
Fast Sampling of Diffusion Models with Exponential Integrator

Anonymous Author(s)

Affiliation

Address

email

Abstract

1 Our goal is to develop a fast sampling method for Diffusion models (DMs) with
2 a small number of steps while retaining high sample quality. To achieve this, we
3 systematically analyze the sampling procedure in DMs and identify key factors that
4 affect the sample quality, among which the method of discretization is most crucial.
5 By carefully examining the learned diffusion process, we propose Diffusion
6 Exponential Integrator Sampler (DEIS). It is based on the Exponential Integrator
7 designed for discretizing ordinary differential equations (ODEs) and leverages
8 a semilinear structure of the learned diffusion process to reduce the discretization
9 error. The proposed method can be applied to any DMs and can generate
10 high-fidelity samples in as few as 10 steps. By directly using pre-trained DMs,
11 we achieve superior sampling performance when the number of score function
12 evaluation (NFE) is limited, e.g., 4.17 FID with 10 NFEs, 2.86 FID with only 20
13 NFEs on CIFAR10.

14 1 Introduction

15 The Diffusion model (DM) [10] is a generative modeling method developed recently that relies on the
16 basic idea of reversing a given simple diffusion process. A time-dependent score function is learned
17 for this purpose and DMs are thus also known as score-based models [27]. Compared with other
18 generative models such as generative adversarial networks (GANs), in addition to great scalability,
19 the DM has the advantage of stable training; it avoids mode-collapsing and is not hyperparameter
20 sensitive [6, 18]. DMs have recently achieved impressive performances on a variety of tasks,
21 including unconditional image generation [10, 27, 24, 8], text conditioned image generation [22, 23],
22 text generation [12, 2], 3D point cloud generation [21], inverse problem [16, 29], etc.

23 However, the remarkable performance of DMs comes at the cost of extremely slow sampling; it
24 takes much longer time to produce high-quality samples compared with GANs. See [Appendix A](#) for
25 discussions on existing methods. The objective of this work is to establish a principled discretization
26 scheme for the learned backward diffusion processes in DMs so as to achieve fast sampling. Since
27 the most expensive part in sampling a DM is the evaluation of the neural network that parameterizes
28 the backward diffusion, we seek a discretization method that requires a small number of network
29 function evaluation (NFE). We start with a family of marginal equivalent SDEs/ODEs associated
30 with DMs and investigate numerical error sources, which include fitting error and discretization
31 error. We observe that even with the same trained model, different discretization schemes can have
32 dramatically different performances in terms of discretization error. We find out that the *Exponential*
33 *Integrator (EI)* [11] that utilizes the semilinear structure of the backward diffusion has minimum
34 error. To further reduce the discretization error, we propose to either use high order polynomials to
35 approximate the nonlinear term in the ODE or employ Runge Kutta methods on a transformed ODE.



Figure 1: Generated images with various DMs. Latent diffusion [24] (Left), 256×256 image with text *A shirt with inscription "World peace"* (15 NFE). VE diffusion [27] (Mid), FFHQ 256×256 (12 NFE). VP diffusion [10] (Right), CIFAR10 (7 NFE) and CELEBA (5 NFE).

36 The resulting algorithms, termed *Diffusion Exponential Integrator Sampler (DEIS)*, achieve the best
 37 sampling quality with limited NFEs.

38 Our contributions are summarized as follows: 1) We investigate a family of marginal equivalent
 39 SDEs/ODEs for fast sampling and conduct a systematic error analysis for their numerical solvers. 2)
 40 We propose DEIS, an efficient sampler that can be applied to any DMs to achieve superior sampling
 41 quality with a limited number of NFEs. 3) We conduct comprehensive experiments to validate the
 42 efficacy of DEIS. For instance, with a pre-trained model [27], DEIS is able to reach 4.17 FID with 10
 43 NFEs, and 2.86 FID with 20 NFEs on CIFAR10.

44 2 Background on Diffusion Models

45 A DM consists of a fixed forward diffusion (noising) process that adds noise to the data, and a learned
 46 backward diffusion (denoising) process that gradually removes the added noise.

47 **Forward noising diffusion:** The forward diffusion of a DM for D -dimensional data is a linear
 48 diffusion described by the stochastic differential equation (SDE) [25]

$$d\mathbf{x} = \mathbf{F}_t \mathbf{x} dt + \mathbf{G}_t d\mathbf{w}, \quad (1)$$

49 where $\mathbf{F}_t \in \mathbb{R}^{D \times D}$ denotes the linear drift coefficient, $\mathbf{G}_t \in \mathbb{R}^{D \times D}$ denotes the diffusion coefficient,
 50 and \mathbf{w} is a standard Wiener process. The diffusion Eq (1) is initiated at the training data and simulated
 51 over a fixed time window $[0, T]$. Denote by $p_t(\mathbf{x}_t)$ the marginal distribution of \mathbf{x}_t and by $p_{0t}(\mathbf{x}_t|\mathbf{x}_0)$
 52 the conditional distribution from \mathbf{x}_0 to \mathbf{x}_t , then $p_0(\mathbf{x}_0)$ represents the underlying distribution of
 53 the training data. The simulated trajectories are represented by $\{\mathbf{x}_t\}_{0 \leq t \leq T}$. The parameters \mathbf{F}_t
 54 and \mathbf{G}_t are chosen such that the conditional marginal distribution $p_{0t}(\mathbf{x}_t|\mathbf{x}_0)$ is a simple Gaussian
 55 distribution, denoted as $\mathcal{N}(\mu_t \mathbf{x}_0, \Sigma_t)$, and the distribution $\pi(\mathbf{x}_T) := p_T(\mathbf{x}_T)$ is easy to sample from.

56 **Backward denoising diffusion:** Under mild assumptions [1, 27], the forward diffusion Eq (1) is
 57 associated with a reverse-time diffusion process

$$d\mathbf{x} = [\mathbf{F}_t \mathbf{x} dt - \mathbf{G}_t \mathbf{G}_t^T \nabla \log p_t(\mathbf{x})] dt + \mathbf{G}_t d\mathbf{w}, \quad (2)$$

58 where \mathbf{w} denotes a standard Wiener process in the reverse-time direction. The distribution of the
 59 trajectories of Eq (2) with terminal distribution $\mathbf{x}_T \sim \pi$ coincides with that of Eq (1) with initial
 60 distribution $\mathbf{x}_0 \sim p_0$, that is, Eq (2) matches Eq (1) in probability law.

61 **Training:** The basic idea of DMs is to use a time-dependent network $s_\theta(\mathbf{x}, t)$, known as a score
 62 network, to approximate the score $\nabla \log p_t(\mathbf{x})$. This is achieved by score matching techniques [13,
 63 31] where the score network s_θ is trained by minimizing the denoising score matching loss

$$\mathcal{L}(\theta) = \mathbb{E}_{t \sim \text{Unif}[0, T]} \mathbb{E}_{p(\mathbf{x}_0) p_{0t}(\mathbf{x}_t|\mathbf{x}_0)} [\|\nabla \log p_{0t}(\mathbf{x}_t|\mathbf{x}_0) - s_\theta(\mathbf{x}_t, t)\|_{\Lambda_t}^2]. \quad (3)$$

64 Here $\nabla \log p_{0t}(\mathbf{x}_t|\mathbf{x}_0)$ has a closed form expression as $p_{0t}(\mathbf{x}_t|\mathbf{x}_0)$ is a simple Gaussian distribution,
 65 and Λ_t denotes a time-dependent weight. We refer the reader to [10, 27] for more details on choices
 66 of Λ_t and training techniques.

67 3 Fast Sampling with learned score models

68 Once the score network $s_\theta(\mathbf{x}, t) \approx \nabla \log p_t(\mathbf{x})$ is trained, it can be used to generate new samples
 69 by solving the backward SDE Eq (2) with $\nabla \log p_t(\mathbf{x})$ replaced by $s_\theta(\mathbf{x}, t)$. It turns out there are
 70 infinitely many diffusion processes one can use. In this work, we consider a family of SDEs

$$d\hat{\mathbf{x}} = [\mathbf{F}_t \hat{\mathbf{x}} - \frac{1 + \lambda^2}{2} \mathbf{G}_t \mathbf{G}_t^T s_\theta(\hat{\mathbf{x}}, t)] dt + \lambda \mathbf{G}_t d\mathbf{w}, \quad (4)$$

71 parameterized by $\lambda \geq 0$. Here we use $\hat{\mathbf{x}}$ to distinguish the solution to the SDE associated with the
 72 learned score from the ground truth \mathbf{x} in Eq (1) and (2). When $\lambda = 0$, Eq (4) reduces to an ODE
 73 known as the *probability flow ODE* [27]. The reverse-time diffusion Eq (2) with an approximated
 74 score is a special case of Eq (4) with $\lambda = 1$. The following Proposition (Proof in Appendix B)
 75 justifies the usage of Eq (4) for generating samples.

76 **Proposition 1.** *When $s_\theta(\mathbf{x}, t) = \nabla \log p_t(\mathbf{x})$ for all \mathbf{x}, t , and $\hat{p}_T^* = \pi$, the marginal distribution \hat{p}_t^*
 77 of Eq (4) matches p_t of the forward diffusion Eq (1) for all $0 \leq t \leq T$.*

78 To generate a new sample, one can sample $\hat{\mathbf{x}}_T^*$ from π and solve Eq (4) to obtain a sample $\hat{\mathbf{x}}_0^*$. The
 79 objective of this work is to develop an efficient sampling scheme from Eq (4) with less discretization
 80 errors. In this section, we focus on the ODE approach with $\lambda = 0$.

81 We investigate the discretization error of solving the probability flow ODE ($\lambda = 0$)

$$\frac{d\hat{\mathbf{x}}}{dt} = \mathbf{F}_t \hat{\mathbf{x}} - \frac{1}{2} \mathbf{G}_t \mathbf{G}_t^T s_\theta(\hat{\mathbf{x}}, t). \quad (5)$$

82 Eq (5) is a semilinear stiff ODE [11]. The exact solution to this ODE is

$$\hat{\mathbf{x}}_t = \Psi(t, s) \hat{\mathbf{x}}_s + \int_s^t \Psi(t, \tau) [-\frac{1}{2} \mathbf{G}_\tau \mathbf{G}_\tau^T s_\theta(\hat{\mathbf{x}}_\tau, \tau)] d\tau, \quad (6)$$

83 where $\Psi(t, s)$ satisfying $\frac{\partial}{\partial t} \Psi(t, s) = \mathbf{F}_t \Psi(t, s)$, $\Psi(s, s) = \mathbf{I}$ is known as the transition matrix
 84 associated with \mathbf{F}_τ . We study the discretization error in solving Eq (5) to reduce gap between
 85 numerical results within a small number of NFEs and exact result Eq (6).

86 **Exponential Integrator over Euler method.** The Euler method is an elementary explicit numerical
 87 method for ODEs and is widely used in numerical softwares [32]. When applied to Eq (5), it reads

$$\hat{\mathbf{x}}_{t-\Delta t} = \hat{\mathbf{x}}_t - [\mathbf{F}_t \hat{\mathbf{x}}_t - \frac{1}{2} \mathbf{G}_t \mathbf{G}_t^T s_\theta(\hat{\mathbf{x}}_t, t)] \Delta t. \quad (7)$$

88 This is used in many existing works in DMs [27, 9]. This approach however has low accuracy and is
 89 sometimes unstable when the stepsize is not sufficiently small. To improve the accuracy, we propose
 90 to use the *Exponential Integrator (EI)*, a method that leverages the semilinear structure of Eq (5).
 91 When applied to Eq (5), the EI reads

$$\hat{\mathbf{x}}_{t-\Delta t} = \Psi(t - \Delta t, t) \hat{\mathbf{x}}_t + [\int_t^{t-\Delta t} -\frac{1}{2} \Psi(t - \Delta t, \tau) \mathbf{G}_\tau \mathbf{G}_\tau^T d\tau] s_\theta(\hat{\mathbf{x}}_t, t). \quad (8)$$

92 It is effective if the nonlinear term $s_\theta(\hat{\mathbf{x}}_t, t)$ does not change much along the solution. In fact, for any
 93 given Δt , Eq (8) solves Eq (5) exactly if $s_\theta(\hat{\mathbf{x}}_t, t)$ is constant over the time interval $[t - \Delta t, t]$.

94 **Parametrization: $\epsilon_\theta(\mathbf{x}, t)$ over $s_\theta(\mathbf{x}, t)$.** We find another source of large discretization error
 95 is caused by rapidly changing score $\nabla \log p_t(\mathbf{x})$. It is found that the parameterization [10]
 96 $\nabla \log p_t(\mathbf{x}) \approx -\mathbf{L}_t^{-T} \epsilon_\theta(\mathbf{x}, t)$, where \mathbf{L}_t can be any matrix satisfying $\mathbf{L}_t \mathbf{L}_t^T = \Sigma_t$, leads to signifi-
 97 cant improvements of accuracy. The network ϵ_θ tries to follow ϵ which is sampled from a standard
 98 Gaussian and thus has a small magnitude. In comparison, the parameterization $s_\theta = -\mathbf{L}_t^{-T} \epsilon_\theta$ can
 99 take large value as $\mathbf{L}_t \rightarrow 0$ as t approaches 0. It is thus better to approximate ϵ_θ than s_θ with a neural
 100 network. We adopt this parameterization and rewrite Eq (5) as

$$\frac{d\hat{\mathbf{x}}}{dt} = \mathbf{F}_t \hat{\mathbf{x}} + \frac{1}{2} \mathbf{G}_t \mathbf{G}_t^T \mathbf{L}_t^{-T} \epsilon_\theta(\hat{\mathbf{x}}, t). \quad (9)$$

101 Applying the EI to Eq (9) yields

$$\hat{\mathbf{x}}_{t-\Delta t} = \Psi(t - \Delta t, t) \hat{\mathbf{x}}_t + [\int_t^{t-\Delta t} \frac{1}{2} \Psi(t - \Delta t, \tau) \mathbf{G}_\tau \mathbf{G}_\tau^T \mathbf{L}_\tau^{-T} d\tau] \epsilon_\theta(\hat{\mathbf{x}}_t, t). \quad (10)$$

NFE	FID for various DEIS									
	DDIM	ρ 2Heun	ρ 3Kutta	ρ 4RK	ρ AB1	ρ AB2	ρ AB3	t AB1	t AB2	t AB3
5	26.91	108 ⁺¹	185 ⁺¹	193 ⁺³	22.28	21.53	21.43	19.72	16.31	15.37
10	11.14	14.72	13.19 ⁺²	28.65 ⁺²	7.56	6.72	6.50	6.09	4.57	4.17
20	5.47	3.50	2.97 ⁺¹	3.92	3.70	3.32	3.17	3.54	3.05	2.86
50	3.27	2.60	2.55⁺¹	2.57 ⁺²	2.70	2.62	2.59	2.67	2.59	2.57

Table 1: DEIS for VPSDE on CIFAR10 with limited NFE. For ρ RK-DEIS, the upper right number indicates extra NFEs used. Bold numbers denote the best performance achieved with similar NFE.

102 Then we develop several fast sampling algorithms, all coined as the *Diffusion Exponential Integrator*
103 *Sampler (DEIS)*, based on Eq (10), for DMs. Interestingly, the discretization Eq (10) based on EI
104 coincides with the popular deterministic DDIM when the forward diffusion Eq (1) is VPSDE [26].
105 The update Eq (10) can be further improved by using a polynomial of time, rather than a constant,
106 to approximation ϵ_θ over the interval $[t - \Delta t, t]$. The resulting approach resembles the classical
107 Adams–Bashforth [11] method, thus we term it t AB-DEIS. Another major factor that affects the
108 performance of sampling is the choice of time discretization.

109 4 Exponential Integrator: simplify probability Flow ODE

110 Next we present a different perspective to DEIS based on ODE transformations. The probability
111 ODE Eq (9) can be transformed into a simple non-stiff ODE, and then off-the-shelf ODE solvers
112 can be applied to solve the ODE effectively. To this end, we introduce variable $\hat{\mathbf{y}}_t := \Psi(t, 0)\hat{\mathbf{x}}_t$ and
113 rewrite Eq (9) into

$$\frac{d\hat{\mathbf{y}}}{dt} = \frac{1}{2}\Psi(t, 0)\mathbf{G}_t\mathbf{G}_t^T\mathbf{L}_t^{-T}\epsilon_\theta(\Psi(0, t)\hat{\mathbf{y}}, t). \quad (11)$$

114 Note that, departing from Eq (9), Eq (11) does not possess semi-linear structure. Thus, we can
115 apply off-the-shelf ODE solvers to Eq (11) without worrying about the semi-linear structure. This
116 transformation Eq (11) can be further improved by taking into account the analytical form of
117 Ψ , \mathbf{G}_t , \mathbf{L}_t . Here we present treatment for VPSDE; the results can be extended to other (scalar) DMs
118 such as VESDE. See Appendix C for the proof.

119 **Proposition 2.** For the VPSDE, with $\hat{\mathbf{y}}_t = \sqrt{\frac{\alpha_0}{\alpha_t}}\hat{\mathbf{x}}_t$ and the time-scaling $\beta(t) = \sqrt{\alpha_0}\left(\sqrt{\frac{1-\alpha_t}{\alpha_t}} - \sqrt{\frac{1-\alpha_0}{\alpha_0}}\right)$, Eq (9) can be transformed into

$$\frac{d\hat{\mathbf{y}}}{d\rho} = \epsilon_\theta\left(\sqrt{\frac{\alpha\beta^{-1}(\rho)}{\alpha_0}}\hat{\mathbf{y}}, \beta^{-1}(\rho)\right), \quad \rho \in [\beta(0), \beta(T)]. \quad (12)$$

121 Based on the transformed ODE Eq (12), we propose two variants of the DEIS algorithm: ρ RK-DEIS
122 when applying classical RK methods, and ρ AB-DEIS when applying Adams-Bashforth methods.
123 We remark that the difference between t AB-DEIS and ρ AB-DEIS lies in the fact that t AB-DEIS fits
124 polynomials in t which may not be polynomials in ρ .

125 5 Experiments and Conclusion

126 We conduct experiment on CIFAR10 with pre-trained
127 model from [27]. As in Fig 2, compared with other
128 samplers, ODE sampler based on RK45 [27], SDE
129 samplers based on Euler-Maruyama (EM) [27] and
130 SDE adaptive step size solver [14], DEIS can converge
131 much faster. We also include comparison among various
132 DEIS algorithms in Tab 1 (See Appendix D for
133 more experiment results). In summary, by utilizing
134 structural information in Eq (5), DEIS can significantly accelerate DM sampling.

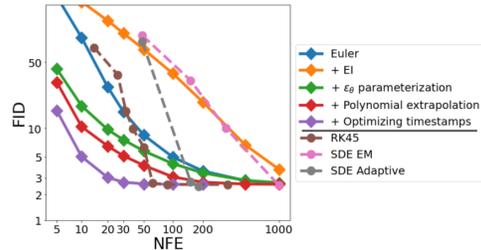


Figure 2: The effects of EI, parametrization, polynomial approximation, and time discretization.

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224 A Related works

225 A lot of research has been conducted to speed up the sampling of DMs. In [19, 34] the authors optimize
 226 denosing process by modifying the underlying stochastic process. However, such acceleration can not
 227 generate high quality samples with a small number of discretization steps. In [26] the authors use a
 228 non-Markovian forward noising. The resulted algorithm, DDIM, achieves significant acceleration than
 229 DDPMs. More recently, the authors of [3] optimize the backward Markovian process to approximate
 230 the non-Markovian forward process and get an analytic expression of optimal variance in denoising
 231 process. Another strategy to make the forward diffusion nonlinear and trainable [36, 30, 7, 33, 4] in
 232 the spirit of Schrödinger bridge [5]. This however comes with a heavy training overhead.

233 More closely related to our method is [20], which interprets update step in stochastic DDIM as a
 234 combination of gradient estimation step and transfer step. It modifies high order ODE methods to
 235 provide an estimation of the gradient and uses DDIM for transfer step. However, the decomposition
 236 of DDIM into two separate components is not theoretically justified. Based on our analysis on
 237 Exponential Integrator, Liu et al. [20] uses Exponential Integral but with a Euler discretization-
 238 based approximation of the nonlinear term. This approximation is inaccurate and may suffer large
 239 discretization error if the step size is large.

240 The semilinear structure presented in probability flow ODE has been widely investigated in physics
 241 and numerical simulation [11, 35], from which we get inspirations. The stiff property of the ODEs
 242 requires more efficient ODE solvers instead of black-box solvers that are designed for general ODE
 243 problems. In this work, we investigate solvers for differential equations in diffusion model and take
 244 advantage of the semilinear structure.

245 B Proof of Proposition 1

246 The proof is inspired by [36]. We show that the marginal distribution induced by Eq (4) does not
 247 depend on the choice of λ and equals the marginal distribution induced by Eq (2) when the score
 248 model is perfect.

249 Consider the distribution q induced by the SDE

$$d\mathbf{x} = [\mathbf{F}_t \mathbf{x} - \frac{1 + \lambda^2}{2} \mathbf{G}_t \mathbf{G}_t^T \nabla \log q_t(\mathbf{x})] dt + \lambda \mathbf{G}_t d\mathbf{w}. \quad (13)$$

250 Eq (13) is simulated from $t = T$ to $t = 0$. According to the Fokker-Planck-Kolmogorov (FPK)
 251 Equation, q solves the partial differential equation

$$\begin{aligned} \frac{\partial q_t(\mathbf{x})}{\partial t} &= -\nabla \cdot \{[\mathbf{F}_t \mathbf{x} - \frac{1 + \lambda^2}{2} \mathbf{G}_t \mathbf{G}_t^T \nabla \log q_t(\mathbf{x})] q_t(\mathbf{x})\} - \frac{\lambda^2}{2} \langle \mathbf{G}_t \mathbf{G}_t^T, \frac{\partial^2}{\partial x_i \partial x_j} q_t(\mathbf{x}) \rangle \\ &= -\nabla \cdot \{[\mathbf{F}_t \mathbf{x} - \frac{1}{2} \mathbf{G}_t \mathbf{G}_t^T \nabla \log q_t(\mathbf{x})] q_t(\mathbf{x})\} + \nabla \cdot \{[\frac{\lambda^2}{2} \mathbf{G}_t \mathbf{G}_t^T \nabla \log q_t(\mathbf{x})] q_t(\mathbf{x})\} - \\ &\quad \frac{\lambda^2}{2} \langle \mathbf{G}_t \mathbf{G}_t^T, \frac{\partial^2}{\partial x_i \partial x_j} q_t(\mathbf{x}) \rangle, \end{aligned}$$

252 where $\nabla \cdot$ denotes the divergence operator. Since

$$\nabla \cdot \{[\frac{\lambda^2}{2} \mathbf{G}_t \mathbf{G}_t^T \nabla \log q_t(\mathbf{x})] q_t(\mathbf{x})\} = \nabla \cdot [\frac{\lambda^2}{2} \mathbf{G}_t \mathbf{G}_t^T \nabla q_t(\mathbf{x})] = \langle \frac{\lambda^2}{2} \mathbf{G}_t \mathbf{G}_t^T, \frac{\partial^2}{\partial x_i \partial x_j} q_t(\mathbf{x}) \rangle, \quad (14)$$

253 we obtain

$$\frac{\partial q_t(\mathbf{x})}{\partial t} = -\nabla \cdot \{[\mathbf{F}_t \mathbf{x} - \frac{1}{2} \mathbf{G}_t \mathbf{G}_t^T \nabla \log q_t(\mathbf{x})] q_t(\mathbf{x})\}. \quad (15)$$

254 Eq (15) shows that the above partial differential equation does not depend on λ . Thus, the marginal
 255 distribution of Eq (13) is independent of the value of λ .

256 C Proof of Proposition 2

257 We start our proof with Eq (11). In VPSDE, Eq (11) reduce to

$$\frac{d\hat{\mathbf{y}}}{dt} = -\frac{1}{2} \sqrt{\frac{\alpha_0}{\alpha_t}} \frac{d \log \alpha_t}{dt} \frac{1}{\sqrt{1 - \alpha_t}} \epsilon_\theta(\Psi(0, t) \hat{\mathbf{y}}, t). \quad (16)$$

258 Now we consider a rescaled time ρ , which satisfies the following equation

$$\frac{d\rho}{dt} = -\frac{1}{2} \sqrt{\frac{\alpha_0}{\alpha_t}} \frac{d \log \alpha_t}{dt} \frac{1}{\sqrt{1-\alpha_t}}. \quad (17)$$

259 Plugging Eq (17) into Eq (16), we reach

$$\frac{d\hat{\mathbf{y}}}{d\rho} = \epsilon_\theta(\Psi(0, t)\hat{\mathbf{y}}, t). \quad (18)$$

260 In VPSDE, we α_t is a monotonically decreasing function with respect to t . Therefore, there exists a
 261 bijective mapping between ρ and t based on Eq (17), which we define as β and $\rho = \beta(t)$. Furthermore,
 262 we can solve Eq (17) for β

$$\beta(t) = \sqrt{\alpha_0} \left(\sqrt{\frac{1-\alpha_t}{\alpha_t}} - \sqrt{\frac{1-\alpha_0}{\alpha_0}} \right). \quad (19)$$

263 D More experiment details

264 D.1 Important technical details and modifications

- 265 • It is found that correcting steps and an extra denoising step can improve image quality at
 266 additional NFE costs [27, 14]. For a fair comparison, we disable the correcting steps, extra
 267 denoising step, or other heuristic clipping tricks for all methods and experiments in this
 268 work unless stated otherwise.
- 269 • Due to numerical issues, we set ending time t_0 in DMs during sampling a non-zero number.
 270 Song et al. [27] suggests $t_0 = 10^{-3}$ for VPSDE and $t_0 = 10^{-5}$ for VESDE. In practice,
 271 we find the value of t_0 and time scheduling have huge impacts on FIDs. This finding is
 272 not new and has been pointed out by existing works [14, 17, 26]. Interestingly, we found
 273 different algorithms have different preferences for t_0 and time scheduling. We report the
 274 best FIDs for each method among different choices of t_0 and time scheduling in Tab 1.
 275 We use t_0 suggested by the original paper and codebase for different checkpoints and
 276 quadratic time scheduling suggested by Song et al. [26] unless stated otherwise. We include
 277 a comprehensive study about t_0 and time scheduling in Appendix D.3
- 278 • Because PNDM needs 12 NFE for the first 3 steps, we compare PNDM only when NFE is
 279 great than 12. However, our proposed iPNDM can work when NFE is less than 12.
- 280 • We include the comparison against A-DDIM [3] with its official checkpoints and implemen-
 281 tation in Appendix D.5.
- 282 • We only provide qualitative results for text-to-image experiment with pre-trained model [23].
- 283 • We include proposed r -th order iPNDM in Appendix D.2. We use $r = 3$ by default unless
 284 stated otherwise.

285 D.2 Improved PNDM

286 By Eq (10), PNDM can be viewed as a combination of Exponential Integrator and linear multistep
 287 method based on the Euler method. More specifically, it uses a linear combination of multiple score
 288 evaluations instead of using only the latest score evaluation. PNDM follows the steps

$$\hat{\epsilon}_t^{(3)} = \frac{1}{24}(55\epsilon_t - 59\epsilon_{t+\Delta t} + 37\epsilon_{t+2\Delta t} - 9\epsilon_{t+3\Delta t}), \quad (20)$$

$$\hat{\mathbf{x}}_{t-\Delta t} = \sqrt{\frac{\alpha_{t-\Delta t}}{\alpha_t}} \hat{\mathbf{x}}_t + [\sqrt{1-\alpha_{t-\Delta t}} - \sqrt{\frac{\alpha_{t-\Delta t}}{\alpha_t}} \sqrt{1-\alpha_t}] \hat{\epsilon}_t^{(4)}, \quad (21)$$

289 where $\epsilon_t = \epsilon_\theta(\hat{\mathbf{x}}_t, t)$, $\epsilon_{t+\Delta t} = \epsilon_\theta(\hat{\mathbf{x}}_{t+\Delta t}, t + \Delta t)$. The coefficients in Eq (20) are derived based
 290 on black-box ODE Euler discretization with fixed step size. Similarly, there exist lower order
 291 approximations

$$\hat{\epsilon}_t^{(0)} = \epsilon_t \quad (22)$$

$$\hat{\epsilon}_t^{(1)} = \frac{3}{2}\epsilon_t - \frac{1}{2}\epsilon_{t+\Delta t} \quad (23)$$

$$\hat{\epsilon}_t^{(2)} = \frac{1}{12}(23\epsilon_t - 16\epsilon_{t+\Delta t} + 5\epsilon_{t+2\Delta t}). \quad (24)$$

Table 2: Comparison between PNDM and t AB-DEIS. The bold results denote the best result with a fixed NFE on each dataset. The advantage of DEIS is obvious when NFE is small.

FID \ NFE	5	10	20	50	FID \ NFE	5	10	20	50
Method					Method				
PNDM	-	-	6.42	3.03	PNDM	-	-	7.60	3.51
iPNDM	70.07	9.36	4.21	3.00	iPNDM	59.87	7.78	5.58	3.34
DDIM	30.64	11.71	6.12	4.25	0-DEIS	30.42	13.53	6.89	4.17
t AB1	20.01	6.09	3.81	3.32	1-DEIS	26.65	8.81	4.33	3.19
t AB2	16.53	4.57	3.41	3.09	2-DEIS	25.13	7.20	3.61	3.04
t AB3	16.10	4.17	3.33	2.99	3-DEIS	25.07	6.95	3.41	2.95

(a) CIFAR10
(b) CELEBA

292 Originally, PNDM uses Runge-Kutta for warming start and costs 4 score network evaluation for
 293 each of the first 3 steps. To reduce the NFE in sampling, the improved PNDM (iPNDM) uses lower
 294 order multistep for warming start. We summarize iPNDM in Alg 1. We include a comparison with
 295 t AB-DEIS in Tab 2, we adapt uniform step size for t AB-DEIS when NFE=50 in CIFAR10 as we find
 296 its performance is slightly better than the quadratic one.

Algorithm 1 Improved PNDM (iPNDM)

Input: $\{t_i\}_{i=0}^N, t_i = i\Delta t$, order r
Instantiate: \mathbf{x}_{t_N} , Empty ϵ -buffer
for i in $N, N-1, \dots, 1$ **do**
 $j = \min(N-i+1, r)$
 ϵ -buffer.append($\epsilon_\theta(\hat{\mathbf{x}}_{t_i}, t_i)$)
 Simulate $\hat{\epsilon}_{t_i}^{(j)}$ based on j and ϵ -buffer
 $\hat{\mathbf{x}}_{t_{i-1}} \leftarrow$ Simulate Eq (21) with $\hat{\mathbf{x}}_{t_i}$ and $\hat{\epsilon}_{t_i}^{(j)}$
end for

297 **D.3 Impact of t_0 and time scheduling on FIDs**

298 We present a study about sampling with difference t_0 and time scheduling based VPSDE. We consider
 299 two choices of t_0 ($10^{-3}, 10^{-4}$) and three choices for time scheduling. The first time scheduling
 300 follows the power function in t

$$t_i = \left(\frac{N-i}{N} t_0^{\frac{1}{\kappa}} + \frac{i}{N} t_N^{\frac{1}{\kappa}} \right)^\kappa, \quad (25)$$

301 the second time scheduling follows power function in ρ

$$\rho_i = \left(\frac{N-i}{N} \rho_0^{\frac{1}{\kappa}} + \frac{i}{N} \rho_N^{\frac{1}{\kappa}} \right)^\kappa, \quad (26)$$

302 and the last time scheduling follows a uniform step in $\log \rho$ space

$$\log \rho_i = \frac{N-i}{N} \log \rho_0 + \frac{i}{N} \log \rho_N. \quad (27)$$

303 We include the comparison between different t_0 and time scheduling in Tab 3 to 5. We notice t_0 has a
 304 huge influence on image FIDs, which is also noticed and investigated across different studies [17, 9].
 305 Among various scheduling, we observe t AB-DEIS has obvious advantages when NFE is small and
 306 ρ RK-DEIS is competitive when we NFE is relatively large.

307 **D.4 More ablation study**

308 We include more quantitative comparisons of the introduced ingredients in Tab 6 for Fig 2. Since
 309 ingredients ϵ_θ -based parameterization and polynomial extrapolation are only compatible with the

FID for various DEIS with $\kappa = 1$ in Eq (25)										
NFE	DDIM	$\rho 2\text{Heun}$	$\rho 3\text{Kutta}$	$\rho 4\text{RK}$	ρAB1	ρAB2	ρAB3	$t\text{AB1}$	$t\text{AB2}$	$t\text{AB3}$
5	47.59	207 ⁺¹	238 ⁺¹	212 ⁺³	35.14	32.51	32.02	25.99	25.06	44.29
10	16.60	84.55	66.81 ⁺²	78.57 ⁺²	10.47	8.85	8.18	9.51	7.71	7.18
15	10.39	46.36 ⁺¹	47.45	41.27 ⁺¹	6.69	5.70	5.24	6.47	5.51	5.01
20	7.93	34.87	28.35 ⁺¹	27.21	5.27	4.56	4.24	5.20	4.50	4.14
50	4.36	11.58	7.00 ⁺¹	7.48 ⁺²	3.32	3.08	2.99	3.32	3.09	2.99
FID for various DEIS with $\kappa = 2$ in Eq (25)										
NFE	DDIM	$\rho 2\text{Heun}$	$\rho 3\text{Kutta}$	$\rho 4\text{RK}$	ρAB1	ρAB2	ρAB3	$t\text{AB1}$	$t\text{AB2}$	$t\text{AB3}$
5	30.64	256 ⁺¹	357 ⁺¹	342 ⁺³	24.58	23.60	23.48	20.01	16.52	16.10
10	11.71	56.62	56.51 ⁺²	103 ⁺²	7.56	6.72	6.50	6.09	4.57	4.17
15	7.67	10.62 ⁺¹	14.96	36.15 ⁺¹	4.93	4.40	4.26	4.29	3.57	3.37
20	6.11	6.33	4.74 ⁺¹	12.81	4.16	3.84	3.77	3.81	3.41	3.33
50	4.24	3.88	3.75 ⁺¹	3.78 ⁺²	3.70	3.68	3.69	3.62	3.61	3.36
FID for various DEIS with $\kappa = 3$ in Eq (25)										
NFE	DDIM	$\rho 2\text{Heun}$	$\rho 3\text{Kutta}$	$\rho 4\text{RK}$	ρAB1	ρAB2	ρAB3	$t\text{AB1}$	$t\text{AB2}$	$t\text{AB3}$
5	34.07	356 ⁺¹	388 ⁺¹	377 ⁺³	29.80	29.35	29.38	24.87	22.57	22.06
10	14.59	115	171 ⁺²	267 ⁺²	10.73	10.16	10.11	8.11	6.36	5.97
15	9.22	32.94 ⁺¹	77.44	103 ⁺¹	6.45	6.03	5.98	5.21	4.26	4.05
20	7.27	13.06	11.55 ⁺¹	50.56	5.17	4.83	4.78	4.45	3.88	3.75
50	4.64	3.76	3.68 ⁺¹	3.74 ⁺²	3.92	3.82	3.79	3.81	3.72	3.71
FID for various DEIS with Eq (27)										
NFE	DDIM	$\rho 2\text{Heun}$	$\rho 3\text{Kutta}$	$\rho 4\text{RK}$	ρAB1	ρAB2	ρAB3	$t\text{AB1}$	$t\text{AB2}$	$t\text{AB3}$
5	54.58	216 ⁺¹	335 ⁺¹	313 ⁺³	49.25	48.56	48.47	37.99	28.45	26.11
10	20.03	14.72	13.19 ⁺²	28.65 ⁺²	14.05	12.63	12.18	10.36	7.03	5.71
15	11.99	5.03 ⁺¹	5.88	6.88 ⁺¹	7.72	6.67	6.29	6.22	4.69	4.13
20	8.92	4.12	3.97 ⁺¹	4.14	5.79	5.05	4.78	4.97	4.10	3.80
50	5.05	3.67	3.75 ⁺¹	3.73 ⁺²	4.01	3.84	3.79	3.89	3.74	3.72

Table 3: DEIS for VPSDE on CIFAR10 with $t_0 = 10^{-3}$.

310 exponential integrator, we cannot combine them with the Euler method. We also provide performance
311 when applying quadratic timestamp scheduling to Euler Tab 7 directly. We find sampling with small
312 NFE and large NFE have different preferences for time schedules.

313 We also report the performance of the RK45 ODE solver for VPSDE on CIFAR10 in Tab 8¹. As a
314 popular and well-developed ODE solver, RK45 has decent sampling performance when $\text{NFE} \geq 50$.
315 However, the sampling quality with limited NFE is not satisfying. Such results are within expectation
316 as RK45 does not take advantage of the structure information of diffusion models. The overall
317 performance of RK45 solver is worse than iPNDM and DEIS when NFE is small.

318 D.5 Comparison with Analytic-DDIM (A-DDIM) [3]

319 We also compare our algorithm with Analytic-DDIM (A-DDIM) in terms of fast sampling perfor-
320 mance. We failed to reproduce the significant improvements claimed in [3] in our default CIFAR10
321 checkpoint. There could be two factors that contribute to this. First, we use a score network trained
322 with continuous time loss objective and different weights [27]. However, Analytic-DDIM is proposed
323 for DDPM with discrete times and finite timestamps. Second, some tricks have huge impacts on the
324 sampling quality in A-DDIM. For instance, A-DDIM heavily depends on clipping value in the last
325 few steps [3]. A-DDIM does not provide high-quality samples without proper clipping when NFE is
326 low.

¹We use `scipy.integrate.solve_ivp` and tune tolerance to get different performances on different NFE. We find different combinations of absolute tolerance and relative tolerance may result in the same NFE but different FID. We report the best FID in that case.

FID for various DEIS with $\kappa = 1$ in Eq (25)										
NFE	DDIM	ρ_2 Heun	ρ_3 Kutta	ρ_4 RK	ρ_{AB1}	ρ_{AB2}	ρ_{AB3}	t_{AB1}	t_{AB2}	t_{AB3}
5	42.38	239 ⁺¹	232 ⁺¹	199 ⁺³	33.09	31.06	30.67	26.01	20.57	42.35
10	17.23	143	95.13 ⁺²	130 ⁺²	12.44	11.04	10.41	12.01	10.57	8.04
15	12.06	99.76 ⁺¹	77.37	88.56 ⁺¹	9.12	8.25	7.79	9.08	8.20	7.50
20	9.71	82.89	57.54 ⁺¹	66.61	7.57	6.89	6.50	7.60	6.90	6.45
50	5.76	31.56	13.10 ⁺¹	15.73 ⁺²	4.64	4.25	4.06	4.67	4.28	4.10
FID for various DEIS with $\kappa = 2$ in Eq (25)										
NFE	DDIM	ρ_2 Heun	ρ_3 Kutta	ρ_4 RK	ρ_{AB1}	ρ_{AB2}	ρ_{AB3}	t_{AB1}	t_{AB2}	t_{AB3}
5	26.91	271 ⁺¹	362 ⁺¹	348 ⁺³	22.28	21.53	21.43	19.72	16.31	15.37
10	11.14	66.25	63.53 ⁺²	111 ⁺²	7.65	6.89	6.67	6.74	5.49	5.02
15	7.06	13.48 ⁺¹	17.15	44.83 ⁺¹	4.69	4.16	3.99	4.38	3.78	3.50
20	5.47	6.62	4.15 ⁺¹	15.14	3.70	3.32	3.17	3.57	3.19	3.03
50	3.27	2.65	2.55 ⁺¹	2.57 ⁺²	2.70	2.62	2.59	2.70	2.61	2.59
FID for various DEIS with $\kappa = 3$ in Eq (25)										
NFE	DDIM	ρ_2 Heun	ρ_3 Kutta	ρ_4 RK	ρ_{AB1}	ρ_{AB2}	ρ_{AB3}	t_{AB1}	t_{AB2}	t_{AB3}
5	32.11	364 ⁺¹	393 ⁺¹	383 ⁺³	28.87	28.58	28.62	25.78	23.66	23.38
10	13.18	135	199 ⁺²	298 ⁺²	9.89	9.38	9.33	7.74	6.20	5.77
15	7.92	42.04 ⁺¹	99.64	122 ⁺¹	5.41	4.99	4.91	4.48	3.65	3.37
20	5.92	17.05	16.66 ⁺¹	64.40	4.04	3.69	3.60	3.54	3.05	2.86
50	3.36	2.77	2.57 ⁺¹	2.71 ⁺²	2.73	2.63	2.60	2.67	2.59	2.57
FID for various DEIS with Eq (27)										
NFE	DDIM	ρ_2 Heun	ρ_3 Kutta	ρ_4 RK	ρ_{AB1}	ρ_{AB2}	ρ_{AB3}	t_{AB1}	t_{AB2}	t_{AB3}
5	54.85	230 ⁺¹	382 ⁺¹	370 ⁺³	51.94	51.62	51.58	43.84	39.91	38.76
10	19.80	23.35	25.08 ⁺²	82.17 ⁺²	14.63	13.43	13.07	11.14	7.78	6.02
15	11.29	5.63 ⁺¹	7.46	8.90 ⁺¹	7.31	6.28	5.90	5.89	4.35	3.71
20	7.91	3.84	3.05 ⁺¹	4.14	4.91	4.19	3.91	4.23	3.35	3.00
50	3.82	2.60	2.56 ⁺¹	2.59 ⁺²	2.86	2.70	2.64	2.79	2.63	2.58

Table 4: DEIS for VPSDE on CIFAR10 with $t_0 = 10^{-4}$ in Eq (25)

FID for various DEIS with $\kappa = 7$ in Eq (26)										
NFE	DDIM	ρ_2 Heun	ρ_3 Kutta	ρ_4 RK	ρ_{AB1}	ρ_{AB2}	ρ_{AB3}	t_{AB1}	t_{AB2}	t_{AB3}
5	53.20	108 ⁺¹	185 ⁺¹	193 ⁺³	47.56	46.36	46.13	36.98	28.76	25.76
10	18.99	18.75	20.27 ⁺²	54.92 ⁺²	13.38	11.84	11.21	10.92	8.26	6.87
15	10.91	4.89 ⁺¹	6.31	9.79 ⁺¹	6.90	5.86	5.42	6.12	4.86	4.33
20	7.81	3.50	2.97 ⁺¹	3.92	4.84	4.10	3.80	4.48	3.69	3.38
50	3.84	2.60	2.58 ⁺¹	2.59 ⁺²	2.86	2.69	2.64	2.82	2.66	2.61

Table 5: DEIS for VPSDE on CIFAR10 with t_0 and time scheduling suggested by Karras et al. [15]

327 To compare with A-DDIM, we conduct another experiment with checkpoints provided by [3] and
328 integrate iPNDM and DEIS into the provided codebase; the results are shown in Tab 9. We use
329 piecewise linear function to fit discrete SDE coefficients in [3] for DEIS. Without any ad-hoc tricks,
330 the plugin-and-play iPNDM is comparable or even slightly better than A-DDIM when the NFE
331 budget is small, and DEIS is better than both of them.

332 D.6 Sampling quality on ImageNet 32×32

333 We conduct experiments on ImageNet 32×32 with pre-trained VPSDE model provided in [28].
334 Again, we observe significant improvement over DDIM and iPNDM methods when the NFE budget

Method	FID with various NFE								
	5	10	20	30	50	100	200	500	1000
Euler	246.16	90.52	27.38	14.99	8.46	4.96	3.54	2.81	2.62
+ EI	283.67	216.47	137.20	100.74	68.03	37.93	18.81	6.66	3.69
+ ϵ_θ	42.38	17.23	9.71	7.56	5.76	4.24	3.37	2.83	2.67
+ Poly	30.67	10.41	6.50	5.13	4.06	3.07	2.69	2.58	2.57
+ Opt $\{t_i\}$	15.37	5.02	3.03	2.70	2.59	2.57	2.56	2.56	2.56

Table 6: Quantitative comparison in Fig 2 for introduced ingredients, Exponential Integrator (EI), ϵ_θ -based score parameterization, polynomial extrapolation, and optimizing time discretization $\{t_i\}$, where we change uniform stepsize to quadratic one $t_0 = 10^{-4}$. We include Tab 3 to 5 for more ablation studies regarding time discretization.

Method	FID with various NFE								
	5	10	20	30	50	100	200	500	1000
Uniform	246.16	90.52	27.38	14.99	8.46	4.96	3.54	2.81	2.62
Quadratic	294.01	138.73	39.82	19.26	8.49	3.96	2.88	2.61	2.57

Table 7: Effects of different timesteps on the Euler method. We use $t_0 = 10^{-4}$ which has lower FID score compared with the default $t_0 = 10^{-3}$ [27] in the experiments.

335 is low. Even with 50 NFE, DEIS is able to outperform blackbox ODE solver in terms of sampling
336 quality.

337 D.7 More results on VPSDE

338 We include mean and standard deviation for CELEBA in Tab 11.

339 D.8 More results on VESDE

340 Though VESDE does not achieve the same accelerations as VPSDE, our method can significantly
341 accelerate VESDE sampling compared with previous method for VESDE. We show the accelerated
342 FID for VESDE on CIFAR10 in Tab 12 and sampled images in Fig 3.

343 D.9 Checkpoint used and code licenses

344 Our code will be released in the future. We implemented our approach in Jax and PyTorch. We have
345 also used code from a number of sources in Tab 13.

346 We list the used checkpoints and the corresponding experiments in Tab 14.

NFE	14	26	32	38	50	62	88.2	344
FID	61.11	36.64	15.18	9.88	6.32	2.63	2.56	2.55

Table 8: Quantitative performance of RK45 ODE solver with $t_0 = 10^{-4}$ in Fig 2.

FID \ NFE	Method			
	5	10	20	50
A-DDIM	51.47	14.06	6.74	4.04
1-iPNDM	30.13	13.01	8.25	5.65
2-iPNDM	84.00	10.45	6.79	4.73
3-iPNDM	105.38	14.03	5.79	4.24
t AB1-DEIS	20.45	8.11	4.91	3.88
t AB2-DEIS	18.87	7.47	4.66	3.79
t AB3-DEIS	18.43	7.12	4.53	3.78

Table 9: Comparison with A-DDIM on the checkpoint and time scheduling provided by [3] on CIFAR10

FID \ NFE	Method			
	5	10	20	50
iPNDM	54.62	15.32	9.26	8.26
DDIM	49.08	23.52	13.69	9.44
t AB1-DEIS	34.69	13.94	9.55	8.41
t AB2-DEIS	29.50	11.36	8.79	8.29
t AB3-DEIS	28.09	10.55	8.58	8.25

Table 10: Sampling quality on VPSDE ImageNet 32×32 with the checkpoint provided by Song et al. [28]. Blackbox ODE solver reports FID 8.34 with ODE tolerance 1×10^{-5} (NFE around 130).

Dataset	FID \ NFE	Method			
		5	10	20	50
CELEBA	PNDM	-	-	7.60±0.12	3.51±0.03
	iPNDM	59.87±1.01	7.78±0.18	5.58±0.11	3.34±0.04
	DDIM	30.42±0.87	13.53±0.48	6.89±0.11	4.17±0.04
	t AB1-DEIS	26.65±0.63	8.81±0.23	4.33±0.07	3.19±0.03
	t AB2-DEIS	25.13±0.56	7.20±0.21	3.61±0.05	3.04±0.02
	t AB3-DEIS	25.07±0.49	6.95±0.09	3.41±0.04	2.95±0.03

Table 11: Mean and standard deviation of multiple runs with 4 different random seeds on the checkpoint and time scheduling provided by Liu et al. [20] on CELEBA.

SDE	FID \ NFE	Method			
		5	10	20	50
VESDE	t AB0-DEIS	103.52±2.09	46.90±0.38	27.64±0.05	19.86±0.03
	t AB1-DEIS	56.33±0.87	26.16±0.12	18.52±0.03	16.64±0.01
	t AB2-DEIS	58.65±0.25	20.89±0.09	16.94±0.03	16.33±0.02
	t AB3-DEIS	96.70±0.90	25.01±0.03	16.59±0.03	16.31±0.02

Table 12: FID results of DEIS on VESDE CIFAR10. We note the Predictor-Corrector algorithm proposed in [27] have ≥ 100 FID if sampling with limited NFE budget (≤ 50).

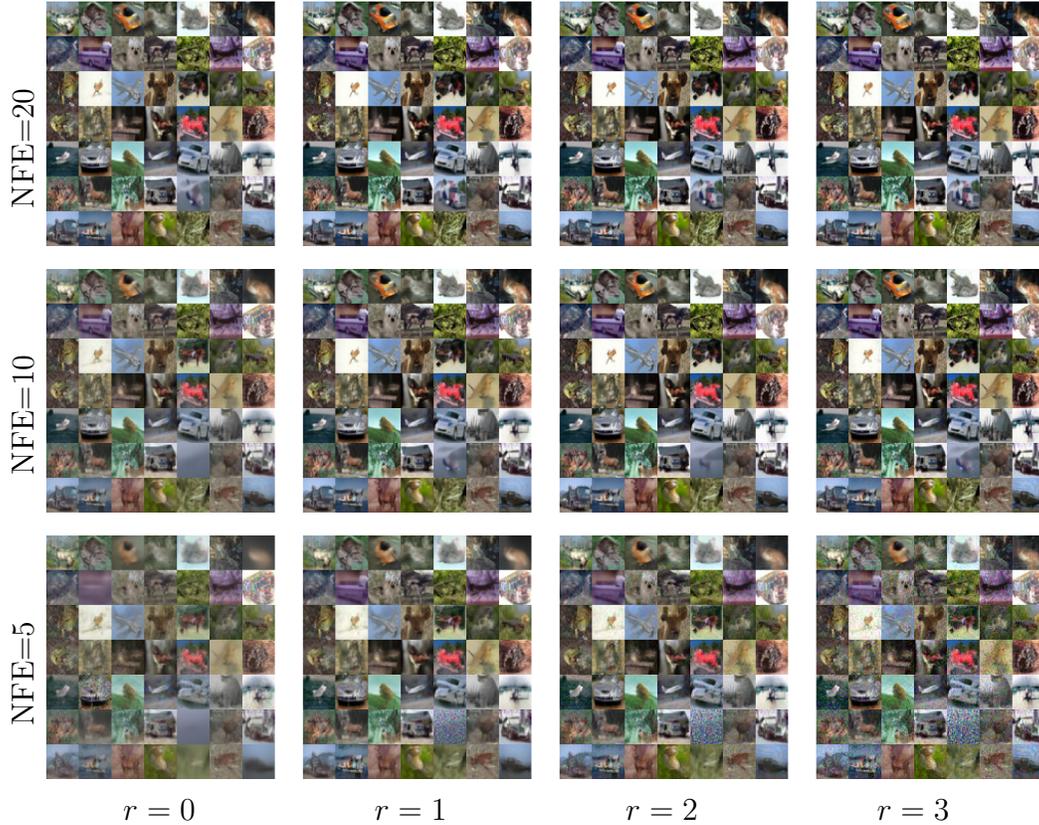


Figure 3: Generated images with *tABr-DEIS* on VESDE CIFAR10.

URL	Citation	License
https://github.com/yang-song/score_sde	[27]	Apache License 2.0
https://github.com/luping-liu/PNDM	[20]	Apache License 2.0
https://github.com/CompVis/latent-diffusion	[24]	MIT
https://github.com/baofff/Analytic-DPM	[3]	Unknown

Table 13: Code Used and License

Experiment	Citation	License
CIFAR10 Tab 1, 3 to 5, 8, 11 and 12 , FFHQ Fig 1	[27]	Apache License 2.0
CIFAR10 Tab 9	[3]	Unknown
CELEBA Tab 11	[20]	Apache License 2.0
ImageNet 32×32 Tab 10	[28]	Unknown
Text-to-image	[24]	MIT

Table 14: Checkpoints for experiments