7.2 Natural Language Processing

Natural language processing is the research area that aims to understand, model, and manage human languages. Text generation is also referred as natural language generation, has become one of the most critical and challenging tasks in natural language processing [187]. It aims to produce plausible and readable text in human language given input data (e.g., a sequence and keywords) or random noise. Researchers have developed numerous techniques for a wide range of applications of text generation [188, 189]. Discrete Denoising Diffusion Probabilistic Models (D3PMs) [7] introduce diffusion-like generative models for character-level text generation [190]. They generalize the multinomial diffusion model [191] through going beyond corruption processes with uniform transition probabilities.

Large autoregressive language models (LMs) is able to generate high-quality text [105, 192, 193, 194]. For the purpose of reliably deploying these LMs in real-world applications, the text generation process is usually expects to be controllable. It means that we need to generate text which can satisfy desired requirements (e.g., topic, syntactic structure). Controlling the behavior of language models (LMs) without re-training is a major and important problem in text generation [195, 196]. Although recent works have achieved remarkable successes on controlling simple sentence attributes (e.g., sentiment) [197, 198], there is little progress on complex, fine-grained controls (e.g., syntactic structure). In order to tackle more complex controls, Diffusion-LM [151] proposes a new language model based on continuous diffusions. Diffusion-LM starts with a sequence of Gaussian noise vectors, and incrementally denoises them into vectors corresponding to words. The gradual denoising steps help producing hierarchical continuous latent representations. This hierarchical and continuous latent variable can make it possible for simple, gradient-based methods to accomplish complex control. Analog Bits [152] first generates the analog bits to represent the discrete variables and further improves the sample quality with self-Conditioning and asymmetric time intervals.

7.3 Waveform Signal Processing

In electronics, acoustics, and some related fields, the waveform of a signal is denoted by the shape of its graph as a function of time, independent of its time and magnitude scales. Generative models for waveform are important in speech generation tasks. WaveGrad [8] introduces a conditional model for waveform generation that estimates gradients of the data density. The model is constructed with the basis on prior score matching and diffusion probabilistic models. It receives a Gaussian white noise signal as input, and iteratively refines the signal with gradient-based sampler. WaveGrad naturally trades inference speed for sample quality through adjusting the amount of refinement steps, and make a connection between non-autoregressive and autoregressive models with respect to audio quality. DiffWave [9] presents a versatile and powerful diffusion probabilistic model for conditional or unconditional waveform generation. The model is non-autoregressive, and it is efficiently trained by optimizing a variant of variational bound on the data likelihood. Moreover, it produces high-fidelity audio in different waveform generation tasks, such as class-conditional generation, and unconditional generation.

7.4 Multi-Modal Learning

7.4.1 Text-to-Image Generation

Vision-language models have attracted a lot of attentions recently due to the number of potential applications [199]. Text-to-Image generation is the task to generate a corresponding image from a descriptive text [200]. Blended diffusion [10] utilizes both pre-trained DDPM [1] and CLIP [199] models, and it firstly proposes a solution region-based image editing for general purpose, which uses natural language guidance and is applicable to real and diverse images. unCLIP [153] proposes a two-stage model, a prior model that can generate a CLIP-based image embedding conditioned on a text caption, and a diffusion-based decoder that can generate an image conditioned on the image embedding. Imagen [11] proposes a text-to-image diffusion model with a better language understanding and an unprecedented degree of photorealism. Inspired by the ability of guided diffusion models [1, 201] to generate photorealistic samples and the ability of text-to-image models to handle free-form prompts, GLIDE [154] applies guided diffusion to the application of text-conditioned image synthesis. VQ-Diffusion [63] proposes a vector-quantized diffusion model for text-to-image generation, and it eliminates the unidirectional bias and avoids accumulative prediction errors.

7.4.2 Text-to-Audio Generation

Text-to-audio generation is the task to transform normal language texts to voice outputs [159, 160]. Grad-TTS [157] presents a novel text-to-speech model with a score-based decoder and diffusion models. It gradually transforms noise predicted by encoder, and is further aligned with text input by the method of Monotonic Alignment Search [202]. Grad-TTS2 [163] improves Grad-TTS in an adaptive way. DiffSound [158] presents a non-autoregressive decoder based on the discrete diffusion model [28, 61], which first predicts all the mel-spectrogram tokens in each single step, and then refines the predicted tokens in the following steps. EditTTS [161] leverages the score-based text-to-speech model to refine a mel-spectrogram prior that is coarsely modified. Instead of estimating the gradient of data density, ProDiff [162] parameterizes the denoising diffusion model through directly predicting the clean data.

7.5 Molecular Graph Modeling

Graph Neural Networks [203, 204, 205, 206] and corresponding representation learning [207] techniques have achieved great success [208, 209, 210, 211, 212, 213] in many areas, including modeling molecule graph in various tasks ranging from property prediction [214, 215] to molecule generation [216, 217], where a molecule is naturally represented by a node-edge graph. Despite their effectiveness in different applications, more intrinsic and informative properties begin to be combined with diffusion models for enhancing molecular graph modeling. Torsional diffusion [13] presents a new diffusion framework that makes operations on the space of torsion angles with a diffusion process on the hyper space, and an extrinsic-to-intrinsic scoring model. Equivariant diffusion [14] proposes a diffusion model for 3D molecule generation which is equivariant to Euclidean transformations. Another equivariant diffusion model [16] presents a fully data-driven denoising diffusion probabilistic model for protein structure and sequence, which is able to generate highly realistic proteins across the full range of domains in the Protein DataBank (PDB) [218]. Motivated by the classical force field methods for simulating molecular dynamics, ConfGF [166] directly estimates the gradient fields of the log density of atomic coordinates in molecular molecular conformation generation. Dynamic Graph Score Matching (DGSM) [167] dynamically constructs graph structures between atoms according to their spatial correlations in both training and testing processes, and thus can model both local and long-range interactions for predicting molecular conformation. Geometric diffusion [64] firstly treats each atom as a particle, and learns to reverse the diffusion process as a Markov chain. A general solution to motif-scaffolding problem [164] proposes a 3D protein-backbone generative model and is able to generate backbone samples that structurally agree with AlphaFold2 [219] predictions.

7.6 Time Series Modeling

7.6.1 Time Series Imputation

Time series data are widely used and important in real-world dynamic applications [220, 221, 222, 185]. Nevertheless, time series usually contain missing values due to multiple reasons, caused by mechanical or artificial errors [223, 224, 225]. In recent years, imputation methods based on deep neural networks have shown remarkable success for both deterministic imputation [226, 227, 228] and probabilistic imputation [229]. These imputation methods typically utilize a variant form of autoregressive models to process time series, and recent work begin to utilize powerful diffusion models to handle this problem. CSDI [168] presents a novel time series imputation method that leverages score-based diffusion models. Specifically, for the purpose of exploiting correlations within temporal data, it adopts the form of self-supervised training to optimize diffusion models. And its application in some real-world datasets reveal the superiority over previous methods. CSDE [170] proposes a novel probabilistic framework for modeling stochastic

dynamics with a neural controlled stochastic differential equation. SSSD [169] integrates conditional diffusion models and structured state space models [230] to particularly capture long-term dependencies in time series. And it performs well in both time series imputation and forecasting tasks.

7.6.2 Time Series Forecasting

Time series forecasting is the task to forecast or predict the future value over a period of time. Neural methods have recently become popular for solving the prediction problem with univariate point forecasting methods [231] or univariate probabilistic methods [232]. In the multivariate setting, we also have point forecasting methods [233] as well as probabilistic methods, which explicitly model the data distribution using Gaussian copulas [234], GANs [235], or normalizing flows [17]. TimeGrad [171] presents an autoregressive model for forecasting multivariate probabilistic time series which samples from the data distribution at each time step through estimating its gradient. To this end, it utilizes diffusion probabilistic models, which is closely connected with score matching and energy-based methods. Specifically, TimeGrad learns gradients by optimizing a variational bound on the data likelihood, and transforms white noise into a sample of the distribution of interest through a Markov chain using Langevin sampling [31] during inference time.

7.7 Adversarial Purification

Adversarial purification [236, 175, 174, 172, 173] denotes a class of defense methods that eliminate adversarial perturbations using a generative model [172]. While adversarial training [237] is viewed as a standard defense method against adversarial attacks for image classifiers, adversarial purification has shown significant performances as an alternative defense method [173], which purifies attacked images into clean images with a standalone purification model. Given an adversarial example, DiffPure [172] first diffuses it with a small amount of noise following a forward diffusion process, and then restore the clean image with a reverse generative process. Adaptive Denoising Purification (ADP) [173] demonstrates that an Energy-Based Model EBM trained with Denoising Score-Matching (DSM) can effectively purify attacked images within just a few steps. It further proposes an effective randomized purification scheme, injecting random noises into images before purification. Projected Gradient Descent (PGD) [18] presents a novel stochastic diffusion-based pre-processing robustification, which aims to be a model-agnostic adversarial defense and yield a high-quality denoised outcome.

Some works propose to apply a guided diffusion process for advance adversarial purification. Guided Diffusion Model for Purification (GDMP) [174] incorporates purification into the diffusion-denoising process of a DDPM, therefore its diffusion process could submerge the adversarial perturbations with Gaussian noises that are gradually added, and both of these noises can be simultaneously eliminated following a guided denoising process. [175] uncovers the fundamental correlations between the unguided diffusion model based adversarial purification and randomized smoothing techniques, producing a provable defense mechanism.

8 Future Directions

Re-Examining Practical Conditions. We still need to check some commonly-believed premises in diffusion models. For example, it is a general belief in practice that the forward process of diffusion models will transform data to standard Gaussian noise. However, finite time solution of the forward diffusion SDE still remember the distribution of original data. [53] have studied this issue, but their result only works when one can accurately estimate the score function. Thus there is a trade-off needed to be further considered between long-term diffusion and short-term diffusion. Long-term diffusion ensures that the perturbed data distribution is close to the given prior while short diffusion time can reduce fitting error and sampling time. Nevertheless, the ideal conditions are hard to acquire, and thus operations in practice would lead to mismatches. We should realize this situation and design proper diffusion models.

From Discrete to Continuous Time. Due to the flexibility of diffusion model, there are many empirical methods that can be strengthened through further analysis [33, 238, 239, 240]. For example, studies have found that analysing the continuous time diffusion model can yield better sample quality [61, 57]. Thus one can transform the discrete time diffusion model to a corresponding continuous time diffusion model, then analyse and design the model. This line of researches are promising, especially when one has already confirmed the noise type and schedule in discrete time setting [240, 57].

New Generation Procedure. The diffusion models generate sample through two major approaches: one is discretizing the reverse diffusion SDE and then generating samples through the discrete reverse SDE, another is using the property of Markov chain in the reverse process to denoise the sample step by step. However, for some diffusion models,

it is hard to apply these approaches to generate sample in practice. For example, it is hard for discrete states diffusion models to find the corresponding reverse SDE, since these diffusion models usually utilize random walk or masking noises and thus can not estimate the transition kernel of reverse diffusion chain without introducing extra variance. Therefore, new generation procedures should be further studied [7, 240].

Generalizing to Complex Scenarios and More Research Areas. As illustrated in Section.7, diffusion models have been applied in seven different types of scenarios, ranging from computer vision to adversarial purification. However, there still exist some scenarios remaining underexplored, such as text-to-audiovisual speech synthesis [241] and visual question answering (VQA) [242]. Additionally, we can obviously find that most of existing applications are limited in single input/output or simple input/output. Therefore, it is critical and challenging for researchers to enable the diffusion models to process complex inputs and generate multiple outputs, and achieve better performance in real-world scenarios. Although diffusion models have been investigated in some research areas like robust learning, representative learning, and reinforcement learning, there still exist opportunities in connecting with more research areas [243, 244].

9 Conclusion

In this paper, we first propose a new and systematical taxonomy of both diffusion models and their applications. Specifically, We categorize the existing diffusion models into three categories: sampling-acceleration, likelihood-maximization, and data-generalization, with respect to different aspects of diffusion models enhancement. Moreover, we categorize the applications of diffusion models into seven categories: computer vision, natural language processing, waveform signal processing, multi-modal learning, molecular graph generation, time series modeling, and adversarial purification. Finally, we propose new perspectives with respect to the development of diffusion models in both algorithms and applications.

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