Google DeepMind

# Simplified and Generalized Masked Diffusion for Discrete Data







in Shi

Kehang Han



Zhe Wang



Arnaud Doucet



Michalis K. Titsias

# Why Diffusion Models for Discrete Data

• Generating discrete data with parallel sampling



# Why Diffusion Models for Discrete Data

• AR models require imposing an ordering which may be unnatural for many data types



HGFGTLEHPIYKVAKQWSMVHDTTVYFSCGLHVAAHPATYVSMQAWKSTNDFPCRQHDNI TMLYHINMESFVNLEFCNFQTDDKYLEDPWARHEKYPIRKAIKWEGLPNMQRLHMLHWIN VSMDPNHGPVYCAKWDTILYMGKDGKERRTSAYMFTGVDEQHCRYEYRKFCGKHKAPKLM GRLFRITKSCWWGCCTLDNMKPDKAKACAEDMRRCRNIPVVQNFQQCGKYWKATSQDNTK RNSKCRAIEWEIFQYWINCSTVVKTFAPCMFGFQFRFHYGYNYMFWVTIKLSVYRWMPGV DRETPVHAVNIINIWSAYKMTRYWCRIQCDSYWLWSGMTWRWCRWNREQPEWLSHDDMVQ CWEGSYKLMFCGWWRHFISKSMVTLGGHKKDDGRRWMLQSTHHLHFPATINIHDDWFPHG





# Challenge

#### Diffusion yet to match AR performance on discrete data



Gulrajani & Hashimoto (2024). Likelihood-based diffusion language models.



# Masked Diffusion Models data mask data $\begin{cases} \text{w/ prob.} \frac{\alpha_s - \alpha_t}{1 - \alpha_t} p(x_0 = j | x_t), \text{ unmask to state } j \\ \text{w/ prob.} \frac{1 - \alpha_s}{1 - \alpha_t}, \text{ remain masked} \end{cases}$ time 0

## MD4 Objective: Weighted Cross-Entropy Losses

Continuous-time Negative ELBO  $(T \rightarrow \infty)$ 

$$\mathscr{L}_{\infty} = \int_{0}^{1} \frac{\alpha_{t}'}{1 - \alpha_{t}} \mathbb{E}_{q(x_{t}|x_{0})} [\delta_{x_{t},m} \cdot x_{0}^{\mathsf{T}} \log \mu_{\theta}(x_{t},t)] dt$$



#### Perplexity on GPT-2 Zero-Shot Eval

Size	Method	LAMBADA	WikiText2	PTB	WikiText103	IBW
Small	GPT-2 (WebText)*	45.04	42.43	138.43	41.60	75.20
	D3PM	$\leq 93.47$	$\leq 77.28$	$\leq 200.82$	$\leq$ 75.16	$\leq$ 138.92
	Plaid	$\leq 57.28$	$\leq 51.80$	$\leq 142.60$	$\leq 50.86$	$\leq$ 91.12
	SEDD Absorb	$\leq 50.92$	$\leq 41.84$	$\leq 114.24$	$\leq 40.62$	$\leq$ 79.29
	SEDD Absorb (reimpl.)	$\leq$ 49.73	$\leq$ 38.94	$\leq 107.54$	$\leq$ 39.15	$\leq$ 72.96
	MD4 (Ours)	$\leq$ 48.43	$\leq$ 34.94	$\leq$ 102.26	$\leq$ 35.90	$\leq$ 68.10
Medium	GPT-2 (WebText)*	35.66	31.80	123.14	31.39	55.72
	SEDD Absorb	$\leq$ 42.77	$\leq 31.04$	$\leq 87.12$	$\leq 29.98$	$\leq 61.19$
	MD4 (Ours)	$\leq$ 44.12	$\leq$ 25.84	$\leq$ 66.07	$\leq$ 25.84	<i>≤</i> <b>51.45</b>

# Pixel-level Image Modeling

CIFAR-10



ImageNet 64x64

# Sampling



- The masking schedule controls the the quantity of simultaneously predicted tokens.
- The cosine schedule that gradually increases parallel predictions works best.

### **Concurrent Work**

#### Simple and Effective Masked Diffusion Language Models

#### Your Absorbing Discrete Diffusion Secretly Models the Conditional Distributions of Clean Data

Subham Sekhar Sahoo Cornell Tech, NYC, USA. ssahoo@cs.cornell.edu Marianne Arriola Cornell Tech, NYC, USA. ma2238@cornell.edu

Aaron Gokaslan Cornell Tech, NYC, USA. akg87@cs.cornell.edu

Edgar Marroquin Cornell Tech, NYC, USA. emm392@cornell.edu Justin T Chiu Cornell Tech, NYC, USA. jtc257@cornell.edu

Yair Schiff

Cornell Tech, NYC, USA

yzs2@cornell.edu

Alexander Rush Cornell Tech, NYC, USA. ar459@cornell.edu Volodymyr Kuleshov Cornell Tech, NYC, USA. kuleshov@cornell.edu Jingyang Ou<sup>1</sup> Shen Nie<sup>1</sup> Kaiwen Xue<sup>1</sup> Fengqi Zhu<sup>1</sup> Jiacheng Sun<sup>2</sup> Zhenguo Li<sup>2</sup> Chongxuan Li<sup>1\*</sup> <sup>1</sup>Gaoling School of Artificial Intelligence, Renmin University of China <sup>2</sup> Huawei Noah's Ark Lab {oujingyang, nieshen,kaiwenxue,chongxuanli}@ruc.edu.cn; fengqizhu@whu.edu.cn;{sunjiacheng1,li.zhenguo}@huawei.com;

## Thanks



ImageNet 64x64 unconditional generation

Conditional text generation

skydiving is a fun sport, but it's extremely risky. You can have so many injuries one time and then one next time. There are so many ways you can hurt, so, neuroconcussions, especially from Skydiving, are continuing to rise every year Though antibacterial products are a poison, the skin needs a chemical solution that protects it from bacteria and spots that form within it that is why I always shampoo twice a day and shower three times a day.