000 001 002 THINK WHILE YOU GENERATE: DISCRETE DIFFUSION WITH PLANNED DENOISING

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ABSTRACT

Discrete diffusion has achieved state-of-the-art performance, outperforming or approaching autoregressive models on standard benchmarks. In this work, we introduce *Discrete Diffusion with Planned Denoising* (DDPD), a novel framework that separates the generation process into two models: a planner and a denoiser. At inference time, the planner selects which positions to denoise next by identifying the most corrupted positions in need of denoising, including both initially corrupted and those requiring additional refinement. This plan-and-denoise approach enables more efficient reconstruction during generation by iteratively identifying and denoising corruptions in the optimal order. DDPD outperforms traditional denoiser-only mask diffusion methods, achieving superior results on language modeling benchmarks such as text8, OpenWebText, and token-based generation on ImageNet 256×256 . Notably, in language modeling, DDPD significantly reduces the performance gap between diffusion-based and autoregressive methods in terms of generative perplexity.

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1 INTRODUCTION

027 028 029 030 031 032 033 034 035 Generative modeling of discrete data has recently seen significant advances across various applications, including text generation [\[5\]](#page-11-0), biological sequence modeling [\[25,](#page-12-0) [4\]](#page-11-1), and image synthesis [\[8,](#page-11-2) [9\]](#page-11-3). Autoregressive transformer models have excelled in language modeling but are limited to sequential sampling, with performance degrading without annealing techniques such as nucleus (top-p) sampling [\[20\]](#page-12-1). In contrast, diffusion models offer more flexible and controllable generation, proving to be more effective for tasks that lack natural sequential orderings, such as biological sequence modeling [\[25,](#page-12-0) [1\]](#page-11-4) and image token generation [\[8\]](#page-11-2). In language modeling, the performance gap between discrete diffusion and autoregressive models has further narrowed recently, thanks to improved training strategies [\[29,](#page-12-2) [36,](#page-13-0) [34,](#page-12-3) [13\]](#page-11-5), however, a gap still remains on some tasks [\[36,](#page-13-0) [29\]](#page-12-2).

036 037 038 039 State-of-the-art discrete diffusion methods train a denoiser (or score) model that determines the transition rate (or velocity) from the current state to predicted values. During inference, the generative process is discretized into a finite number of steps. At each step, the state values are updated based on the transition probability, which is obtained by integrating the transition rate over the timestep period.

040 041 042 043 044 045 046 047 048 In order to further close the performance gap with autoregressive models, we advocate for a rethinking of the standard discrete diffusion design methodology. We propose a new framework Discrete **Diffusion with Planned Denoising** (DDPD), that divides the generative process into two key components: a planner and a denoiser, facilitating a more adaptive and efficient sampling procedure. The process starts with a sequence of tokens initialized with random values. At each timestep, the planner model examines the sequence to identify the position most likely to be corrupted and in need of denoising. The denoiser then predicts the value for the selected position, based on the current noisy sequence. The key insight behind our plan-and-denoise approach is that the generative probability at each position can be factorized into two components: 1) planning: the probability that a position is corrupted, and 2) denoising: the probability of denoising it according to the data distribution.

- **049 050** Our framework offers two primary advantages:
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1. Simplified Learning Process: By decomposing the generative task into planning and denoising, each sub-task becomes easier to learn. Planning, in particular, is significantly

less complex than denoising. Traditional uniform diffusion models, in contrast, require a single neural network to handle both tasks simultaneously, which can lead to inefficiencies. 2. Improved Sampling Algorithm: The plan-and-denoise framework enables an adaptive sampling procedure that dynamically adjusts based on the planner's predictions.

As shown in Fig. [1,](#page-1-0) this process provides enhanced robustness:

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- **Adaptive Time Discretization:** When the planner identifies that the sequence is noisier than expected at a given timestep, it increases the number of denoising moves within the remaining time to ensure thorough refinement.
- Error Correction: The planner can identify errors introduced in earlier steps. If necessary, it adjusts time backward, allowing the denoiser to revisit and correct mistakes. This ensures all corrupted tokens are reconstructed accurately, yielding higher-quality generations.

- **076 077 078 079 080 081** Figure 1: An example generation trajectory from $t = 0$ to 1 with a sequence of 5 letters. At each step, the *planner* predicts the probability of each token being corrupted (indicated by the numbers next to the tokens). Based on these probabilities, a position is selected, and the *denoiser* makes its prediction. The *actual time* progression may not always align with the scheduled timestep, and is determined based on planner's assessment of the noise level of the sequence. For instance, in step 2, the denoiser makes minimal improvement and time progresses slower than scheduled. In step 4, the denoiser made an unintended error, the time progression is effectively backward. Sampling continues until all corrupted tokens are reconstructed.
	- Our contributions are as follows:
		- We introduce Discrete Diffusion with Planning and Denoising (DDPD), a novel framework for discrete generative modeling that decomposes the generation process into planning and denoising.
		- Our proposed plan-and-denoise framework introduces an adaptive sampling scheme, guided by the planner's output, enabling continuous self-correction of errors in an optimal order. This results in improved generation by scaling the number of sampling steps.
		- We derive simple and effective training objectives for the planner and denoiser models, grounded in maximizing the Evidence Lower Bound (ELBO) for discrete diffusion processes.
		- In experiments on GPT-2 scale language modeling and 256×256 image token generation, DDPD significantly outperforms its mask diffusion counterparts when using the same denoiser. Furthermore, we demonstrate that incorporating a planner substantially enhances generation quality, even when using a smaller or weaker denoiser model compared to baseline methods.

2 PRELIMINARIES

100 We begin by introducing the problem setup and notations. Following [\[7,](#page-11-6) [13\]](#page-11-5), we then explain the Continuous Time Markov Chain (CTMC) framework [\[31\]](#page-12-4), which is used to define the forward and reverse processes of discrete diffusion, and how the discrete timestep version is derived from it.

101 102 103 104 105 106 Setup and Notations. We aim to model discrete data where a sequence $x \in \{1, \dots, S\}^D$ is D-dimensional and each element x^d takes S possible states. $x^{\setminus d}$ denotes all dimensions except d. For clarity in presentation, we assume $D = 1$ and all results hold for $D > 1$ (see Section [3.1\)](#page-2-0). We use $p(x)$ to denote the probability mass function (PMF). The $\delta\{i, j\}$ is the Kronecker delta function, which is 1 when $i = j$ and 0 otherwise.

107 Continuous Time Markov Chains and Discretization. We adopt the CTMC framework to define the discrete diffusion process. A realization of the CTMC dynamics is defined by a trajectory x_t over

108 109 110 111 112 time $t \in [0, 1]$ that makes jumps to another state after a random waiting period known as the holding time. The transition rates and the next states are governed by the rate matrix $R_t \in \mathbb{R}^{S \times S}$ (analogous to the velocity field ν_t in continuous state spaces), where the off-diagonal elements, representing jumps to different states, are non-negative. For an infinitesimal timestep dt , the probability of transitioning from x_t to a different state j is given by $R_t(x_t, j)dt$.

113 114 115 In practice, the trajectory is simulated using finite time intervals Δt . As a result, the transition probability follows a categorical distribution with the PMF [\[39\]](#page-13-1):

$$
p_{t+\Delta t|t}(j|x_t) = \delta\{x_t, j\} + R_t(x_t, j)\Delta t,\tag{1}
$$

117 118 119 where we denote this as $\text{Cat}(\delta \{x_t, j\} + R_t(x_t, j) \Delta t)$, and $R_t(x_t, x_t) := -\sum_{s \neq x_t} R_t(x_t, s)$ to ensure that the transition probabilities sum to 1.

120 121 122 123 124 125 Forward Corruption Process. Following [\[7,](#page-11-6) [34,](#page-12-3) [13\]](#page-11-5), which were inspired by flow matching in continuous state space [\[26,](#page-12-5) [27,](#page-12-6) [2\]](#page-11-7), we construct the forward process by interpolating from noise $p_0(x_0) = p_{\text{noise}}(x_0)$ to clean data $p_1(x_1) = p_{\text{data}}(x_1)$. Common choices for the noise distribution include: (i) $p_{\text{noise}}^{\text{unif}}(x_t) = 1/s$, a uniform distribution over $\{1, \dots, S\}$; and (ii) $p_{\text{noise}}^{\text{mask}}(x_t) = \delta \{\mathbb{M}, x_t\}$, a delta PMF concentrated on an artificially introduced mask state M. Let α_t be the noise schedule that introduces noise to the data over time t. For example, a linear schedule is given by $\alpha_t = t$. The conditional marginal $p_{t|1}(x_t|x_1)$ is given in closed form:

$$
p_{t|1}^{\text{unif}}(x_t|x_1) = \text{Cat}(\alpha_t \delta\{x_1, x_t\} + (1 - \alpha_t)\frac{1}{S}),
$$
\n(2)

$$
p_{t|1}^{\text{mask}}(x_t|x_1) = \text{Cat}(\alpha_t \delta \{x_1, x_t\} + (1 - \alpha_t) \delta \{\mathbb{M}, x_t\}).
$$
\n(3)

130 131 132 At $t = 1$, the conditional marginal converges to the datapoint x_1 , i.e. $\delta \{x_1, x_t\}$. At $t = 0$, the conditional marginal converges to the noise distribution $p_{\text{noise}}(x_t)$.

133 134 135 136 Reverse Generation Process. Sampling from p_{data} is achieved by learning a generative rate matrix $R_t(x_t, j)$ to reverse simulate the process from $t = 0$ to $t = 1$ using Eq. [\(1\)](#page-2-1), such that we begin with samples of p_{noise} and end with samples of p_{data} . The datapoint conditional reverse rate $R_t(x_t, j|x_1)$ $R_t(x_t, j|x_1)$ $R_t(x_t, j|x_1)$ for $j \neq x_t^{-1}$ under the uniform or mask noise distributions is given by [\[7,](#page-11-6) [13\]](#page-11-5):

$$
R_t^{\text{unif}}(x_t, j|x_1) = \frac{\dot{\alpha}_t}{1 - \alpha_t} \delta\{x_1, j\} (1 - \delta\{x_1, x_t\}), \quad R_t^{\text{mask}}(x_t, j|x_1) = \frac{\dot{\alpha}_t}{1 - \alpha_t} \delta\{x_1, j\} \delta\{x_t, M\}.
$$

[\[7,](#page-11-6) [13\]](#page-11-5) show that the rate we aim to learn for generating p_{data} is the expectation of the data-conditional rate, taken over the denoising distribution, i.e., $R_t(x_t, j) := \mathbb{E}_{p_{1|t}(x_1|x_t)} [R_t(x_t, j|x_1)]$:

$$
R_t^{\text{unif}}(x_t, j) = \frac{\dot{\alpha}_t}{1 - \alpha_t} p_{1|t}(x_1 = j | x_t), \quad R_t^{\text{mask}}(x_t, j) = \frac{\dot{\alpha}_t}{1 - \alpha_t} \delta\{x_t, \mathbb{M}\} p_{1|t}(x_1 = j | x_t). \tag{4}
$$

The goal is to approximate this rate using a neural network. During inference, the generative process is simulated with the learned rate by taking finite timesteps, as described in Eq. [\(1\)](#page-2-1).

3 METHOD

3.1 DECOMPOSING GENERATION INTO PLANNING AND DENOISING

151 152 153 154 155 Recent state-of-the-art discrete diffusion methods [\[39,](#page-13-1) [29,](#page-12-2) [7,](#page-11-6) [36,](#page-13-0) [34,](#page-12-3) [13\]](#page-11-5) have converged on parameterizing the generative rate using a denoising neural network and deriving cross-entropy-based training objectives. This enables simplified and effective training, leading to better and SOTA performance in discrete generative modeling compared to earlier approaches [\[3,](#page-11-8) [6\]](#page-11-9). In Table [1,](#page-3-0) we summarize the commonalities and differences in the design choices across various methods.

156 157 158 159 Based on the optimal generative rate in Eq. [\(4\)](#page-2-2), we propose a new approach to parameterizing the generative rate by dividing it into two distinct components: planning and denoising. We begin by examining how the generative rate in mask diffusion can be interpreted within our framework, followed by a derivation of the decomposition for uniform diffusion.

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¹For simplicity, we only derive the rates for $j \neq x_t$. The rate for $j = x_t$ can be computed as $R_t(x_t, x_t | x_1) :=$ $-\sum_{s\neq x_t} R_t(x_t,s|x_1).$

[‡] DFM assumes a linear schedule. ^{*} MD4 also supports learnable schedule of α_t .

[†] $\lambda_{\theta}(x_i)$ is the total rate of jump determined by the planner.

Mask Diffusion. For mask diffusion, the planning part is assigning probability of $\frac{\dot{\alpha}_t}{1-\alpha_t} \delta \{x_t, M\} \Delta t$ for the data to be denoised with an actual value. $\delta \{x_t, M\}$ tells if the data is noisy (M) or clean. $\frac{\alpha_t}{1-\alpha_t}$ is the rate of denoising, which is determined by the remaining time according to the noise schedule. The denoiser $p_{1|t}$ assigns probabilities to the possible values to be filled in if this transition happens.

> $R_t^{\text{mask}}(x_t, j) \Delta t = \frac{\dot{\alpha_t}}{1}$ $\frac{\alpha_t}{1-\alpha_t} \delta\left\{x_t, M\right\}$ rate of making correction $\Delta t \, p_{1|t} \, (x_1 = j | x_t)$ prob. of denoising (5)

188 Uniform Diffusion. Similarly, we would want to decompose the transition probability into two parts: the planning probability based on if the data is corrupted and the denoising probability that determines which value to change to. But in contrast to the mask diffusion case, the noise/clean state of the data is not given to us during generation. We use $z_t^d \in \{N, D\}$ as a latent variable to denote if a dimension is corrupted, with N denoting noise and D denoting data.

192 193 194 From Bayes rule, for $j \neq x_t$, since $p_{1|t}$ $(x_1 = j | x_t, z_t = D) = \frac{p(x_t | x_1 = j, z_t = D)p(x_1 = j)}{p(x_t | z_t = D)} = 0$

$$
p_{1|t}(x_1 = j|x_t) = \sum_{z_t \in \{N, D\}} p(z_t|x_t) p_{1|t}(x_1 = j|x_t, z_t) = \underbrace{p(z_t = N|x_t)}_{\text{prob. of being corrupted}} \underbrace{p_{1|t}(x_1 = j|x_t, z_t = N)}_{\text{prob. of denoising}} \tag{6}
$$

The first part of the decomposition is the posterior probability of x_t being corrupted, and the second part gives the denoising probability to recover the value of x_t if x_t is corrupted. Plugging Eq. [\(6\)](#page-3-1) into Eq. [\(4\)](#page-2-2), we arrive at:

$$
R_t^{\text{unif}}(x_t, j)\Delta t = \underbrace{\frac{\dot{\alpha}_t}{1 - \alpha_t} p(z_t = N | x_t)}_{\text{rate. of making correction}} \Delta t \underbrace{p_{1|t}(x_1 = j | x_t, z_t = N)}_{\text{prob. of denoising}} \tag{7}
$$

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205 206 207 208 209 210 By comparing Eq. [\(7\)](#page-3-2) and Eq. [\(5\)](#page-3-3), we find that they share the same constant part $\frac{\dot{\alpha}_t}{1-\alpha_t}$ which represents the rate determined by the current time left according to the noise schedule. The main difference is in the middle part that represents the probability of x_t being corrupted. In mask diffusion case, this can be readily read out from the M token. But in the uniform diffusion case, we need to compute/approximate this probability instead. The last part is the denoising probability conditioned on x_t being corrupted, which again is shared by both and needs to be computed/approximated.

211 212 Generative Rate for Multi-Dimensions. The above mentioned decomposition extends to $D > 1$. We have the following reverse generative rate [\[7,](#page-11-6) [13\]](#page-11-5) for mask diffusion:

$$
R_t^{\text{mask}}(x_t, j^d) \Delta t = \frac{\dot{\alpha}_t}{1 - \alpha_t} \Delta t \ \delta \left\{ x_t^d, \mathbb{M} \right\} p_{1|t} \left(x_1^d = j^d | x_t \right), \quad \forall j^d \neq x_t^d,
$$
\n
$$
(8)
$$

and we derive the following decomposition result for uniform diffusion (proof in Appendix [A.3\)](#page-19-0):

216 217 218 Proposition 3.1. *The reverse generative rate at* d*-th dimension can be decomposed into the product of recovery rate, probability of corruption and probability of denoising:*

$$
R_t^{\text{unif}}(x_t, j^d) \Delta t = \frac{\dot{\alpha}_t}{1 - \alpha_t} p_{1|t} \left(x_1^d = j^d | x_t \right) \Delta t
$$
\n
$$
= \underbrace{\frac{\dot{\alpha}_t}{1 - \alpha_t}}_{\text{noise removal rate prob. of corruption}} \underbrace{p \left(z_t^d = N | x_t \right)}_{\text{prob. of denoising}} p_{1|t} \left(x_1^d = j^d | x_t, z_t^d = N \right) \Delta t, \quad \forall j^d \neq x_t^d
$$
\n(9)

where
$$
p\left(z_t^d = N|x_t\right) = 1 - p_{1|t}\left(x_1^d = x_t^d|x_t\right) \frac{\alpha_t}{\alpha_t + (1 - \alpha_t)/S}
$$
(10)

 $p_{1|t}\left(x_1^d=j^d|x_t, z_t^d=N\right)=\frac{p_{1|t}\left(x_1^d=j^d|x_t\right)}{p(z^d-N|x_t)}$

 $p(z_t^d = N|x_t)$

(11)

$$
\begin{array}{c} 225 \\ 226 \end{array}
$$

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We observe that the term $p(z_t^d = N|x_t)$ determines how different dimensions are reconstructed at different rates, based on how likely the dimension is clean or noise given the current context.

232 Previous Parameterization. In the case of mask diffusion, as studied in recent works [\[29,](#page-12-2) [7,](#page-11-6) [36,](#page-13-0) [34,](#page-12-3) [13\]](#page-11-5), the most effective parameterization for learning is to directly model the denoising probability with a neural network, as this is the only component that needs to be approximated.

233 234 235 236 237 In the case of uniform diffusion, the conventional approach uses a single model to approximate the generative rate as a whole, by modeling the posterior $p_{1|t}$ $(x_1^d = j^d | x_t)$ as shown in Eq. [\(9\)](#page-4-1). However, despite its theoretically greater flexibility – allowing token values to be corrected throughout sampling, akin to the original diffusion process in the continuous domain – its performance has not always outperformed mask diffusion, particularly in tasks like image or language modeling.

238 239 240 Plan-and-Denoise Parameterization. Based on the observation made in Proposition [3.1,](#page-3-4) we take the view that generation should consist of two models: a planner model for deciding which position to denoise and a denoiser model for making the denoising prediction for a selected position.

$$
R_{t, \text{jump}}^{\text{unif}}\left(x_{t}, j^{d}\right) \Delta t = \underbrace{\frac{\dot{\alpha}_{t}}{1 - \alpha_{t}}}_{\text{noise removal rate}} \Delta t}_{\text{plane}} \underbrace{p_{\theta}\left(z_{t}^{d} = N | x_{t}\right)}_{\text{planner}} \underbrace{p_{1|t}^{\theta}\left(x_{1}^{d} = j^{d} | x_{t}, z_{t}^{d} = N\right)}_{\text{denoiser}}, \quad \forall x_{t} \neq j^{d} \tag{12}
$$

245 246 247 248 249 This allows us to utilize the planner's output to design an improved sampling algorithm that optimally identifies and corrects errors in the sequence in the most effective denoising order. Additionally, the task decomposition enables separate training of the planner and denoiser, simplifying the learning process for each neural network. Often, a pretrained denoiser is already available, allowing for computational savings by only training the planner, which is generally faster and easier to train.

250 251 252 253 254 Remark 3.2. *Under this perspective, masked diffusion (Eq.* [\(8\)](#page-3-5)*) can be interpreted as a denoiser-only* modeling paradigm with a fixed planner, i.e., $p_\theta\left(z^d_t=N|x_t\right)=\delta\left\{x^d_t,\mathbb{M}\right\}$, which assumes that *mask tokens represent noise while actual tokens represent clean data. This planner is optimal under the assumption of a perfect denoiser, which rarely holds in practice. When the denoiser makes errors, this approach does not provide a mechanism for correcting those mistakes.*

255 256 257 Next, we demonstrate how our plan-and-denoise framework enables an improved sampling algorithm that effectively leverages the planner's predictions. From this point forward, we assume uniform diffusion by default and use $R_{t,\text{jump}}$ to denote the reverse jump rate, unless explicitly stated otherwise.

259 3.2 SAMPLING

261 262 263 264 265 266 267 268 269 Prior Works: Tau-leaping Sampler. The reverse generative process is a CTMC that consists of a sequence of jumps from $t = 0$ to $t = 1$. The most common way [\[6,](#page-11-9) [39,](#page-13-1) [29,](#page-12-2) [36,](#page-13-0) [34,](#page-12-3) [13\]](#page-11-5) is to discretize it into equal timesteps and simulate each step following the reverse generative rate using an approximate simulation method called tau-leaping. During step $[t, t + \Delta t]$, all the transitions happening according to Eq. [\(1\)](#page-2-1) are recorded first and simultaneously applied at the end of the step. When the discretization is finer than the number of denoising moves required, some steps may be wasted when no transitions occur during those steps. In such cases when no transition occurs during $[t - \Delta t, t]$, a neural network forward pass can be saved for step $[t, t + \Delta t]$ by using the cached $p_{1|t}(x_1^d | x_{t-\Delta t})$ from the previous step [\[10,](#page-11-10) [34\]](#page-12-3), assuming the denoising probabilities remain unchanged during $[t - \Delta t, t]$. However, as discussed in literature [\[6,](#page-11-9) [39,](#page-13-1) [29,](#page-12-2) [7\]](#page-11-6), such modeling of the reverse denoiser is predicting single dimension transitions but not joint transitions of all dimensions.

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270 271 272 Therefore, the tau-leaping simulation will introduce approximation errors if multiple dimensions are changed during the same step.

273 274 275 276 277 278 279 280 281 Gillespie Sampler. Instead, we adopt the Gillespie algorithm [\[15,](#page-11-11) [16,](#page-11-12) [41\]](#page-13-2), a simulation method that iteratively repeats the following two-step procedure: (1) sampling Δt , the holding time spent at current state until the next jump and (2) sampling which state transition occurs. In the first step, the holding time Δt is drawn from an exponential distribution, with the rate equal to the total jump rate, defined as the sum of all possible jump rates in Eq. [\(12\)](#page-4-2): $R_{t, \text{total}}(x_t) := \sum_{d} \sum_{j \neq x_t^d} R_{t, \text{jump}}(x_t, j^d)$. For the second step, the event at the jump is sampled according to $R_{t, \text{jump}}(x_t, j^d)/R_{t, \text{total}}(x_t)$, such that the likelihood of the next state is proportional to the rate from the current position. A straightforward way is using ancestral sampling by first selecting the dimension d , followed by sampling the value to jump to $j^{\bar{d}}$:

$$
\bar{d} \sim \text{Cat}\left(\sum_{j\bar{d}\neq x_{t}^{\bar{d}}} R_{t, \text{jump}}(x_{t}, j^{\bar{d}})/R_{t, \text{total}}(x_{t})\right), \quad j^{\bar{d}} \sim \text{Cat}\left(R_{t, \text{jump}}(x_{t}, j^{\bar{d}})/\sum_{j\bar{d}\neq x_{t}^{\bar{d}}} R_{t, \text{jump}}(x_{t}, j^{\bar{d}})\right)
$$

.

284 285 286 We find we can simplify the calculation of the total jump rate and next state transition by introducing the possibility of self-loop jumps into the CTMC. These allow the trajectory to remain in the current state after a jump occurs. This modification results in an equivalent but simpler simulated process with our plan-and-denoise method, formalized in the following proposition:

Proposition 3.3. *The original CTMC defined by the jump rate* $R_{t,jump}$ *given by Eq.* [\(12\)](#page-4-2) *has the same distribution over trajectories as the modified self-loop CTMC with rate matrix*

$$
\tilde{R}_t(x_t, j^d) = \frac{\dot{a}_t}{1 - \alpha_t} p_\theta(z_t^d = N | x_t) p_{1|t}^\theta(x_1^d = j^d | x_t, z_t^d = N), \quad \forall x_t, j^d
$$

For this self-loop Gillespie algorithm, the total jump rate and next state distribution have the form

$$
\sum_{d,j^d} \tilde{R}_t(x_t, j^d) = \frac{\dot{\alpha}_t}{1 - \alpha_t} \sum_d p_\theta(z_t^d = N | x_t) \bar{d} \sim \text{Cat}\left(p_\theta(z_t^{\bar{d}} = N | x_t)\right), \quad j^{\bar{d}} \sim \text{Cat}\left(p_{1|t}^\theta(x_1^{\bar{d}} = j^{\bar{d}} | x_t, z_t^{\bar{d}} = N)\right).
$$

Intuitively, the modification preserves the inter-state jump rates, ensuring that the distribution of effective jumps remains unchanged. A detailed proof is provided in Appendix [A.3.](#page-17-0)

300 301 302 303 304 Remark 3.4. *The Gillespie algorithm sets* ∆t *adaptively, which is given by the holding time until the next transition. This enables a more efficient discretization of timesteps, such that one step leads to one token denoised (if denoising is correct). In contrast, tau-leaping with equal timesteps can result in either no transitions or multiple transitions within the same step. Both scenarios are suboptimal: the former wastes a step, while the latter introduces approximation errors.*

306 307 308 309 Adaptive Time Correction. According to the sampled timesteps Δt , the sampling starts from noise at $t = 0$ and reaches data at 1. However, in practice, the actual time progression can be faster or slower than scheduled. For example, sometimes the progress is faster in the beginning when the starting sequence contains some clean tokens. More often, later in the process, the denoiser makes mistakes and hence time progression is slower than the scheduled Δt or even negative for some steps.

310 311 312 313 314 315 316 317 318 319 320 321 322 323 This raises the question: can we leverage the signal from the planner to make adaptive adjustments? For example, even if scheduled time is reaches $t = 1.0$, but according to the planner 10% of the data is still corrupted, the actual time progression under a linear schedule should be closer to $t = 0.9$. The reasonable approach is to assume the process is not yet complete and continue the plan-anddenoise sampling. Under this 'time correction' mechanism, the stopping criterion is defined as continuing the sampling procedure until the planner determines that all positions are denoised, i.e., when $p_{\theta}\left(z_t^d=N|\dot{x}_t\right) \approx 0$. In practice, we don't need to know the exact time; instead, we can continue sampling until either the stopping criterion is satisfied or the maximum budget of steps, T , is reached. The pseudo-algorithm for our proposed sampling method is presented in Algorithm [1.](#page-6-0) In cases where the denoiser use time information as input, we find it helpful to use the estimated time \tilde{t} from the planner. At time t, from the noise schedule, we expect there to be $(1 - \alpha_t)D$ noised positions. The estimate of the number of noised positions from the denoiser is $\sum_{d'} p_{\theta}(z_t^{d'} = N|x_t)$. Therefore, the planner's estimate of the corruption time is $\tilde{t} = \alpha_t^{-1} (1 - \sum_{d'} p_{\theta}(z_t^{d'} = N | x_t) / D)$ where α_t^{-1} is the inverse noise schedule. This adjustment better aligns the time-data pair with the distribution that the denoiser was trained on.

324 325 326 327 328 329 330 331 Based on the decomposition of the generation into planning and denoising, the proposed sampling method maximally capitalizes on the available sampling steps budget. The Gillespie-based plan-anddenoise sampler allows for exact simulation and ensures no step is wasted by prioritizing the denoising of noisy tokens first. The time correction mechanism enables the planner to identify both initial and reintroduced noisy tokens, continuously denoising them until all are corrected. This mechanism shares similarities with the stochastic noise injection-correction step in EDM [\[22\]](#page-12-7). Instead of using hyperparameters for deciding how much to travel back, our time correction is based on the planner's estimate of the noise removal progress.

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Algorithm 1 DDPD Sampler

2: while $i < T$ or $p_{\theta}(z_i^d = N | x_i) < \epsilon, \forall d$ do

3: Plan sample dimension $\bar{d} \sim \text{Cat}\left(p_{\theta}(z_i^{\bar{d}} = N|x_i)\right)$

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339 340 4: if denoiser uses time as input then 5: $t \leftarrow \alpha_t^{-1} \left(1 - \sum_{d'} p_{\theta}(z_t^{d'} = N | x_t) / D \right)$ 6: Denoise sample $j^{\bar{d}} \sim \text{Cat}\left(p_{1|t}^{\theta}(x_1^{\bar{d}}=j^{\bar{d}}|x_i, z_i^{\bar{d}}=N)\right), x_{i+1}^{\bar{d}} \leftarrow j^{\bar{d}}$

1: **init** $i \leftarrow 0, x_0 \sim p_0$, planner p_θ , denoiser $p_{1|t}^\theta$, maximum steps T, stopping criteria ϵ

- 7: $i \leftarrow i + 1$ 8: return x_i
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Utilizing a Pretrained Mask Diffusion Denoiser. In language modeling and image generation, mask diffusion denoisers have been found to be more accurate than uniform diffusion counterparts [\[3,](#page-11-8) [29\]](#page-12-2), with recent efforts increasingly focused on training mask diffusion denoisers [\[36,](#page-13-0) [34,](#page-12-3) [13\]](#page-11-5). The following proposition offers a principled way to sample from the uniform denoiser by leveraging a strong pretrained mask diffusion denoiser, coupled with a separately trained planner.

Proposition 3.5. From the following marginalization over z_t , which indicates if tokens are noise or *data:*

$$
p_{1|t}\left(x_1^d|x_t, z_t^d = N\right) = \sum_{z_t} p\left(z_t|x_t, z_t^d = N\right) p_{1|t}(x_1^d|x_t, z_t),\tag{13}
$$

samples from $p_{1|t,uniform}(x_1^d|x_t, z_t^d = N)$ can be drawn by first sampling z_t from $p(z_t|x_t, z_t^d = N)$ and then using a mask diffusion denoiser to sample x_1^d with $p_{1|t,mask}\left(x_1^d|\tilde{x}_t\right)$, where \tilde{x}_t is the masked *version of* x_t *according to* z_t *.*

356 357 358 359 360 361 362 363 In practice, we can approximately sample $z^{\setminus d}$ from $p(z_t|x_t, z_t^d = N) \approx \prod_{d' \neq d} p_{\theta}(z_t^{d'}|x_t)$. This approximation becomes exact if $p(z_t^d|x_t)$ is either very close to 0 or 1, which holds true for most dimensions during generation. We validated this holds most of time in language modeling in Appendix [E.5.](#page-33-0) Even if approximation errors in z_t occasionally lead to increased denoising errors, our sampling algorithm can effectively mitigate this by using the planner to identify and correct these unintentional errors. In our controlled experiments, we validate this and observe improved generative performance by replacing the uniform denoiser with a mask diffusion denoiser trained on the same total number of tokens, while keeping the planner fixed.

4 TRAINING

367 368 369 370 371 372 373 374 375 Training objectives. Our plan-and-denoise parameterization in Eq. [\(12\)](#page-4-2) enables us to use two separate neural networks for modeling the planner and the denoiser. Alternatively, both the planner and denoiser outputs can be derived from a single uniform diffusion model, $p_{1|t}^{\theta}(x_1^d|x_t)$, as described in Proposition [3.1.](#page-3-4) This approach may offer an advantage on simpler tasks, where minimal approximation errors for neural network training can be achieved, avoiding the sampling approximation introduced in Proposition [3.5.](#page-6-1) However, in modern generative AI tasks, training is often constrained by neural network capacity and available training tokens, making approximation errors inevitable. By using two separate networks, we can better decompose the complex task, potentially enabling faster training – especially since planning is generally easier than denoising.

376 377 The major concern with decomposed modeling is that joint modeling could introduce unnecessarily coupled training dynamics, hindering effective backpropagation of the training signal across different models. However, as we prove in Theorem [4.1,](#page-7-0) the evidence lower bound (ELBO) of discrete

378 379 380 diffusion decomposes neatly, allowing the use of direct training signals from the noise corruption process for independent training of the planner and denoiser (proof in Appendix [A.3\)](#page-19-0).

Theorem 4.1. Let x_1 be a clean data point, and x_t , z_t represent a noisy data point and its state of *corruption drawn from* $p_{t|1}(x_t, z_t|x_1)$ *. The ELBO for uniform discrete diffusion simplifies into the sum of the following separate cross-entropy-type objectives. The training of the planner* p_{θ} *reduces to a binary classification, where the goal is to estimate the corruption probability by maximizing:*

$$
\mathcal{L}_{\text{planner}} = \mathbb{E}_{\mathcal{U}(t;0,1)p_{\text{data}}(x_1)p_{t|1}(z_t,x_t|x_1)} \left[\frac{\dot{\alpha}_t}{1-\alpha_t} \sum_{d=1}^D \log p_{\theta} \left(z_t^d | x_t \right) \right]. \tag{14}
$$

The denoiser $p_{1|t}^{\theta}$ is trained to predict clean data reconstruction distribution:

$$
\mathcal{L}_{denoiser} = \mathbb{E}_{\mathcal{U}(t;0,1)p_{\text{data}}(x_1)p(x_t,z_t|x_1)} \left[\frac{\alpha_t}{1-\alpha_t} \sum_{d=1}^D \delta\{z_t^d, N\} \log p_{1|t}^\theta(x_1^d | x_t, z_t^d = N) \right]. \tag{15}
$$

Standard transformer architectures can be used to parameterize both the denoiser and the planner, where the denoiser outputs S logits and the planner outputs a single logit per dimension.

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5 RELATED WORK

396 397 398 399 400 401 402 403 404 405 Discrete Diffusion/Flow Models. Previous discrete diffusion/flow methods, whether in discrete time [\[3,](#page-11-8) [21,](#page-12-8) [34\]](#page-12-3) or continuous time [\[6,](#page-11-9) [39,](#page-13-1) [29,](#page-12-2) [7,](#page-11-6) [36,](#page-13-0) [13\]](#page-11-5), adopt the denoiser-only or score-modeling perspective. In contrast, we introduce a theoretically grounded decomposition of the generative process into planning and denoising. DFM [\[7\]](#page-11-6) and the Reparameterized Diffusion Model (RDM) [\[46\]](#page-13-3) introduce stochasticity into the reverse flow/diffusion process, allowing for adjustable random jumps between states. This has been shown to improve the generation quality by providing denoiser more opportunities to correct previous errors. Additionally, RDM uses the denoiser's prediction confidence as a heuristic [\[14,](#page-11-13) [35,](#page-12-9) [8\]](#page-11-2) for determining which tokens to denoise first. Lee et al. [\[24\]](#page-12-10) introduces another heuristic in image generation that aims at correcting previous denoising errors by first generating all tokens and then randomly regenerating them in batches.

406 407 408 409 410 Self-Correction Sampling. Predictor-corrector sampling methods are proposed for both continuous and discrete diffusion [\[37,](#page-13-4) [6\]](#page-11-9) that employ MCMC steps for correction after each predictor step. However, for continuous diffusion, this approach has been found to be less effective compared to the noise-injection stochasticity scheme [\[22,](#page-12-7) [42\]](#page-13-5). In the case of discrete diffusion, an excessively large number of corrector steps is required, which limits the method's overall effectiveness.

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6 EXPERIMENT

414 415 416 417 Before going into details, we note that DDPD incurs 2 NFE v.s. 1 NFE per step in denoiser-only approaches, an extra cost we pay for planning. To ensure a fair comparison, we also evaluate denoiseronly methods that are either $2\times$ large or use $2\times$ steps. Our findings show that spending compute on planning is more effective than doubling compute on denoising when cost is a factor.

418 419 420 421 422 423 424 425 426 427 428 429 Text8. We first evaluate DDPD on the small-scale character-level text modeling benchmark, text8 [\[30\]](#page-12-11), which consists of 100 million characters extracted from Wikipedia, segmented into chunks of 256 letters. Our experimental setup follows that of [\[7\]](#page-11-6). Methods for comparison include 1) autoregressive model 2) DFM: discrete flow model (and $2 \times$ param. version) [\[7\]](#page-11-6), the best available discrete diffusion/flow model for this task, 3) DFM-Uni: original DFM uniform diffusion using tau-leaping, 4) DDPD-DFM-Uni: DDPD using uniform diffusion model as planner and denoiser, 5) DDPD-UniD: DDPD with separately trained planner and uniform denoiser, 6) DDPD-MaskD: DDPD with separately planner and mask denoiser. Details in the sampling differences are summarized in Table [3.](#page-23-0) All models are of same size (86M) and trained for 750k iterations of batch size 2048, except for autoregressive model, which requires fewer iterations to converge. Generated samples are evaluated using the negative log-likelihood (NLL) under the larger language model GPT-J-6B [\[40\]](#page-13-6). Since NLL can be manipulated by repeating letters, we also measure token distribution entropy. High-quality samples should have both low NLL and entropy values close to the data distribution.

430 431 Fig. [2](#page-8-0) shows the performance of various methods with different sampling step budgets. DFM methods use tau-leaping while DDPD methods use our proposed adaptive Gillespie sampler. The original mask diffusion (DFM, $\eta = 0$) and uniform diffusion (DFM-Uni) perform similarly, and

432 433 434 435 adding stochasticity ($\eta = 15$) improves DFM's sample quality. Our proposed plan-and-denoise DDPD sampler consistently enhances the quality vs. diversity trade-off and significantly outperforms significantly outperforms DFM with $2\times$ parameters. Moreover, DDPD makes more efficient use of the inference-time budget (Fig. [2,](#page-8-0) middle), continuously refining the generated sequences.

436 437 438 439 440 441 442 443 444 We observe that DDPD with a single network (DDPD-DFM-Uni) outperforms using separately trained planner and denoiser, as the task simplicity allows all models to achieve $\geq 90\%$ denoising accuracy at $t = 0.85$. The benefit of reducing each model's burden is outweighed by compounded approximation errors (Section [3.2\)](#page-6-2). The weaker performance of τ -leaping (P×MaskD in Fig. [7\)](#page-27-0) confirms this issue lies in approximation errors, not the sampling scheme. To emulate a practical largerscale task where the models are undertrained due to computational or capacity budget limitations, we reduced training steps from $750k$ to $20k$ (Fig. [2,](#page-8-0) right). With only $20k$ steps, using separate planner and denoiser performs comparably to DFM at 750k, while the single model suffers mode collapse due to larger approximation errors, highlighting the benefits of faster separate learning.

445 446 447 448 449 450 451 452 453 Further ablation studies on imperfect training of either the planner or denoiser (Figs. [5](#page-26-0) and [6\)](#page-26-1) show that performance remains robust to varying levels of denoiser imperfection, thanks to the self-correction mechanism in the sampling process. An imperfect planner has a greater impact, shifting the quality-diversity Pareto front. In this case, training separate models proves more robust in preserving diversity and preventing mode collapse compared to training a single model. The ablation in Fig. [7](#page-27-0) examines the individual effects of the modifications introduced in the DDPD sampler. We also measure the denoising error terms in the ELBO for the planner + denoiser setup vs. the single neural network approach, as shown in Tables [4](#page-27-1) to [6](#page-28-0) of Appendix [E.1.3,](#page-25-0) which further validates the performance difference of various design choices. In Appendix [E.2,](#page-25-1) we tested how fast the sampling converges and reported statistics of dimensions be adjusted during the process.

Figure 2: Negative log-likelihood measured with GPT-J versus sample entropy (in terms of tokens), with logit temperatures of the denoiser swept over {0.8, 0.9, 1.0}. *Left*: DDPD v.s. SOTA baselines. *Middle*: Varying sampling steps from 256 to 1024; both DFM and DDPD use the same mask-based denoiser. *Right*: DDPD single-neural-network v.s. DDPD planner + mask denoiser, both trained for 20k iterations. DFM at 750k iter.

467 468 469 470 471 472 473 474 475 476 477 OpenWebText Language Modeling. In Fig. [3,](#page-9-0) we compare DDPD with SEDD [\[29\]](#page-12-2), both trained on the larger OpenWebText dataset [\[18\]](#page-12-12). We maintained the same experimental settings as in SEDD, with token vocabulary size $S = 50257$ and $D = 1024$, to validate whether planning improves generative performance under controlled conditions. We use the same pretrained SEDD-small or SEDD-medium score model as a mask diffusion denoiser, based on the conversion relationship outlined in Table [1.](#page-3-0) A separate planner network, with the same configuration as SEDD-small (90M), is trained for 400k iterations with batch size 512. We evaluated the quality of unconditional samples using generative perplexity, measured by larger language models GPT-2-L (774M) [\[33\]](#page-12-13) and GPT-J (6B) [\[40\]](#page-13-6). Both SEDD and DDPD were simulated using 1024 to 4096 steps, with top- $p = 1.0$. SEDD used tau-leaping, while DDPD employed our newly proposed sampler. We also include GPT-2 [\[33\]](#page-12-13) as the autoregressive baseline, with top-p sweeping from 0.7 to 1.0. We experimented DDPD sampler with both softmax selection (Fig. [9\)](#page-29-0) and proportional selection (Fig. [10\)](#page-29-1).

478 479 480 481 SEDD shows marginal improvement with additional steps, similar to DFM in text8. In contrast, DDPD leveraged planning to continuously improve sample quality, with the most improvements in early stages and diminishing returns in later steps as the sequence gets mostly corrected. This shows that the planner optimally selects the denoising order and adaptively corrects accumulated mistakes.

482 483 484 485 ImageNet 256×256 Generation with Discrete Tokens. An image is represented using discretevalued tokens with a pre-trained tokenizer and a decoder. The generative model is used for generating sequences in the token space. We focus on understanding how DDPD compares to existing sampling methods using the same denoiser, instead of aiming for SOTA performance. The pretrained tokenizer and mask denoiser from Yu et al. [\[45\]](#page-13-7) is used, where the token length of an image is $D = 128$.

Figure 3: Generative perplexity ↓ v.s. entropy ↑ (both plotted in log-scale) of SEDD, DDPD and GPT-2.

495 496 497 498 499 500 501 502 We compare DDPD with two mask diffusion type baselines: 1) standard mask diffusion and 2) MaskGIT [\[8\]](#page-11-2), which selects the next tokens based on the denoiser's confidence of its predicted logits. To prevent MaskGIT from making overly greedy selections, random noise is added to the confidence scores, with its magnitude annealed to zero following a linear schedule. We test all methods from 8 to 128 steps. Parallel sampling is used if $\#$ steps $<$ 128. The results on FID scores ([\[19\]](#page-12-14), lower is better) are presented in Table [2.](#page-9-1) More results on inception scores and comparison with SOTA are in Appendix [E.4.](#page-28-1) Generated samples are in Appendix [F.3.](#page-41-0) In DDPD, the sampling process is divided into two stages: the first half follows a parallel sampling schedule, while the second half adopts an adaptive step size based on the noise level, allowing for finer discretization towards the end of sampling.

503 504 505 506 507 508 509 510 511 Notably, we observe that the standard mask performs poorly, with no significant improvement even with more sampling steps. This is attributed to the low accuracy of the denoiser, which is much worse than in OpenWebText language modeling $(3\% \text{ v.s. } 60\% \text{ at } t = 0.85)$. The confidence-based sampling of MaskGIT proves effective, but its greedy selection, despite the added randomness, sacrifices the sample diversity for quality, leading to higher FID values compared to DDPD. This issue becomes particularly pronounced when more steps are used, resulting in an overly greedy sampling order. While DDPD requires a minimum number of sampling steps to correct sampling errors from earlier stages, it achieves the best results and more steps do not lead to worse FID. We also conducted ablation to study the effect of increasing number of second-stage steps for DDPD in Fig. [12.](#page-31-0)

512 513 514 515 516 517 518 519 520 521 To enhance the empirical performance in image token generation, we tested all methods with logit temperature annealing, a common approach to lower sampling temperature τ for improved denoising accuracy. We found $\tau = 0.6$ gives the best results among $\tau = 1.0, 0.9, 0.8, 0.7, 0.6, 0.5$, greatly improving mask diffusion and resulting in competitive FID scores. However, for MaskGIT, this reduces sample diversity, leading to even higher FID scores compared to no annealing. We also tried another annealing trick from Yu et al. [\[45\]](#page-13-7), where τ is linearly reduced from 1.0 to 0.0 during generation. This trick worked well for mask diffusion, allowing for further improvement over fixedtemperature annealing. For DDPD, performance remained relatively stable, with minor improvements or degradations compared to no annealing. Our method is designed based on the original sampling process without heuristics or classifier-free guidance, but we also evaluate its performance with these additions (Appendix [E.4.1\)](#page-30-0) and discuss their effects and interplay with DDPD.

522 523 Table 2: FID score (\downarrow) on ImageNet 256 \times 256. MaskD refers to mask diffusion. The denoiser and parallel sampling schedule are kept the same as [\[45\]](#page-13-7), without classifier-free guidance.

	No Logit Annealing			Logit temp 0.6			Logit temp $1.0 \rightarrow 0.0$		
Steps T		MaskD MaskGIT DDPD			MaskD MaskGIT DDPD			MaskD MaskGIT DDPD	
8	38.06	5.51	6.8	5.69	10.02	5.71	4.99	8.53	5.99
16	32.44	6.66	5.12	4.85	11.24	4.92	4.69	9.21	5.03
32	29.12	8.09	4.75	4.86	11.93	4.91	4.62	9.9	4.98
64	27.54	9.08	4.73	4.98	12.26	5.14	4.6	10.35	5.26
128	26.83	9.34	4.89	5.13	12.52	5.39	4.89	10.2	5.54

7 CONCLUSION

533 534 535 536 537 538 539 We introduced Discrete Diffusion with Planned Denoising (DDPD), a novel framework that decomposes the discrete generation process into planning and denoising. We propose a new adaptive sampler that leverages the planner for more effective and robust generation by adjusting time step sizes and prioritizing the denoising of the most corrupted positions. Additionally, it simplifies the learning process by allowing each model to focus specifically on either planning or denoising. The incorporation of planning makes the generative process more robust to errors made by the denoiser during generation. On GPT-2 scale language modeling and ImageNet 256×256 token generation, DDPD enables a significant performance boost compared to denoiser-only discrete diffusion models.

8 REPRODUCIBILITY STATEMENT

 To facilitate reproducibility, we provide comprehensive details of our method in the main paper and Appendix [D.](#page-22-0) This includes the model designs, hyper-parameters in training, sampling schemes and evaluation protocols for all the experiments. We further provide PyTorch pseudocode for the proposed adaptive Gillespie sampling algorithm.

9 ETHICS STATEMENT

 This work raises ethical considerations common to deep generative models. While offering potential benefits such as generating high-quality text/image contents, these models can also be misused for malicious purposes like creating deepfakes or generating spam and misinformation. Mitigating these risks requires further research into guardrails for reducing harmful contents and collaboration with socio-technical experts.

 Furthermore, the substantial resource costs associated with training and deploying deep generative models, including energy and water consumption, present environmental concerns. This work is able save cost on training by reusing a pretrained denoisers and just focusing on training different planner models for slightly different tasks. At inference time, our newly proposed sampler is able to generate at better quality as compared to existing methods that use same amount of compute.

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Appendix

A PROOFS

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A.1 PROOF OF PROPOSITION [3.1](#page-3-4)

Part 1: Calculate $p\left(z^d_t=N|x_t\right)$ in Eq. [\(10\)](#page-4-4).

We first derive how to calculate $p(z_t^d = N|x_t)$ in Eq. [\(10\)](#page-4-4) using $p_{1|t}$.

766 767 First, from law of total probability,

$$
p(z_t^d = N|x_t) = \sum_{\bar{j}^d} p_{1|t} (x_1^d = \bar{j}^d | x_t) p(z_t^d = N | x_1^d = \bar{j}^d, x_t)
$$
 (16)

770 771 772 Next we derive closed form of $p(z_t^d = N | x_1^d = \overline{j}^d, x_t)$.

According to the noise schedule,

$$
p(z_t^d, x_t^d | x_1) = \begin{cases} \alpha_t & \text{if } z_t^d = D, x_t^d = x_1^d\\ 0 & \text{if } z_t^d = D, x_t^d \neq x_1^d\\ (1 - \alpha_t)/S & \text{if } z_t^d = N, x_t^d = x_1^d\\ (1 - \alpha_t)/S & \text{if } z_t^d = N, x_t^d \neq x_1^d \end{cases}
$$
(17)

Using Bayes rule $p\left(z_t^d|x_t^d, x_1\right) = p\left(z_t^d, x_t^d|x_1\right) / p\left(x_t^d|x_1\right)$, we have

$$
p(z_t^d | x_t^d, x_1) = \begin{cases} \frac{\alpha_t}{\alpha_t + (1 - \alpha_t)/S} & \text{if } z_t^d = D, x_t^d = x_1^d\\ 0 & \text{if } z_t^d = D, x_t^d \neq x_1^d\\ \frac{(1 - \alpha_t)/S}{\alpha_t + (1 - \alpha_t)/S} & \text{if } z_t^d = N, x_t^d = x_1^d\\ 1 & \text{if } z_t^d = N, x_t^d \neq x_1^d \end{cases}
$$
(18)

Plugging Eq. [\(18\)](#page-14-0) into Eq. [\(16\)](#page-14-1), we have

$$
p(z_t^d = N|x_t) = \sum_{\bar{j}^d} p(x_1^d = \bar{j}^d | x_t) p(z_t^d = N | x_1^d = \bar{j}^d, x_t)
$$
\n(19)

$$
= \sum_{\bar{j}^d \neq x_t^d} p\left(x_1^d = \bar{j}^d | x_t\right) \cdot 1 + p\left(x_1^d = x_t^d | x_t\right) \cdot \frac{(1 - \alpha_t)/S}{\alpha_t + (1 - \alpha_t)/S} \tag{20}
$$

$$
= \sum_{\bar{j}^d \neq x_t^d} p\left(x_1^d = \bar{j}^d | x_t\right) \cdot 1 + p\left(x_1^d = x_t^d | x_t\right) \cdot \left(1 - \frac{\alpha_t}{\alpha_t + (1 - \alpha_t)/S}\right) \tag{21}
$$

$$
= 1 - p\left(x_1^d = x_t^d | x_t\right) \frac{\alpha_t}{\alpha_t + (1 - \alpha_t)/S}
$$
\n⁽²²⁾

which gives us the form in Eq. (10) .

Part 2: Calculate $p_{1|t}\left(x_1^d=j^d| x_t, z_t^d=N\right)$ in Eq. [\(11\)](#page-4-5).

From Bayes rule, we have

$$
p_{1|t}\left(x_1^d = j^d | x_t, z_t^d = N\right) = \frac{p\left(x_1^d = j^d, z_t^d = N | x_t\right)}{p\left(z_t^d = N | x_t\right)}
$$
\n⁽²³⁾

$$
= \frac{p(x_1^d = j^d | x_t) p(z_t^d = N | x_t, x_1^d = j^d)}{p(z_t^d = N | x_t)} \tag{24}
$$

$$
= \frac{p\left(x_1^d = j^d | x_t\right)}{p\left(z_t^d = N | x_t\right)}, \quad \forall x_t^d \neq j^d \tag{25}
$$

Eq. [\(25\)](#page-14-2) is by plugging in the following from Eq. [\(18\)](#page-14-0) that $p(z_t^d = N | x_t, x_1^d = j^d) = 1$ if $x_t^d \neq j^d$.

810 811 Part 3: Verify equivalence to the original optimal rate in Eq. [\(9\)](#page-4-1).

812 By plugging in Eq. (10) and Eq. (11) into Eq. (9) , we have

$$
R_t^{\text{unif}}(x_t, j^d) = \underbrace{\frac{\dot{\alpha}_t}{1 - \alpha_t}}_{\text{recovery rate}} p(z_t^d = N | x_t) p_{1|t} (x_1^d = j^d | x_t, z_t^d = N)}_{\text{prob. of denoising}} = \underbrace{\frac{\dot{\alpha}_t}{1 - \alpha_t}}_{\text{recovery rate}} \underbrace{p_{1|t} (x_1^d = j^d | x_t)}_{\text{recovery rate}}
$$
\n
$$
R_{\text{R15}}^{\text{unif}}(x_t, j^d) = \underbrace{\frac{\dot{\alpha}_t}{1 - \alpha_t}}_{\text{recovery rate}} p(z_t^d = N | x_t) p_{1|t} (x_1^d = j^d | x_t, z_t^d = N)}_{\text{prob. of denoising}} = \underbrace{\frac{\dot{\alpha}_t}{1 - \alpha_t}}_{\text{recovery rate}}
$$
\n
$$
R_{\text{R26}}
$$
\n
$$
R_{\text{R37}}
$$
\n
$$
R_{\text{R48}}
$$
\n
$$
R_{\text{R58}}
$$
\n
$$
R_{\text{R68}}
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\n
$$
R_{\text{R78}}
$$
\n
$$
R_{\text{R88}}
$$
\n

This derivation follows the Continuous Time Markov Chain framework. We refer the readers to Appendix C.1 of Campbell et al. [\[7\]](#page-11-6) for a primer on CTMC. Here we provide the proof for $D = 1$ case. The result holds for $D > 1$ case following same arguments from Appendix E of Campbell et al. [\[7\]](#page-11-6).

836 837 838 839 840 Let W be a CTMC trajectory, fully described by its jump times T_1, \dots, T_n and state values between jumps $W_0, W_{T_0}, \cdots, W_{T_n}$. At time T_k , the state jumps from $W_{T_{k-1}}$ to W_{T_k} . With its path measure properly defined, we start with the following result from Campbell et al. [\[7\]](#page-11-6) Appendix C.1, the ELBO of $\mathbb{E}_{p_{data}(x_1)} [\log p_{\theta}(x_1)]$ is given by introducing the corruption process as the variational distribution:

$$
\mathbb{E}_{p_{\text{data}}(x_1)}\left[\log p_{\theta}(x_1)\right] \ge \int p_{\text{data}}(\mathrm{d}x_1) \mathbb{Q}^{|x_1}(\mathrm{d}\omega) \log \frac{\mathrm{d}\mathbb{P}^{\theta}}{\mathrm{d}\mathbb{Q}^{|x_1}}(\omega),\tag{27}
$$

where

826

828

$$
\frac{\mathrm{d}\mathbb{P}^{\theta}}{\mathrm{d}\mathbb{Q}^{|x_1}}(\omega) = \frac{p_0(W_0) \exp\left(-\int_{t=0}^{t=1} R_t^{\theta}(W_t^-) \mathrm{d}t\right) \prod_{t:W_t \neq W_t^-} R_t^{\theta}(W_t^-, W_t)}{p_{0|1}(W_0|x_1) \exp\left(-\int_{t=0}^{t=1} R_t(W_t^-|x_1) \mathrm{d}t\right) \prod_{t:W_t \neq W_t^-} R_t(W_t^-, W_t|x_1)}.
$$
(28)

Intuitively, the measure (probability) of a trajectory is determined by: the starting state from the prior distribution $p_0(W_0)$, and the product of the probability of waiting from T_{k-1} to T_k (which follows an Exponential distribution) and the transition rate of the jump from W_t^- to W_t .

851 852 853 854 For our method, when simulating the data corruption process, we augment W_t^{aug} to record both state values W_t and its latent value $Z_t \in \{N, D\}^D$. The jump is defined to happen when the latent value jumps from Z_{k-1} to Z_k with one of the dimensions corrupted and the state value jumps from W_{k-1} to \hat{W}_k . Similarly, the ELBO of $\mathbb{E}_{p_{data}(x_1)}$ [log $p_{\theta}(x_1)$] can be defined as:

$$
\mathbb{E}_{p_{\text{data}}(x_1)}\left[\log p_{\theta}(x_1)\right] \ge \int p_{\text{data}}(\mathrm{d}x_1) \mathbb{Q}^{|x_1}(\mathrm{d}\omega^{\text{aug}})\log \frac{\mathrm{d}\mathbb{P}^{\theta}}{\mathrm{d}\mathbb{Q}^{|x_1}}(\omega^{\text{aug}}) \tag{29}
$$

where the Radon-Nikodym derivative is given by:

$$
\frac{\mathrm{d}\mathbb{P}^{\theta}}{\mathrm{d}\mathbb{Q}^{|x_{1}}}(\omega^{\text{aug}}) = \frac{p_{0}\left(W_{0}\right)\exp\left(-\int_{t=0}^{t=1}R_{t}^{\theta}\left(W_{t}^{-}\right)\mathrm{d}t\right)\prod_{t}R_{t}^{\theta}\left(W_{t}^{-},W_{t}\right)}{p_{0|1}\left(W_{0},Z_{0}\mid x_{1}\right)\exp\left(-\int_{t=0}^{t=1}R_{t}\left(W_{t}^{-},Z_{t}^{-}\mid x_{1}\right)\mathrm{d}t\right)\prod_{t}R_{t}\left(W_{t}^{-},W_{t},Z_{t}^{-},Z_{t}\mid x_{1}\right)}\tag{30}
$$

862 863

By plugging in Eq. [\(30\)](#page-15-1) into Eq. [\(29\)](#page-15-2), we arrive at

866

$$
\frac{867}{868}
$$

$$
\mathcal{L}_{ELBO} = \int p_{data} (dx_1) \int_{\omega^{\text{aug}}:\mathbb{Q}^{|\,x_1}(\omega^{\text{aug}}) > 0} \mathbb{Q}^{|\,x_1}(\mathrm{d}\omega^{\text{aug}}) \left\{ - \int_{t=0}^{t=1} R_t^{\theta} (W_t^-) dt + \sum_t \log R_t^{\theta} (W_t^-, W_t) \right\}
$$
\n
$$
= \int p_{data} (dx_1) \int_{\omega^{\text{aug}}:\mathbb{Q}^{|\,x_1}(\omega^{\text{aug}}) > 0} \mathbb{Q}^{|\,x_1}(\mathrm{d}\omega^{\text{aug}}) \left\{ - \int_{t=0}^{t=1} \frac{\dot{\alpha}_t}{1 - \alpha_t} p_{\theta} (Z_t^- = N | W_t^-) \right\}
$$
\n
$$
+ \sum_t \log \frac{\dot{\alpha}_t}{1 - \alpha_t} p_{\theta} (Z_t^- = N | W_t^-) p_{1|t}^{\theta} (x_1 = W_t | W_t^-, Z_t^- = N) \right\}
$$
\n
$$
= \int p_{data} (dx_1) \int_{\omega^{\text{aug}}:\mathbb{Q}^{|\,x_1}(\omega^{\text{aug}}) > 0} \mathbb{Q}^{|\,x_1}(\mathrm{d}\omega^{\text{aug}}) \left\{ - \int_{t=0}^{t=1} \frac{\dot{\alpha}_t}{1 - \alpha_t} p_{\theta} (Z_t^- = N | W_t^-) \right\}
$$
\n
$$
+ \sum_{t \in \{T_1, \cdots, T_N\}} \left(\log \frac{\dot{\alpha}_t}{1 - \alpha_t} p_{\theta} (Z_t^- = N | W_t^-) + \log p_{1|t}^{\theta} (x_1 = W_t | W_t^-, Z_t^- = N) \right) \right\}
$$
\n(31)

 $\sqrt{ }$

 \mathcal{L}

879 880 881

Eq. [\(31\)](#page-16-0) contain terms that depend on the planner $p_{\theta}(z_t = N|x_t)$ and the denoiser $p_{1|t}^{\theta}(x_1 = j | x_t, z_t = N)$. Next, we show those terms can be separated into two parts:

$$
\mathcal{L}_{\text{denoiser}} = \mathbb{E}_{\mathcal{U}(t;0,1)p_{\text{data}}(x_1)p(x_t,z_t|x_1)} \left[\frac{\dot{\alpha}_t}{1-\alpha_t} \delta\{z_t, N\} \log p_{1|t}^{\theta}(x_1|x_t,z_t=N) \right]
$$
(32)

$$
\mathcal{L}_{\text{planner}} = \mathbb{E}_{\mathcal{U}(t;0,1)p_{\text{data}}(x_1)p_{t|1}(z_t,x_t|x_1)} \left[\frac{\dot{\alpha}_t}{1-\alpha_t} \log p_{\theta}\left(z_t|x_t\right) \right]
$$
(33)

First part: cross-entropy loss on
$$
x_1
$$
 denoising.

All terms associated with $p_{1|t}^{\theta}$ $(x_1 = W_t|W_t^-, Z_t^- = N)$ are:

$$
\mathcal{L}_{\text{denoising}} = \int p_{\text{data}} \left(\mathrm{d}x_{1}\right) \int_{\omega^{\text{aug}}} \mathbb{Q}^{|x_{1}}(\mathrm{d}\omega^{\text{aug}}) \sum_{t} \log p_{1|t}^{\theta}\left(x_{1} = W_{t}|W_{t}^{-}, Z_{t}^{-} = N\right)
$$
\n
$$
= \int p_{\text{data}} \left(\mathrm{d}x_{1}\right) \int_{\omega^{\text{aug}}} \mathbb{Q}^{|x_{1}}(\mathrm{d}\omega^{\text{aug}}) \int_{t=0}^{t=1} \sum_{(y,u)} R_{t}\left((W_{t}, Z_{t}), (y,u)|x_{1}\right) \log p_{1|t}^{\theta}\left(x_{1} = W_{t}|W_{t}^{-}, Z_{t}^{-} = N\right) \text{ Dynkin}
$$
\n
$$
= \int p_{\text{data}} \left(\mathrm{d}x_{1}\right) \int_{\omega^{\text{aug}}} \mathbb{Q}^{|x_{1}}(\mathrm{d}\omega^{\text{aug}}) \int_{t=0}^{t=1} \sum_{(y,u)} \frac{\dot{\alpha}_{t}}{1 - \alpha_{t}} \delta\{Z_{t}, N\} \delta\{u, D\} \delta\{y, x_{1}\} \log p_{1|t}^{\theta}\left(x_{1} = W_{t}|W_{t}^{-}, Z_{t}^{-} = N\right)
$$
\n
$$
= \int \int_{t=0}^{t=1} p_{\text{data}} \left(\mathrm{d}x_{1}\right) \int_{\omega^{\text{aug}}} \mathbb{Q}^{|x_{1}}(\mathrm{d}\omega^{\text{aug}}) \frac{\dot{\alpha}_{t}}{1 - \alpha_{t}} \delta\{Z_{t}, N\} \log p_{1|t}^{\theta}\left(x_{1} = W_{t}|W_{t}^{-}, Z_{t}^{-} = N\right)
$$
\n
$$
= \mathbb{E}_{\mathcal{U}(t;0,1)p_{\text{data}}(x_{1})p_{t|1}(z_{t}, x_{t}|x_{1})} \left[\frac{\dot{\alpha}_{t}}{1 - \alpha_{t}} \delta\{z_{t}, N\} \log p_{1|t}^{\theta}\left(x_{1}|x_{t}, z_{t} = N\right)\right]
$$

At the second equation, we use Dynkin's formula

$$
\int p_{\text{data}}\left(\mathrm{d}x_{1}\right) \mathbb{Q}^{\mid x_{1}}\left(\mathrm{d}\omega\right) \sum_{t:\text{all jump times}} f\left(W_{t}^{-}, W_{t}\right) = \int p_{\text{data}}\left(\mathrm{d}x_{1}\right) \mathbb{Q}^{\mid x_{1}}\left(\mathrm{d}\omega\right) \int_{t=0}^{t=1} \sum_{y} R_{t}\left(W_{t}, y \mid x_{1}\right) f\left(W_{t}, y\right) \mathrm{d}t
$$

911 912 which allows us to switch from a sum over jump times into a full integral over time interval weighted by the probability of the jump happening and the next state the jump goes to.

913 Second part: cross-entropy loss on $z_t = N$ prediction.

914 915 The remaining terms are associated with $\frac{\dot{\alpha_t}}{1-\alpha_t} p_\theta (Z_t^- = N|W_t^-)$ which is the jump rate at W_t^- , i.e.

916 $R_{t,\text{jump}}^{\theta}(W_t^-) = \sum_j R_{t,\text{jump}}^{\theta}(W_t^-,j) = \frac{\alpha_t}{1-\alpha_t} p_{\theta} \left(Z_t^- = N|W_t^-\right)$ according to Eq. [\(12\)](#page-4-2). In this proof,

918 919 we will use R_t^{θ} in short for $R_{t,\text{jump}}^{\theta}$. The remaining loss terms

$$
\mathcal{L}_{\text{planner}} = \int p_{\text{data}} \left(dx_{1} \right) \int_{\omega^{\text{aug}}} \mathbb{Q}^{\mid x_{1}} \left(d\omega^{\text{aug}} \right) \left\{ - \int_{t=0}^{t=1} R_{t}^{\theta} \left(W_{t}^{-} \right) dt + \sum_{t} \log R_{t}^{\theta} \left(W_{t}^{-} \right) \right\}
$$
\n
$$
= \int p_{\text{data}} \left(dx_{1} \right) \int_{\omega^{\text{aug}}} \mathbb{Q}^{\mid x_{1}} \left(d\omega^{\text{aug}} \right) \left\{ - \int_{t=0}^{t=1} R_{t}^{\theta} \left(W_{t} \right) dt + \int_{t=0}^{t=1} \sum_{(y,u)} R_{t} \left(\left(W_{t}, Z_{t} \right), (y,u) \right| x_{1} \right) \log R_{t}^{\theta} \left(W_{t} \right) dt \right\}
$$
\nDynkin

925 926 927

$$
= \int p_{\text{data}}\left(\mathrm{d}x_{1}\right) \int_{\omega^{\text{aug}}}\mathbb{Q}^{\mid x_{1}\mid}(\mathrm{d}\omega^{\text{aug}})\left\{-\int_{t=0}^{t=1} R_{t}^{\theta}\left(W_{t}\right) \mathrm{d}t + \int_{t=0}^{t=1} \frac{\dot{\alpha}_{t}}{1-\alpha_{t}} \delta\{Z_{t}, N\}\log R_{t}^{\theta}\left(W_{t}\right) \mathrm{d}t\right\}
$$
\n
$$
= \mathbb{E}_{\mathcal{U}(t;0,1)p_{\text{data}}(x_{1})p(x_{t},z_{t}|x_{1})}\left[-R_{t}^{\theta}\left(x_{t}\right)+\frac{\dot{\alpha}_{t}}{1-\alpha_{t}} \delta\{z_{t}, N\}\log R_{t}^{\theta}\left(x_{t}\right)\right]
$$

We first rewrite the loss as

$$
\mathbb{E}_{\mathcal{U}(t;0,1)p(x_t)p(x_1,z_t|x_t)}\left[-R_t^{\theta}(x_t) + \frac{\dot{\alpha}_t}{1-\alpha_t}\delta\{z_t,N\}\log R_t^{\theta}(x_t)\right]
$$
\n
$$
=\mathbb{E}_{\mathcal{U}(t;0,1)p(x_t)p(x_1,z_t|x_t)}\left[-\frac{\dot{\alpha}_t}{1-\alpha_t}p_{\theta}(z_t=N|x_t) + \frac{\dot{\alpha}_t}{1-\alpha_t}\delta\{z_t,N\}\log\frac{\dot{\alpha}_t}{1-\alpha_t}p_{\theta}(z_t=N|x_t)\right]
$$
\n(34)

If x_t is given fixed, by taking the derivative of $p_\theta(z_t = N|x_t)$ and setting it to zero, we have the optimal solution to be:

$$
p_{\theta}\left(z_{t}=N|x_{t}\right)=\mathbb{E}_{p(x_{1},z_{t}|x_{t})}\delta\{z_{t},N\}
$$

This is equivalent to optimizing the cross-entropy loss, which has the same optimal solution:

$$
\mathbb{E}_{p(x_1, z_t | x_t)} [\delta \{z_t, N\} \log p_\theta (z_t = N | x_t) + (1 - \delta \{z_t, N\}) \log (1 - p_\theta (z_t = N | x_t))]
$$

Plugging this x_t -conditional loss back to Eq. [\(34\)](#page-17-1), we arrive at the cross entropy training loss for the planner:

$$
\mathcal{L}_{\text{planner}} = \mathbb{E}_{\mathcal{U}(t;0,1)p_{\text{data}}(x_1)p_{t|1}(z_t,x_t|x_1)} \left[\frac{\dot{\alpha}_t}{1-\alpha_t} \log p_{\theta}\left(z_t|x_t\right) \right].
$$

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A.3 PROOF OF PROPOSITION [3.3:](#page-5-1) CONTINUOUS TIME MARKOV CHAINS WITH SELF-CONNECTIONS

955 956 957 958 959 960 961 We first describe the stochastic process that includes self-loops as this differs slightly from the standard CTMC formulation. We have a rate matrix $\hat{R}(i, j)$ that is non-negative at all entries, $\overline{R}(i, j) > 0$. To simulate this process, we alternate between waiting for an exponentially distributed amount of time and sampling a next state from a transition distribution. The waiting time is exponentially distributed with rate $\sum_k R(i, k)$. The next state transition distribution is $\tilde{P}(j|i) = \frac{\tilde{R}(i,j)}{\sum_{k} \tilde{R}(i,j)}$ $\frac{R(i,j)}{k \tilde{R}(i,k)}$. Note that $\tilde{P}(i|i)$ can be non-zero due to the self-loops in this style of process.

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964 965 966 967 968 We can find an equivalent CTMC without self-loops that has the same distribution over trajectories as this self-loop process. To find this, we look at the infinitesimal transition distribution from time t to time $t + \Delta t$. We let J denote the event that the exponential timer expires during the period $[t, t + \Delta t]$. We let \bar{J} denote the no jump event. For the self-loop process, the infinitesimal transition distribution is

$$
p_{t+\Delta t|t}(j|i) = \mathbb{P}(J,j|i) + \mathbb{P}(\bar{J},j|i)
$$

$$
= \mathbb{P}(J|i)\mathbb{P}(j|J,i) + \mathbb{P}(\bar{J}|i)\mathbb{P}(j|\bar{J},i)
$$

971

972 973 We have the following relations

$$
\mathbb{P}(J|i) = \sum_{k} \tilde{R}(i,k) \Delta t
$$
 property of exponential distribution

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974

k $\mathbb{P}(j|J,i) = \frac{\tilde{R}(i,j)}{\sum_{k} \tilde{R}(i,k)}$

$$
\begin{array}{c} 978 \\ 979 \\ 980 \end{array}
$$

Our infinitesimal transition distribution therefore becomes

 $\mathbb{P}(j|\bar{J},i) = \delta\{j=i\}$

$$
p_{t+\Delta t|t}(j|i) = \left(\sum_{k} \tilde{R}(i,k)\Delta t\right) \frac{\tilde{R}(i,j)}{\sum_{k} \tilde{R}(i,k)} + \left(1 - \Delta t \sum_{k} \tilde{R}(i,k)\right) \delta\{j = i\}
$$

$$
= \Delta t \tilde{R}(i,j) + \delta \{j = i\} - \delta \{j = i\} \Delta t \sum_{k} \tilde{R}(i,k)
$$

 $\overline{1}$

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$$
= \delta\{i=j\} + \Delta t \left(\tilde{R}(i,j) - \delta\{i=j\}\sum_{k} \tilde{R}(i,k)\right)
$$

We now note that for a standard CTMC without self-loops and rate matrix $R(i, j)$, the infinitesimal transition probability is

$$
p_{t + \Delta t | t}(j|i) = \delta\{i = j\} + \Delta t R(i, j)
$$

Therefore, we can see our self-loop process is equivalent to the CTMC with rate matrix equal to

$$
R(i, j) = \tilde{R}(i, j) \quad i \neq j
$$

$$
R(i, i) = -\sum_{k} \tilde{R}(i, k)
$$

1000 In other words, the CTMC rate matrix is the same as the self-loop matrix except simply removing the diagonal entries and replacing them with negative row sums as is standard.

1002 In our case, the original CTMC without self-loops is defined by rate matrix

$$
R_t(x_t, j^d) = \frac{\dot{\alpha}_t}{1 - \alpha_t} p_\theta(z_t^d = N | x_t) p_{1|t}^\theta(x_1^d = j^d | x_t, z_t^d = N), \qquad \forall x_t^d \neq j^d
$$

1005 1006 We have free choice over the diagonal entries in our self-loop rate matrix and so we set the diagonal entries to be exactly the above equation evaluated at $x_t^d = j^d$.

$$
\tilde{R}_t(x_t, j^d) = \frac{\dot{\alpha}_t}{1 - \alpha_t} p_\theta(z_t^d = N | x_t) p_{1|t}^\theta(x_1^d = j^d | x_t, z_t^d = N), \forall x_t^d, j^d
$$

1010 We can now evaluate the quantities needed for Gillespie's Algorithm. The first is the total jump rate

$$
\sum_{d} \sum_{j^{d}} \tilde{R}_{t}(x_{t}, j^{d}) = \frac{\dot{\alpha}_{t}}{1 - \alpha_{t}} \sum_{d} \sum_{j^{d}} p_{\theta}(z_{t}^{d} = N | x_{t}) p_{1|t}^{\theta}(x_{1} = j^{d} | x_{t}, z_{t}^{d} = N)
$$
(35)

$$
\begin{array}{c} 1013 \\ 1014 \\ 1015 \end{array}
$$

1016

1018 1019 1020

$$
=\frac{\dot{\alpha}_t}{1-\alpha_t}\sum_d p_\theta(z_t^d=N|x_t)
$$
\n(36)

1017 We now need to find the next state jump distribution. To find the dimension to jump to we use

$$
\frac{\sum_{j^d} \tilde{R}_t(x_t, j^d)}{\sum_d \sum_{j^d} \tilde{R}_t(x_t, j^d)} = \frac{\frac{\dot{\alpha}_t}{1 - \alpha_t} p_\theta(z_t^d = N | x_t)}{\frac{\dot{\alpha}_t}{1 - \alpha_t}} = p_\theta(z_t^d = N | x_t)
$$
(37)

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- **1023**
- **1024**

1026 1027 To find the state within the chosen jump, the distribution is

 $\tilde{R}_t(x_t, j^d)$

$$
1028\\
$$

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 $\frac{N_{t}(x_t, y)}{\sum_{j^d} \tilde{R}_t(x_t, j^d)}$ = $\frac{\dot{\alpha}_t}{1-\alpha_t} p_\theta(z_t^d=N|x_t)$ (38)

 $\frac{\dot{\alpha}_t}{1-\alpha_t} p_\theta(z_t^d = N | x_t) p_{1|t}^{\theta}(x_1^d = j^d | x_t, z_t^d = N)$

$$
=p_{1|t}^{\theta}(x_1^d=j^d|x_t, z_t^d=N)
$$
\n(39)

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B GENERAL FORMULATION

B.1 SCORE-ENTROPY BASED: SDDM [\[39\]](#page-13-1), SEDD [\[29\]](#page-12-2)

1040 1041 1042 For coherence, we assume $t = 0$ is noise and $t = 1$ is data, while discrete diffusion literature consider a flipped notion of time. Following Campbell et al. [\[6\]](#page-11-9), (see Sec. H.1 of Campbell et al. [\[7\]](#page-11-6)), the conditional reverse rate of discrete diffusion considered in [\[39,](#page-13-1) [29\]](#page-12-2) is defined to be:

$$
R_t^{\text{diff}}\left(x_t, j^d \mid x_1^d\right) = R_t(j^d, x_t^d) \frac{p_{t|1}\left(j^d \mid x_1^d\right)}{p_{t|1}\left(x_t^d \mid x_1^d\right)}
$$
(40)

1046 1047 with the forward corruption rate $R_t = \frac{\dot{\alpha}_t}{S \alpha_t} (11^\top - S \mathbf{I})$ for uniform diffusion or $R_t = \frac{\dot{\alpha}_t}{\alpha_t} (1 \mathbf{e}_\mathbb{M}^- - \mathbf{I})$ for mask diffusion, such that the corruption schedule is according to α_t .

1048 1049 And the expected reverse rate for $x_t^d \neq j^d$ is given by:

$$
R_t^{\text{diff}}\left(x_t, j^d\right) = \mathbb{E}_{p_{1|t}\left(x_1^d \mid x_t\right)} R_t^{\text{diff}}\left(x_t, j^d \mid x_1^d\right) \tag{41}
$$

$$
= \sum_{x_1^d} p_{1|t} \left(x_1^d \mid x_t \right) R_t(j^d, x_t^d) \frac{p_{t|1} \left(j^d \mid x_1^d \right)}{p_{t|1} \left(x_t^d \mid x_1^d \right)} \tag{42}
$$

$$
= R_t \sum_{x_1^d} p_{1|t} \left(x_1^d \mid x_t \right) \frac{p_{t|1} \left(j^d \mid x_1^d \right)}{p_{t|1} \left(x_t^d \mid x_1^d \right)} \tag{43}
$$

$$
1057\n\n1058\n\n1059\n\n1059\n\n1060\n\n
$$
= R_t \sum_{x_1^d} \frac{p\left(x_t^d \mid x_1^d, x_t^{\lambda d}\right) p\left(x_1^d \mid x_t^{\lambda d}\right)}{p\left(x_t^d \mid x_t^{\lambda d}\right)} \frac{p_{t|1}\left(j^d \mid x_1^d\right)}{p_{t|1}\left(x_t^d \mid x_1^d\right)}\n \tag{44}
$$
$$

$$
= R_t \sum_{x_1^d} \frac{p\left(x_1^d \mid x_t^{\backslash d}\right)}{p\left(x_t^d \mid x_t^{\backslash d}\right)} p_{t|1}\left(j^d \mid x_1^d\right) \tag{45}
$$

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1061

 P_t^{θ} **Parameterization in SDDM.** From here we can derive the rate derived in Eq. (16) in SDDM [\[39\]](#page-13-1) which uses a neural network to parameterize $p^{\theta} \left(x_t^d | x_t^{\setminus d} \right)$

$$
R_t^{\text{diff}}\left(x_t, j^d\right) = R_t \frac{\sum_{x_1^d} p\left(x_1^d \mid x_t^{\setminus d}\right) p_{t|1}\left(j^d \mid x_1^d\right)}{p\left(x_t^d \mid x_t^{\setminus d}\right)} = R_t \frac{p_t^\theta\left(j^d \mid x_t^{\setminus d}\right)}{p_t^\theta\left(x_t^d \mid x_t^{\setminus d}\right)}
$$

1073 1074 1075 1076 S_t^{θ} **Parameterization in SEDD.** SEDD [\[29\]](#page-12-2) introduces the notion of score that directly models $p_t(j^d,x_t^{\setminus d})$ $\frac{p_t(y, x_t, y_t)}{p_t(x_t^d, x_t^{\{d\}})}$ with $s_\theta(x_t)_{x_t^d \to j}$. Hence the reverse rate is parameterized by:

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$$
R_t^{\text{diff}}(x_t, j^d) = R_t \frac{p_t\left(j^d \mid x_t^{\setminus d}\right)}{p_t\left(x_t^d \mid x_t^{\setminus d}\right)} = R_t \frac{p_t\left(j^d, x_t^{\setminus d}\right)}{p_t\left(x_t^d, x_t^{\setminus d}\right)} = R_t s_\theta(x_t)_{x_t^d \to j}
$$

1080 1081 1082 $p_{1|t}^{\theta}$ **Parameterization in SDDM.** In Eq. (24) of Sun et al. [\[39\]](#page-13-1), the alternative parameterization uses a neural network to parameterize $p_{1|t}^{\theta}\left(x_1^d \mid x_t^{\setminus d}\right)$ and the rate is given by:

$$
R_t^{\text{diff}}\left(x_t, j^d\right) = R_t \frac{p\left(j^d \mid x_t^{\backslash d}\right)}{p\left(x_t^d \mid x_t^{\backslash d}\right)}
$$

$$
=R_t\frac{\sum_{x^d_1}p_{1|t}^{\theta}\left(x^d_1\mid x^{\backslash d}_t\right)p_{t|1}\left(j^d\mid x^d_1\right)}{\sum_{x^d_1}p_{1|t}^{\theta}\left(x^d_1\mid x^{\backslash d}_t\right)p_{t|1}\left(x^d_t\mid x^d_1\right)}
$$

Connection to reverse rate in Campbell et al. [\[7\]](#page-11-6). In mask diffusion case, the rate of SD-DM/SEDD coincides with the rate used in Eq. [\(42\)](#page-19-2), i.e. rate of discrete diffusion and discrete flow formulation are the same for the mask diffusion case, $R_t^{\text{diff}} = R_t^{*,\text{DFM}}$. We have for $x_t^d = \mathbb{M}$ and $j^d \neq \mathbb{M}$:

1106 1107 We can find that the parameterization of the generative rate used in DFM is only different from the SDDM/SEDD's parameterization by a scalar.

1108 1109 1110 1111 1112 In the uniform diffusion case, the reverse rate used for discrete diffusion effectively generates the same marginal distribution $p_{t|1}$ and p_t , but the difference lies in that the rate used for discrete diffusion is the sum of the rate introduced in Campbell et al. [\[7\]](#page-11-6) plus a special choice of the CTMC stochasticity that preserve detailed balance: $R_t^{\text{diff}} = R_t^{*,\text{DFM}} + R_t^{\text{DB}}$. Details are proved in H.1 in Campbell et al. [\[7\]](#page-11-6)

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C ADDITIONAL TECHNICAL DETAILS

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1117 C.1 EVALUATING THE ELBO

1119 1120 1121 1122 1123 Note that the ELBO values are only comparable between uniform diffusion methods or mask diffusion methods, since they have different marginal distribution $p_{t|1}$ and hence different trajectory path distribution $\mathbb{Q}(W \in d\omega)$. Based on Eq. [\(29\)](#page-15-2), we write out the ELBO terms for mask diffusion and uniform diffusion. Results about log-likelihood in prior works [\[3,](#page-11-8) [7,](#page-11-6) [29,](#page-12-2) [36,](#page-13-0) [34\]](#page-12-3) are reporting the (denoising) rate transitioning term only, i.e., $\log p_{1|t}^{\theta} \left(x_1^{d'} = W_t^{d'} | W_t^{-} \right)$.

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1126 C.1.1 MASK DIFFUSION ELBO

1128 Term 1: Prior ratio $\log \frac{p_0(W_0)}{p_{0|1}(W_0|x_1)} = 0$.

1129 1130 1131 1132 We observe that $\frac{p_0(W_0)}{p_{0|1}(W_0|x_1)}$ = 1 since the starting noise distribution is the same. Hence $\log \frac{p_0(W_0)}{p_{0|1}(W_0|x_1)}=0.$

Term 2: Rate Matching
$$
\log \frac{\exp(-\int_{t=0}^{t=1} R_t^{\theta}(W_t^{-}) dt)}{\exp(-\int_{t=0}^{t=1} R_t (W_t^{-}|x_1) dt)} = 0.
$$

1134 1135 In the mask diffusion case, this term equals to 1, since

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$$
R_t^{\theta}(W_t^-) = \frac{\dot{\alpha}_t}{1 - \alpha_t} \sum_{d=1}^D \delta \left\{ W_t^{-,d}, \mathbb{M} \right\}, \quad R_t(W_t^- | x_1) = \frac{\dot{\alpha}_t}{1 - \alpha_t} \sum_{d=1}^D \delta \left\{ W_t^{-,d}, \mathbb{M} \right\}
$$

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For any trajectory $W_t, t \in [0,1)$, $R_t^{\theta}(W_t^{-}) = R_t(W_t^{-}|x_1)$ and hence Term 2 equals to 0, i.e. $\log \frac{\exp\left(-\int_{t=0}^{t=1} R_t^{\theta}(W_t^{-}) dt\right)}{\left(\int_{t=1}^{t=1} P_t(W_t^{-}) dt\right)}$

1141 $\frac{\exp(-\int_{t=0}^{t=1} R_t(W_t^{-}|x_1) dt)}{\exp(-\int_{t=0}^{t=1} R_t(W_t^{-}|x_1) dt)} = 0.$

1142
1143 **Term 3: Rate Transitioning**
$$
\log \frac{R_t^{\theta}(W_t^-, W_t)}{R_t(W_t^-, W_t|x_1)}
$$
.

1144 1145 Let the jump at t happens at dimension d' , we have

$$
R_t^{\theta}(W_t^-, W_t) = \frac{\dot{\alpha}_t}{1 - \alpha_t} \delta \left\{ W_t^{-,d'}, \mathbb{M} \right\} p_{1|t}^{\theta} \left(x_1^{d'} = W_t^{d'} | W_t^- \right), \quad R_t(W_t^-, W_t | x_1) = \frac{\dot{\alpha}_t}{1 - \alpha_t} \delta \left\{ W_t^{-,d'}, \mathbb{M} \right\}
$$

1148 1149 1150 1151 Since before the jump $W_t^{-,d'}$ must be at mask state in order for jump to happen, hence this term simplifies to $\log \frac{R_t^{\theta}(W_t^-, W_t)}{P_t(W_t^-, W_t^+)}$ $\frac{R_t^\theta(W_t^-,W_t)}{R_t(W_t^-,W_t|x_1)} = \log p_{1|t}^\theta\left(x_1^{d'} = W_t^{d'}|W_t^-\right).$

1152 1153 C.1.2 UNIFORM DIFFUSION ELBO

1154 Term 1: Prior ratio $\log \frac{p_0(W_0)}{p_{0|1}(W_0|x_1)} = 0$.

1155 1156 1157 1158 We observe that $\frac{p_0(W_0)}{p_{0|1}(W_0|x_1)} = 1$ since the starting noise distribution is the same uniform distribution. Hence $\log \frac{p_0(W_0)}{p_{0|1}(W_0|x_1)} = 0.$

Term 2: Rate Matching
$$
\log \frac{\exp(-\int_{t=0}^{t=1} R_t^{\theta}(W_t^{-}) dt)}{\exp(-\int_{t=0}^{t=1} R_t(W_t^{-}|x_1) dt)}
$$

1161 1162 If the generative process is parameterized by $p_{1|t}^{\theta}(x_1^d|x_t)$ in Eq. [\(4\)](#page-2-2):

1163
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1165

$$
R_t(W_t^{-}) = \frac{\dot{\alpha}_t}{1 - \alpha_t} \sum_{d=1}^D p_{1|t}^{\theta}(x_1^d \neq W_t^{-,d}|x_t), \quad R_t(W_t^{-}|x_1) = \frac{\dot{\alpha}_t}{1 - \alpha_t} \sum_{d=1}^D (1 - \delta \left\{ W_t^{-,d}, x_1^d \right\})
$$

1167 If the reverse generative process is parameterized as our approach in Eq. [\(12\)](#page-4-2):

$$
R_t^{\theta}(W_t^{-}) = \frac{\dot{\alpha}_t}{1 - \alpha_t} \sum_{d=1}^D p^{\theta}(z_t^{-,d} = N | x_t), \quad R_t(W_t^{-}, Z_t^{-} | x_1) = \frac{\dot{\alpha}_t}{1 - \alpha_t} \sum_{d=1}^D \delta \left\{ Z_t^{-,d}, N \right\}
$$

1172 Term 2 simplifies to:

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\n
$$
\int_{t=0}^{t=1} R_t(W_t^-|x_1) dt - \int_{t=0}^{t=1} R_t^{\theta}(W_t^-) dt
$$

\n
$$
= \int_{t=0}^{t=1} [R_t(W_t^-|x_1) - R_t^{\theta}(W_t^-)] dt
$$

$$
= \mathbb{E}_{\mathcal{U}(t;0,1)}\left[R_t\left(W_t^-|x_1\right) - R_t^{\theta}\left(W_t^-\right)\right]
$$

1179 1180 Similarly, it simplifies to $\mathbb{E}_{\mathcal{U}(t;0,1)}\left[R_t\left(W_t^-, Z_t^-| x_1\right) - R_t^{\theta}\left(W_t^-\right)\right]$ for DDPD.

1181 1182 For a given W_t or W_t^{aug} , we can approximate this term with Monte-Carlo samples from $t \sim \mathcal{U}(t;0,1)$.

1183 1184 Term 3: Rate Transitioning $\log \frac{R_t^{\theta}(W_t^-, W_t)}{R_t(W_t^-, W_t)_{\infty}}$ $\frac{R_t(W_t^-, W_t)}{R_t(W_t^-, W_t | x_1)}$.

1185 If using parameterization
$$
p_{1|t}^{\theta}(x_1^d|x_t)
$$
 in Eq. (4):

1186
\n
$$
R_t^{\theta}(W_t^-, W_t) = \frac{\dot{\alpha}_t}{1 - \alpha_t} p_{1|t}^{\theta} \left(x_1^{d'} = W_t^{d'} | W_t^- \right), \quad R_t(W_t^-, W_t | x_1) = \frac{\dot{\alpha}_t}{1 - \alpha_t} \left(1 - \delta \left\{ W_t^{-, d'}, x_1^d \right\} \right) \delta \left\{ W_t^{d'}, x_1^d \right\}
$$

 $\big)$

1188 1189 1190 We know for the trajectory W_t , before the jump $W_t^{-,d'} \neq x_1^d$ and after the jump $W_t^{d'} = x_1^d$, therefore $R_t(W_t^-, W_t | x_1) = \frac{\dot{\alpha_t}}{1 - \alpha_t}$. Hence the term simplifies to

1191 1192

$$
\log \frac{R_t^{\theta}(W_t^-,W_t)}{R_t(W_t^-,W_t|x_1)} = \log p_{1|t}^{\theta}\left(x_1^{d'} = W_t^{d'}|W_t^-\right)
$$

If using our parameterization in Eq. [\(12\)](#page-4-2):

$$
R_t^{\theta}(W_t^-, W_t) = \frac{\dot{\alpha}_t}{1 - \alpha_t} p^{\theta} \left(z_t^{-,d'} = N | W_t^- \right) p_{1|t}^{\theta} \left(x_1^{d'} = W_t^{d'} | W_t^-, z_t^{-,d'} = N \right),
$$

$$
R_t(W_t^-, W_t, Z_t^-, Z_t | x_1) = \frac{\dot{\alpha}_t}{1 - \alpha_t} \delta \left\{ z_t^{-, d'}, N \right\} \delta \left\{ z_t^{d'}, D \right\} \delta \left\{ W_t^{d'}, x_1^d \right\} = \frac{\dot{\alpha}_t}{1 - \alpha_t}
$$

1200 The term simplifies to

$$
\log \frac{R_t^{\theta}(W_t^-, W_t)}{R_t(W_t^-, W_t | x_1)} = \log \left[p^{\theta} \left(z_t^{-, d'} = N | W_t^{-} \right) p_{1|t}^{\theta} \left(x_1^{d'} = W_t^{d'} | W_t^{-}, z_t^{-, d'} = N \right) \right]
$$

D IMPLEMENTATION DETAILS

1207 D.1 TEXT8

1208 1209 1210 1211 1212 1213 1214 1215 1216 1217 1218 1219 1220 1221 Models and training. We used the same transformer architecture from the DFM [\[7\]](#page-11-6) for the denoiser model, with architectural details provided in Appendix I of [\[7\]](#page-11-6). For the planner, we modified the final layer to output a logit value representing the probability of noise. To prevent the planner model from exploiting the the current time step information to cheating on predicting the noise level, we find it necessary to not use time-embedding. Unlike the original DFM implementation, which uses self-conditioning inputs with previously predicted x_1 , we omit self-conditioning in all of our trained models, as we found it had minimal impact on the results. When training the planner and denoiser, we implemented the optimization objectives in Theorem [4.1](#page-7-0) as the cross entropy between target and predicted noise state and tokens, averaged over the corrupted dimensions. A linear noise schedule is used. We do not apply the time-dependent prefactor $\frac{\dot{\alpha}_t}{1-\alpha_t}$ to the training examples, as the signals from each corrupted token are independent. All models follow Campbell et al. [\[7\]](#page-11-6) which is based on the smallest GPT2 architecture (768 hidden dimensions, 12 transformer blocks, and 12 attention heads) and have 86M parameters. We increase the model size to 176M parameters for DFM-2 \times with 1024 hidden dimensions, 14 transformer blocks, and 16 attention heads.

- **1222** The following models were trained for text8:
	- Autoregressive: $p(x^d|x^{1:d-1})$
	- Uniform diffusion denoiser (DFM-Uni): $p_{1|t}(x_1^d|x_t)$
	- Planner: $p(z_t^d|x_t)$
	- Noise-conditioned uniform diffusion denoiser (UniD): $p_{1|t}(x_1^d | x_t, z_t^d = N)$
	- Mask diffusion denoiser (MaskD): $p_{1|t}(x_1^d | x_t, x_t^d = M)$

1231 1232 1233 1234 1235 1236 We maintained the training procedure reported in [\[7\]](#page-11-6), which we reproduce here for completeness. For all models, we used an effective batch size of 2048 with micro-batch 512 accumulated every 4 steps. For optimization, we used AdamW [\[28\]](#page-12-15) with a weight decay factor of 0.1. Learning rate was linearly warmed up to 10⁻⁴ over 1000 steps, and decayed using a cosine schedule to 10⁻⁵ at 1M steps. We used the total training step budget of 750k steps. We saved checkpoints every 150k steps for ablation studies reported in Figs. [5](#page-26-0) and [6.](#page-26-1) EMA was not used for text8 models. We trained our models on four A100 80GB GPUs, and it takes around 100 hours to finish training for 750k iterations.

1238 1239 Sampling schemes. The sampling schemes used for experiments in the main text are outlined in Table [3.](#page-23-0) Gillespie Algorithm options A, B, and C are defined as follows:

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- A: Default DDPD Gillespie sampling in Algorithm [1](#page-6-0)
- \bullet +B: Continue sampling until the maximum time step budget is reached

Table 3: Sampling schemes used for text8 experiments.

 \bullet +C: Use the softmax of noise prediction logits (over the dimension axis) instead of normalized prediction values to select the dimensions that will be denoised

The implementation of these options when the uniform diffusion denoiser (DFM-Uni) is decomposed as a planner and a denoiser is presented in Listing [1.](#page-24-0)

1260 1261 1262 1263 Evaluation. For each specified sampling scheme and sampling time step budget, we sampled 512 sequences with $D = 256$. Using the GPT-J (6B) model [\[40\]](#page-13-6), we computed the average negative loglikelihood for each sequence, and using the same tokenization scheme (BPE in [\[33\]](#page-12-13)), we calculated sequence entropy as the sum over all dimensions.

1264 1265 D.2 OPENWEBTEXT

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1266 1267 1268 1269 1270 1271 1272 1273 1274 1275 1276 1277 1278 1279 Models and training. We used the same model architectures from SEDD [\[29\]](#page-12-2), which are based on the diffusion transformer (DiT) [\[32\]](#page-12-16) and use rotary positional encodings [\[38\]](#page-13-8). We followed their training procedure closely for the OpenWebText experiments. Like the text8 models, we modified the final layer of DiT to serve as a noise probability logit predictor for the planner model. SEDD models use the noise level σ instead of time t for the time embeddings. While we retain this model input by using their $\sigma(t)$, we replace it with zero when training the planner, similarly to the text8 models. All models were trained with a batch size of 128 and gradients were accumulated every 4 steps. We used AdamW [\[28\]](#page-12-15) with a weight decay factor of 0, and the learning rate was linearly warmed up to 3×10^{-4} over the first 2500 steps and then held constant. EMA with a decay factor of 0.9999 was applied to the model parameters. We validated the models on the OpenWebText dataset [\[17\]](#page-11-14). The mask denoisers are taken from the pretrained checkpoints of Lou et al. [\[29\]](#page-12-2). SEDD-small has 90M parameters and SEDD-medium has 320M parameters. We trained our planner models on nodes with four A100 80GB GPUs for 400k iterations. We only trained the planner models in the size of GPT-2-Small, which is 768 hidden dimensions, 12 layers, and 12 attention heads.

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1281 1282 1283 1284 Sampling and evaluation. We employed Tweedie tau-leaping denoising scheme for SEDD, and adaptive Gillespie sampler for DDPD, and different nucleus sampling thresholds (top-p values of 0.8, 0.85, 0.9, and 1.0) for GPT-2. For all models and sampling schemes, we generated 200 samples of sequence length 1024 and evaluated the generative perplexity using the GPT-2 Large [\[33\]](#page-12-13) and GPT-J [\[40\]](#page-13-6) models.

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1287 D.3 IMAGE GENERATION WITH TOKENS

1288 1289 1290 1291 1292 1293 1294 1295 Models and training. For tokenization and decoding of images, we use TiTok-S-128 model [\[45\]](#page-13-7), which tokenizes 256×256 image into $D = 128$ tokens with the codebook size of $S = 4096$. Both mask diffusion denoiser and planner models use the U-Vit model architecture of MaskGIT [\[8\]](#page-11-2) as implemented in the codebase of [\[45\]](#page-13-7), with 768 hidden dimensions, 24 layers, and 16 attention heads. The mask denoisers are taken from pretrained checkpoints from Yu et al. [\[45\]](#page-13-7). The planner is trained with batch size 2048 for 400k iterations on 4 A100-80GB GPUs. We used AdamW [\[28\]](#page-12-15) optimizer with a weight decay factor of 0.03, $\beta_1 = 0.9$, and $\beta_2 = 0.96$, and a learning rate of 2×10^{-4} . The learning rate schedule included a linear warmup over the first 10k steps, followed by cosine annealing down to a final learning rate of 10[−]⁵ . EMA was applied with a decay factor of 0.999.

1301 1302 1303 1304 1305 Listing 1: Gillespie Algorithm sampling loop with uniform diffusion denoiser (DFM-Uni) decomposed as a planner and a denoiser.

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           import torch
           import torch.nn.functional as F
           B = batch\_sizeD = num dimensions
           S = mask\_token\_id = vocab\_sizeeps = stopping_criteria
           samples = torch.randint(0, S, (B, D),dtype=torch.int64)
           time = torch.zeros(B, dtype=torch.float)
           is_time_up = torch.zeros(B, dtype=torch.bool)
           for i in range(timesteps):
               # Planning: compute probabilities of changing each dimension
               logits = model(samples, time) # (B, D, S+1)
                logits[:, :, mask_token_id] = -1e4
pt_x1_probs = F.softmax(logits, dim=-1)
               pt_x1_probs_at_xt = torch.gather(pt_x1_probs, -1, samples[:, :, None]) # (B, D, 1)
               p_{if\_change} = 1 - pt_x1\_probs_at_xt.\nsqueeze()p_if_change = torch.clamp(p_if_change, min=1e-20, max=1.0) # (B, D)
               \verb|total-noise = p_if\_change.sum(-1)# Continue (Gillespie option B) or check stopping criteria
               if allow_time_backwards:
                   pass
               else:
                    \mathtt{is\_time\_up} \ = \ \mathtt{(p\_if\_change \ <\,eps)\mathinner{.\,all}\,(-1)}if is_time_up.all():
                       break
               # Planning: get dimensions that change
               if use_softmax_for_dim_change: # Use softmax instead (Gillespie option C)
                    logits_dim_change = torch.logit(p_if_change.to(torch.float64), eps=1e-10)
                    dim_change = torch.multinomial(
                        torch.softmax(logits_dim_change, dim=-1), 1
                   ).squeeze() # (B,)
               else:
                    dim_change = torch.multinomial(p_if_change, 1).squeeze()
               # Compute time input from planner output
               time = 1.0 - total\_noise / D# Denoising: sample new values for the dimensions that change
               logits = model(samples, time)
               logits[:, :, mask\_token_id] = -1e4pt_x1_probs = F.softmax(logits, dim=-1) # (B, D, S+1)
               probs_change = pt_x1_probs[torch.arange(B), dim_change, :] # (B, S+1)
               probs_change[torch.arange(B), samples[torch.arange(B), dim_change]] = 0.0
               x1_values = torch.multinomial(probs_change, 1).squeeze() # (B,)
               samples[~is_time_up, dim_change[~is_time_up]] = x1_values[~is_time_up]
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1350 1351 1352 1353 Evaluation. We utilize the evaluation code from ADM $[11]$ to compute the FID scores $[19]$ and inception scores. For this evaluation, 50,000 images are generated across all classes. Each image is produced by first generating tokens, followed by decoding with the TiTok-S-128 decoder.

1354 1355 E ADDITIONAL RESULTS

1356 1357 E.1 TEXT8

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1358 E.1.1 EFFECT OF APPROXIMATION ERRORS IN DENOISER AND PLANNER

1359 1360 1361 We conducted experiments to measure the effect of approximation errors in denoiser and planner on the generation quality. Results are summarized in Figs. [4](#page-25-3) to [6.](#page-26-1)

1374 1375 1376 1377 Figure 4: Comparing DDPD sampling under imperfect learning: 1) a single uniform diffusion model as planner + denoiser v.s. 2) separately trained planner + mask denoiser. The single uniform diffusion model converge slower in training and using DDPD sampler results in collapse in sample entropy. Using separate networks for planner and denoiser achieves results more close to SOTA methods in terms of quality v.s. diversity.

1379 E.1.2 ABLATION OF CHANGES INTRODUCED IN DDPD SAMPLER

1381 1382 We conducted controlled experiment to measure the individual effect of the changes we introduced to the sampling process. Results are summarized in Fig. [7](#page-27-0)

1384 E.1.3 MODEL LOG-LIKELIHOODS ON TEST DATA

1385 Following ELBO terms derived in Appendix [C.1,](#page-20-1) we calculate them for three different design choices:

- A single uniform diffusion neural network, but decomposed into planner and denoiser.
- Separate planner network and uniform diffusion denoiser network
- Separate planner network and mask diffusion denoiser network

1391 1392 1393 1394 1395 In Table [4,](#page-27-1) we evaluate the ELBO terms for three methods both trained for 750k iterations (near optimality). We observe that the mask diffusoin denoiser has a better denonising performance even with mask approximation error introduced in the step of Proposition [3.5.](#page-6-1) In Table [5,](#page-27-2) We also observe mask diffusion denoiser performs better than uniform diffusion denoiser in terms the denoising log-likelihood.

1396 1397 E.2 CONVERGENCE OF SAMPLING

1398 1399 We conducted experiments to see the convergence of sampling with regards to number of steps. The results are shown in Fig. [8.](#page-28-3)

- **1400**
- **1401 1402** E.3 OPENWEBTEXT
- **1403** In Figs. [9](#page-29-0) and [10,](#page-29-1) we measure generative perplexity of unconditional samples from GPT-2 small, GPT-2-medium, SEDD-small, SEDD-medium, DDPD-Small: Planner-small + SEDD-

Figure 5: *Left*: Denoiser checkpoints at 450k v.s. 750k iterations. *Right*: Denoiser checkpoints at 150k, 300k, 450k, 600k, 750k iterations. DDPD is able to use an imperfect denoiser to achieve the same performance as the best possible.

Figure 6: More ablation studies on pairing an imperfect denoiser with an imperfect planner.

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1457 small-denoiser, DDPD-Medium: Planner-small + SEDD-small-denoiser. We also tested using sigmoid(logit_if_noise) and softmax(logit_if_noise) for planning. The difference is not as

1482 1483 1484 Figure 7: Ablation on introduced changes to discrete diffusion. A: Original Gillespie sampling. B: Timeadjustment based on the planner, continue sample until maximum number of steps is reached. C: Use softmax(logit_if_noise) instead of sigmoid(logit_if_noise) to pick which dimension to denoise next. The softmax trick makes the planning slightly more greedy than the original planning probability.

1488 1489 Table 4: ELBO terms computed on the test set of text8 in bits-per-character (BPC) with fully trained models. Denoising likelihood only evaluates the probability of correctly denoising, for Planer + Mask Diffusion Denoiser, a mask is first sampled according to the planner.

Method	Rate Matching Transitioning Combined (BPC)	(BPC)	(BPC)
Uniform Diffusion	≤ 0.0131	≤ 2.252	≤ 2.265
Planner + Uniform Diffusion Denoiser	≤ 0.0176	≤ 2.284	< 2.244
Planner + Mask Diffusion Denoiser (given correct mask for denoising)	≤ 0.0176	≤ 2.226	≤ 2.302
Planner + Mask Diffusion Denoiser (use planner-predicted mask for denoising)	≤ 0.0176	≤ 2.605	≤ 2.623

Table 5: Denoising performance in bits-per-character (BPC). Mask Denoiser v.s. Uniform Diffusion Denoiser. Note that those are not entirely comparable as ELBO terms for uniform diffusion and mask diffusion are different.

Method		Denoising (BPC) Denoising Accuracy at $\alpha_t = 0.85$
Uniform Diffusion Denoiser	≤ 2.063	92.2%
Mask Diffusion Denoiser	≤ 1.367	96.8%

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significant as in the text8 case. Using softmax($logit_if_inoise$) slightly increases entropy at the

Table 6: ELBO terms computed on the test set of text8 in bits-per-character (BPC) with imperfect models trained at 20k iterations.

Figure 8: Convergence of sampling along number of sampling steps: *Left Upper:* amount of noise left. *Right Upper:* amount of dimensions that are predicted to haved different z_t^i and z_{t-1}^i between t and t – 1. *Left Down:* how many samples meet the criteria of stopping to sample for $p_{\theta}(z_t^i = N) < 0.05$). *Right Down:* how many samples meet the criteria of stopping to sample for $p_{\theta}(z_t^i = N) < 0.01$.

expense of perplexity. In Fig. [11,](#page-30-2) we find that DDPD using Planner-Small and SEDD-Denoiser-Small outperforms simply scaling up denoiser to SEDD-Medium.

E.4 IMAGENET 256×256

Table 7: Inception Scores (†) on ImageNet 256 \times 256. MaskD refers to mask diffusion. The denoiser and parallel sampling schedule are kept the same as [\[45\]](#page-13-7), without classifier-free guidance.

	No Logit Annealing			Logit temp 0.6			Logit temp $1.0 \rightarrow 0.0$		
Steps T		MaskD MaskGIT DDPD MaskD MaskGIT DDPD MaskD MaskGIT DDPD							
8	33.56	199.83			149.98 149.28 271.73 201.67 157.19			249.86	213.03
16	39.36	248.88		178.17 179.85	281.73	173.48 164.01		263.47	185.25
32	43.30	266.17		169.49 200.33	281.36	156.22 170.73		268.88	158.14
64	45.06	274.56		160.74 206.06	281.14	146.27 171.62		269.45	145.95
128	45.56	276.45		152.61 210.27	278.88		138.55 142.40	272.73	137.19

 We study the effect of planned denoising with an increased number of refinement steps in Table [9.](#page-31-1) The FID first increases and then converges. The inception score also improves with increased refinement

Figure 9: Using softmax($logit_if_noise$) for planning. Generative perplexity evaluated with GPT-2 Large (GPT-2-L) and GPT-J: SEDD v.s. DDPD using the same denoiser.

1616 Figure 10: Using sigmoid($logit_if_nis$) for planning. Generative perplexity evaluated with GPT-2 Large (GPT-2-L) and GPT-J: SEDD v.s. DDPD using the same denoiser.

1619 steps and then converges. From the visualized samples, we can see that plan-and-denoise sampling is very effective at fixing errors without losing its original content.

Figure 11: DDPD SEDD-small denoiser (90M) + Planner-small (90M) v.s. SEDD medium denoiser (320M) v.s. GPT-2-Medium (355M). DDPD with a smaller (less perfect) denoiser achieve better performance than simply using a larger (better) denoiser.

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1658 E.4.1 EFFECT OF CLASSIFIER-FREE GUIDANCE

1659 1660 1661 1662 1663 1664 1665 We also studied the effect of applying classifier-free guidance in ?? for discrete mask diffusion. The effect of classifier-free guidance is similar to temperature annealing. In the case of no logit annealing, it helps mask diffusion to achieve much better FID score. DDPD achieves similar FID scores but much better Inception Scores (which means aesthetically higher quality). When logit temperature $= 0.6$, the inception score of Mask Diffusion is greatly improved, but the composition of logit annealing and classifier-free guidance leads to worse FID score due to less diversity. The same applies to MaskGIT.

1666 1667 1668 1669 1670 1671 1672 We note that the interaction of various sampling heuristics, particularly in configurations that incorporate logit annealing and classifier-free guidance (CFG), is intricate and nuanced. As detailed in Yu et al. [\[45\]](#page-13-7), the best FID scores for MaskGIT are achieved using additional hyperparameter adjustments, specifically inflating the logit and confidence temperatures to 3.0, which are then linearly annealed to 0.0. These unconventional settings are tailored to mitigate the loss of diversity typically caused by the combination of logit annealing and CFG. However, while this approach improves FID scores, it adversely impacts inception scores, underscoring a fundamental quality-diversity trade-off.

1673 To address this trade-off, Table [11](#page-32-0) presents results for MaskGIT with the same configurations as Yu et al. [\[45\]](#page-13-7), where sampling includes logit annealing and logit and confidence temperatures are

Figure 12: DDPD No Annealing, increasing number of refinement steps. The added refinement steps act as "touch-up" to improve the aesthetic quality without losing its original content.

Table 9: FID Scores on ImageNet 256×256 . Increasing the number of refinement steps.

 initialized at 3.0. Interestingly, the initial tokens sampled under these higher temperatures (which tend to introduce more errors) are later corrected during the annealing process, allowing the decoder to reconstruct coherent and high-quality outputs. These techniques are specifically optimized for mask

 Table 10: CFG scale 2.0, Logit Temp 1.0 or 0.6. MaskGIT anneals confidence noise temperature from 1.0 to 0.0. FID/Inception Scores (\downarrow / \uparrow) on ImageNet 256 × 256.

 diffusion with CFG, but do not generalize directly to DDPD, which operates using uniform diffusion. Following this insight, we applied the same configuration to DDPD as an experiment (Table [11\)](#page-32-0). While this approach improved inception scores, it worsened FID scores, further highlighting the quality-diversity trade-off. Upon analysis, we observed that the DDPD planner proactively identified some of the initially generated tokens (under high-temperature settings) as noisy, as they deviated significantly from the original distribution. These tokens were subsequently corrected in later denoising steps, leading to improved visual quality at the expense of reduced diversity. This behavior indicates that DDPD naturally balances quality and diversity differently from MaskGIT.

 Table 11: When using the same hyperparameters as in [1] (8 steps are not enough for DDPD to converge). FID / Inception Scores (\downarrow / \uparrow) .

 E.5 NOISE ESTIMATION ERROR USING INDEPENDENT NOISE OUTPUT $p_{\theta}(z_{t}^d | x_t)$

 We tested the assumption made in utilizing a pretrained mask diffusion denoiser by sampling joint noise latent variables using independent marginal prediction from a transformer for $p(z_t|x_t, z_t^d)$ $N) \approx \prod_{d' \neq d} p_{\theta}(z_i^{d'} | x_t)$ in Table [12.](#page-33-1) We observe that the assumption holds almost perfectly in language modeling such as OpenWebText. On character modeling task text8, the assumption also holds most of the time, especially near the end of generation, but it is more complicated than word tokens due to a much smaller vocabulary. This is also discovered in Table [4](#page-27-1) where we observe the two-step sampling introduces approximation errors and hence makes the log-likelihood for denoising lower.

 Table 12: Accuracy on Mask Prediction for text8 and OpenWebText at fixed times. Mask accuracy measures if the independent sampling matches the joint noise variable values. Almost deterministic measures the assumption $p(z_t^{\overline{d}}|x_t, z_t^d = N) \approx 1$. We set the threshold to be logit.abs() > 3.0.

Fixed Time	text8	OpenWebText			
		$t = 1 \rightarrow 0$ Mask Accuracy If Deterministic Mask Accuracy If Deterministic			
$(Data)$ 1.0	0.9988	0.9975	0.9999	0.9997	
0.95	0.9915	0.9864	0.9985	0.9960	
0.8	0.9623	0.9238	0.9943	0.9851	
0.6°	0.8784	0.6789	0.9847	0.9585	
0.4	0.7416	0.2261	0.9679	0.9100	
0.2	0.7402	0.2125	0.9476	0.8466	
0.05	0.8878	0.4800	0.9599	0.8817	
(Noise) 0.0	0.9465	0.5974	0.9975	0.9906	

1836 1837 F GENERATION EXAMPLES

1944 1945 F.2 GENERATED SAMPLES FROM MODELS TRAINED ON OPENWEBTEXT

In general, samples from DDPD demonstrate a better ability to capture word correlations, leading to greater coherence compared to those generated by SEDD. However, both methods exhibit less coherence in longer contexts when compared to samples from GPT-2 models.

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2256 F.3 GENERATED SAMPLES FROM MODELS TRAINED ON IMAGENET 256×256

2257 2258 In Figs. [13](#page-42-0) to [15,](#page-44-0) we visualize samples of DDPD, Mask Diffusion and MaskGIT.

2259 2260 2261 2262 Without logit temperature annealing, Mask Diffusion captures diversity, but the sample quality suffers due to imperfections in the denoiser. On the other hand, MaskGIT's confidence-based strategy significantly improves sample quality, but at the cost of reduced diversity. DDPD trades off diversity v.s. quality naturally without the need for any annealing or confidence-based tricks.

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(a) DDPD 32 steps (b) Mask Diffusion 32 steps (c) MaskGIT 32 steps

Figure 16: DDPD v.s. Mask Diffusion v.s. MaskGIT, No Logit Annealing

Figure 17: DDPD v.s. Mask Diffusion v.s. MaskGIT, Logit Annealing $1.0 \rightarrow 0.0$

(a) DDPD $16 + 16$ steps (b) DDPD $16 + 32$ steps

Figure 18: DDPD No Annealing, increasing number of refinement steps. The added refinement steps act as "touch-up" to improve the aesthetic quality without losing its original content.