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Fast Solvers for Discrete Diffusion Models:

Theory and Applications of High-Order Algorithms

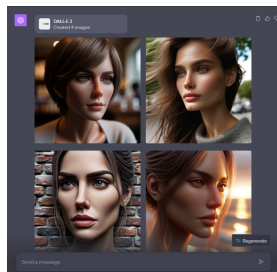
- 1 Discrete Diffusion Models (DMs): an Introduction and the Stochastic Integral Framework
- 2 High-Order Inference Algorithms for Discrete DMs: Formulation and Theory
- 3 Experiments: Toy Model, Text and Image Generation, Math Reasoning

Section 1:

Discrete Diffusion Models (DMs): an Introduction and the Stochastic Integral Framework

Diffusion Models

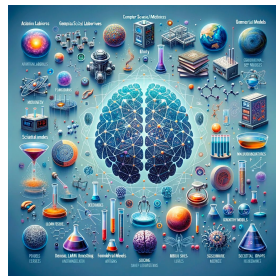
Introduction



(a) DALL-E 3



(b) Stable Diffusion



(c) AI4Science

Figure: Diffusion and flow-based generative models have exerted huge impacts on scientific research in many fields.

Problem Setting: Discrete Diffusion Models

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- **Forward Continuous Time Markov Chain (CTMC):**

$$\frac{d\mathbf{p}_t}{dt} = \mathbf{Q}_t \mathbf{p}_t, \text{ with } Q_t(x, x) = - \sum_{y \neq x} Q_t(y, x) \text{ and } Q_t(x, y) \geq 0 \ (x \neq y)$$

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- **Backward CTMC:**

$$\frac{d\tilde{\mathbf{p}}_s}{ds} = \bar{\mathbf{Q}}_s \tilde{\mathbf{p}}_s, \text{ with } \bar{Q}_s(y, x) = \begin{cases} \frac{\tilde{p}_s(y)}{\tilde{p}_s(x)} \tilde{Q}_s(x, y), & \forall x \neq y \in \mathbb{X}, \\ - \sum_{y' \neq x} \bar{Q}_s(y', x), & \forall x = y \in \mathbb{X}. \end{cases}$$

with $\mathbf{p}_0 = \mathbf{p}_T$ (commonly uniform or Dirac-delta over Δ) and $\tilde{\mathbf{p}}_T = \mathbf{p}_0$

Problem Setting: Discrete Diffusion Models

- **Score Function:** $s_t(x) = (s_t(x, y))_{y \in \mathbb{X}} = \frac{\mathbf{p}_t}{p_t(x)}$ by optimizing

$$\int_0^T \psi_t \mathbb{E}_{x_t \sim p_t} \left[\sum_{y \neq x} \left(-\log \frac{\hat{s}_t^\theta(x, y)}{s_t(x, y)} - 1 + \frac{\hat{s}_t^\theta(x, y)}{s_t(x, y)} \right) s_t(x, y) Q_t(x, y) \right] dt$$

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- **Implementations:**

- Approximate samplers like τ -leaping scheme [Gil01, CBDB⁺22], Euler sampler and Tweedie τ -leaping sampler [LME24]

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- › **Implementations:**

- › Approximate samplers like τ -leaping scheme [Gil01, CBDB⁺22], Euler sampler and Tweedie τ -leaping sampler [LME24]
- › Exact samplers like uniformization [VD92, CY24] and first-hitting sampler [ZCM⁺24]

Mathematical Preliminaries

Poisson Random Measure with Evolving Intensity

$(\Omega, \mathcal{F}, \mathcal{P})$: probability space

$(\mathbb{X}, \mathcal{B}, \nu)$: measure space

$\lambda_t(y)$: a non-negative predictable process on $\mathbb{R}^+ \times \mathbb{X} \times \Omega$ satisfying

$$\int_0^T \int_{\mathbb{X}} 1 \vee |y| \vee |y|^2 \lambda_t(y) \nu(dy) dt < \infty, \text{ a.s..}$$

for any $T > 0$, The random measure $N[\lambda](dt, dy)$ on $\mathbb{R}^+ \times \mathbb{X}$ is called a *Poisson random measure with evolving intensity* $\lambda_t(y)$ if

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- 1 For any $B \in \mathcal{B}$ and $0 \leq s < t$, $N[\lambda]((s, t] \times B) \sim \mathcal{P} \left(\int_s^t \int_B \lambda_\tau(y) \nu(dy) d\tau \right)$;

Interpretation: the number of jumps of magnitude y during the infinitesimal time interval $(t, t + dt]$ is Poisson distributed with mean $\lambda_t(y) \gamma(dy) dt$.

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Interpretation: the number of jumps of magnitude y during the infinitesimal time interval $(t, t + dt]$ is Poisson distributed with mean $\lambda_t(\nu) \gamma(d\nu) dt$.

- 2 For any $t \geq 0$ and disjoint sets $\{B_i\}_{i \in [n]} \subset \mathcal{B}$, $\{N_t[\lambda](B_i) := N[\lambda]((0, t] \times B_i)\}_{i \in [n]}$ are independent stochastic processes.

Stochastic Integral Formulation: True Processes

Forward Process:

$$x_t = x_0 + \int_0^t \int_{\mathbb{D}} \nu N[\lambda](ds, d\nu),$$

where $\mathbb{D}$ is the set of all possible jumps and the intensity function

$$\lambda_t(\nu, \omega) = Q_t^0(x_{t-}(\omega) + \nu, x_{t-}(\omega))$$

if $x_{t-}(\omega) + \nu \in \mathbb{X}$ and 0 otherwise.

True Backward Process ($\tilde{s}_t$ denotes the true score):

$$y_s = y_0 + \int_0^s \int_{\mathbb{D}} \nu N[\mu](ds, d\nu),$$

where the intensity function

$$\mu_\rho(\nu) = \tilde{s}_\rho(y_{\rho-}, y_{\rho-} + \nu) \tilde{Q}_\rho^0(y_{\rho-}, y_{\rho-} + \nu)$$

if $y_{s-} + \nu \in \mathbb{X}$ and 0 otherwise.

Stochastic Integral Formulation: τ -Leaping Scheme

τ -leaping inference scheme (Euler):

$$\hat{y}_{t+\Delta} = \hat{y}_t + \sum_{\nu \in \mathbb{D}} \nu \mathcal{P}(\hat{\mu}_t(\nu) \Delta)$$

with Δ being the time step and the estimated intensity function

$$\hat{\mu}_\rho(\nu) = \hat{s}_\rho^\theta(\hat{y}_{\rho-}, \hat{y}_{\rho-} + \nu) \tilde{Q}_\rho^0(\hat{y}_{\rho-}, \hat{y}_{\rho-} + \nu)$$

Stochastic Integral formulation (equivalent to τ -leaping):

$$\hat{y}_{t+\Delta} = \hat{y}_t + \int_t^{t+\Delta} \int_{\mathbb{D}} \nu N[\hat{\mu}](ds, d\nu)$$

Error bound of τ -leaping [RCRY24]

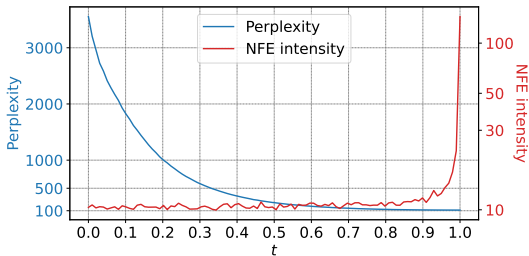
$$D_{\text{KL}}(p_0 \| \hat{q}_T) \lesssim \underbrace{\exp(-T)}_{\text{truncation error}} + \underbrace{\epsilon}_{\text{score estimation error}} + \boxed{\underbrace{\kappa T}_{\text{numerical error}}}$$

Section 2:

High-Order Inference Algorithms for Discrete DMs: Formulation and Theory

Motivation: Redundancy of Exact Samplers

Discrete diffusion models with uniformization for text generation:



- x -axis: time of the backward process; y -axis: frequency of jumps (NFE).
- Perplexity convergence occurs before the NFE grows unbounded!

Methodology: High-Order Numerical Solvers

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$$\hat{x}_{t+\theta\Delta}^* = \hat{x}_t + f_t(\hat{x}_t)\theta\Delta$$

$$\hat{x}_{t+\Delta} = \hat{x}_t + \left[\left(1 - \frac{1}{2\theta}\right) f_t(\hat{x}_t) + \frac{1}{2\theta} f_{t+\theta\Delta}(\hat{x}_{t+\theta\Delta}^*) \right] \Delta.$$

where $\theta \in (0, 1)$.

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where $\theta \in (0, 1)$.

- Notations: *time discretization scheme* $(s_i)_{i \in [0:N]}$ and *θ -section points* $(\rho_n)_{n \in [0:N]}$ are denoted by

$$0 = s_0 < s_1 < \cdots < s_N = T - \delta, \quad \rho_n = (1 - \theta)s_n + \theta s_{n+1}$$

Take $\alpha_1 = \frac{1}{2\theta(1-\theta)}$ and $\alpha_2 = \frac{(1-\theta)^2 + \theta^2}{2\theta(1-\theta)}$ with $\alpha_1 - \alpha_2 = 1$

Methodology: High-Order Numerical Solvers

- **θ -RK-2 Method:** Interpolation between s_n and ρ_n

$$\hat{y}_{\rho_n}^* \leftarrow \hat{y}_{s_n} + \sum_{\nu \in \mathbb{D}} \nu \mathcal{P}(\hat{\mu}_{s_n}(\nu) \theta \Delta_n),$$

$$\hat{y}_{s_{n+1}} \leftarrow \hat{y}_{s_n} + \sum_{\nu \in \mathbb{D}} \nu \mathcal{P}\left(\mathbf{1}_{\hat{\mu}_{s_n} > 0} \left[\left(1 - \frac{1}{2\theta}\right) \hat{\mu}_{s_n} + \frac{1}{2\theta} \hat{\mu}_{\rho_n}^*\right]_+ (\nu) \Delta_n\right).$$

Analogy: SDE [BB96], continuous diffusion model [KAAL22, WCW24] and chemical reaction [BT04]

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- **θ -Trapezoidal Method:** Extrapolation beyond s_n and ρ_n

$$\hat{y}_{\rho_n}^* \leftarrow \hat{y}_{s_n} + \sum_{\nu \in \mathbb{D}} \nu \mathcal{P}(\hat{\mu}_{s_n}(\nu) \theta \Delta_n),$$

$$\hat{y}_{s_{n+1}} \leftarrow \hat{y}_{\rho_n}^* + \sum_{\nu \in \mathbb{D}} \nu \mathcal{P} \left(\left(\alpha_1 \hat{\mu}_{\rho_n}^* - \alpha_2 \hat{\mu}_{s_n} \right)_+ (\nu) (1 - \theta) \Delta_n \right).$$

Analogy: SDE [AM11] and chemical reaction [HLM11]

Theoretical Analysis: Assumptions

- **Exponential convergence of the forward process:**
 $D_{\text{KL}}(p_T \| p_\infty) \lesssim \exp(-T).$
- **Regularity of intensity:** Both the true intensity μ_s and the estimated intensity $\hat{\mu}_s$ are in $\mathcal{C}^2$ and bounded for any $s \in [0, T - \delta]$.
- **Score estimation error:** The following error bounds hold for any grid point or θ -section point $s \in \cup_{n=0}^{N-1} \{s_n, \rho_n\}$:

$$\mathbb{E} \left[\sum_{\nu \in \mathbb{D}} \left(\mu_s(\nu) \left(\log \frac{\mu_s(\nu)}{\hat{\mu}_s(\nu)} - 1 \right) + \hat{\mu}_s(\nu) \right) \right] \leq \epsilon_{\text{I}},$$

$$\mathbb{E} \left[\sum_{\nu \in \mathbb{D}} |\mu_s(\nu) - \hat{\mu}_s(\nu)| \right] \leq \epsilon_{\text{II}}.$$

Theoretical Analysis: Informal Bounds

- **θ -RK-2 Method:** Suppose $\theta \in (0, \frac{1}{2}]$ and $(1 - \frac{1}{2\theta})\hat{\mu}_{[s]} + \frac{1}{2\theta}\hat{\mu}_{\rho_s}^* \geq 0$, then

$$D_{\text{KL}}(p_0 \| \hat{q}_T^{\text{RK}}) \lesssim \exp(-T) + (\epsilon_{\text{I}} + \epsilon_{\text{II}})T + \boxed{\kappa^2 T}$$

- **θ -Trapezoidal Method:** Suppose $\theta \in (0, 1]$ and $\alpha_1 \hat{\mu}_{\rho_s}^* - \alpha_2 \hat{\mu}_{[s]} \geq 0$, then

$$D_{\text{KL}}(p_0 \| \hat{q}_T^{\text{trap}}) \lesssim \exp(-T) + (\epsilon_{\text{I}} + \epsilon_{\text{II}})T + \boxed{\kappa^2 T}$$

Theoretical Analysis: Informal Bounds

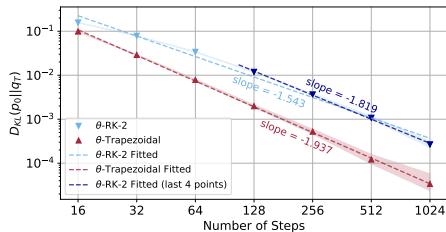
- **Proof Technique:** Change of measure [RCRY24] between stochastic integral with respect to *Poisson random measures*, error decomposition, and the usage of *Dynkin's Formula*;
- **Second-Order Numerical Error Guarantee:** $\mathcal{O}(\kappa^2 T)$ for both θ -RK-2 and θ -Trapezoidal methods vs. $\mathcal{O}(\kappa T)$ for τ -leaping method;
- **Range of θ :** $\theta \in (0, 1/2]$ for RK-2 method and $\theta \in (0, 1]$ for trapezoidal method, which is caused by application of *Jensen's Inequality*.

Section 3:

Experiments: Toy Model,
Text and Image Generation,
Math Reasoning

Experiment: Toy Model

Data: synthetic discrete distribution with $S = 15$ states, dimension $d = 1$



The figure above plots empirical KL divergence between the true and generated distribution of the toy model versus the number of steps. Data are fitted with linear regression with 95% confidence interval by bootstrapping.

Experiment: Text Generation

Data: OpenWebText dataset [GC19], number of states $S = 50258$, dimension $d = 1024$;

Model: RADD [ONX⁺24] (pretrained score of a masked discrete DM, GPT2-level)

Table: Generative perplexity of texts generated by different sampling algorithms on GPT-2 large. Lower values are better, with the best in **bold**.

Method	NFE = 16	NFE = 32	NFE = 64	NFE = 128	NFE = 256	NFE = 512	NFE = 1024
FHS	≤ 307.425	≤ 186.594	≤ 141.625	≤ 122.732	≤ 113.310	≤ 113.026	≤ 109.406
Euler	≤ 277.962	≤ 160.586	≤ 111.597	≤ 86.276	≤ 68.092	≤ 55.622	≤ 44.686
Tweedie τ -leaping	≤ 277.133	≤ 160.248	≤ 110.848	≤ 85.738	≤ 70.102	≤ 55.194	≤ 44.257
τ -leaping	≤ 126.835	≤ 96.321	≤ 69.226	≤ 52.366	≤ 41.694	≤ 33.789	≤ 28.797
Semi-AR	≤ 2857.469	≤ 1543.302	≤ 741.184	≤ 360.793	≤ 222.303	≤ 164.162	≤ 147.406
θ -RK-2	≤ 127.363	≤ 109.351	≤ 86.102	≤ 64.317	≤ 49.816	≤ 40.375	≤ 33.971
θ -Trapezoidal	$\leq \mathbf{123.585}$	$\leq \mathbf{89.912}$	$\leq \mathbf{66.549}$	$\leq \mathbf{49.051}$	$\leq \mathbf{39.959}$	$\leq \mathbf{32.456}$	$\leq \mathbf{27.553}$

Experiment: Text Generation

Table: Generative perplexity of texts generated by different sampling algorithms on LLaMA 3. Lower values are better, with the best in **bold**.

Method	NFE = 16	NFE = 32	NFE = 64	NFE = 128	NFE = 256	NFE = 512	NFE = 1024
FHS	≤ 342.498	≤ 210.742	≤ 155.258	≤ 132.135	≤ 127.526	≤ 123.013	≤ 120.791
Euler	≤ 318.413	≤ 175.555	≤ 125.955	≤ 91.051	≤ 75.245	≤ 59.971	≤ 49.406
Tweedie τ -leaping	≤ 316.744	≤ 172.941	≤ 121.248	≤ 94.253	≤ 75.403	≤ 59.943	≤ 49.239
τ -leaping	≤ 152.867	≤ 117.930	≤ 86.980	≤ 68.090	$\leq \mathbf{53.664}$	≤ 44.676	≤ 38.293
Semi-AR	≤ 2696.883	≤ 1684.973	≤ 829.391	≤ 410.177	≤ 251.963	≤ 166.927	≤ 162.093
θ -RK-2	≤ 150.439	≤ 132.090	≤ 107.066	≤ 80.742	≤ 63.277	≤ 52.563	≤ 44.687
θ -Trapezoidal	$\leq \mathbf{146.027}$	$\leq \mathbf{113.260}$	$\leq \mathbf{83.456}$	$\leq \mathbf{66.071}$	≤ 54.307	$\leq \mathbf{44.293}$	$\leq \mathbf{35.524}$

Experiment: Image Generation

Data: ImageNet [DDS⁺09], number of states $S = 1025$, dimension $d = 256$, (VQ-GAN based tokenization)

Model: MaskGIT [CZJ⁺22]

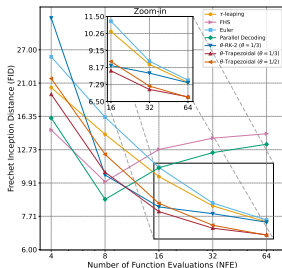


Figure: FID of images generated vs. NFEs with different parameter choices.

Experiment: Image Generation

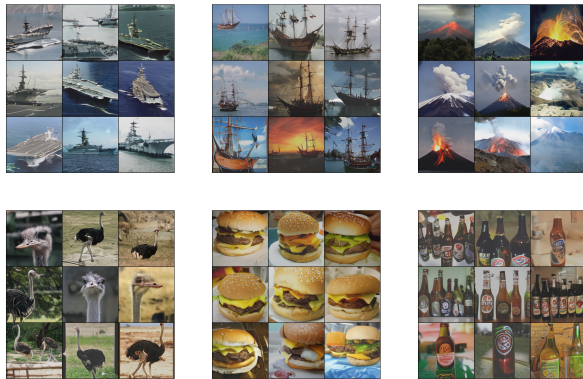


Figure: Visualization of samples generated by θ -Trapezoidal. **Upper Left:** Aircraft carrier (ImageNet-1k class: 933); **Upper Middle:** Pirate; **Upper Right:** Volcano ; **Lower Left:** Ostrich; **Lower Middle:** Cheeseburger ; **Lower Right:** Beer bottle

Experiment: Math Reasoning

Data: GSM8K dataset [CKB⁺21]

Model: Large Language Diffusion Model (LLaDA)-Instruct8B [NZY⁺25]

Table: Response accuracy on GSM8K with different NFEs.

Accuracy (%)	NFE = 64	NFE = 128	NFE = 256
Semi-AR (Conf.)	33.6	32.0	39.1
Semi-AR (Rand.)	33.8	34.3	40.3
θ -Trapezoidal	35.1	38.4	39.7

Thank you for your attention!

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