Constraint Guided Discrete Diffusion Models for CSPs

Justin Jung and Tim Hanson

Abstract

Discrete diffusion models have recently become competitive generative models for text and discrete sequences, rivaling the transformer architecture. We introduce *DDCPS* (Discrete Diffusion for Constraint Satisfaction Problems), applying these models to Sudoku puzzles. By incorporating constraint guidance, analogous to classifier guidance, we enhance diffusion model output. While further improvements are required, our experimental results demonstrate the potential of discrete diffusion models in the constraint satisfaction domain.

Keywords: Constraint satisfaction, discrete diffusion model, classifier guidance

Methods

We employ the Masked Language Model variant of discrete diffusion models (Austin et al.):

1. Forward process: corrupt a discrete sequence $w_0 \to w_T$ using an absorbing transition matrix (defines probability of transitioning to [MASK] token)
2. Reverse process: Learn $w_T \to w_0$ through parameterized denoiser $p_\theta(\hat{w}_0|w_t, t)$

The learning objective is the following log likelihood objective

$$L(\theta) = \mathbb{E}_{w_0,t}\left[-\log p_\theta(w_0|w_t)\right], \; w_t \sim p(w_t|w_0) \tag{2}$$

To generate a sample, iterative apply the learned denoiser to a completely noised sequence w_T.

$$p_\theta(w_{t-1}|w_t) = \sum_{\hat{w}_0} p(w_{t-1}|w_t, \hat{w}_0) p_\theta(\hat{w}_0|w_t, t) \tag{3}$$

with $p(w_{t-1}|w_t, w_0)$ defined by Bayes' rule.

Introduction

- Constraint satisfaction problems (CSPs) such as Sudoku are widely regarded by the symbolic and neuro-symbolic community
- Deep neural networks have been applied to Sudoku, notably Recurrent Transformers (Yang et al. 2023) and Recurrent Relational Networks (Palm et al., 2018)
- Discrete diffusion models have shown promising results on textual texts, outperforming comparably sized GPT-2
- We apply discrete diffusion models to CSPs and add a form of classifier guidance, namely constraint guidance, to improve model output for the CSP setting

Results

Model	Easy SatNet
DDSCP w/o guidance	85.2%
DDSP w/ guidance	90.6%
SEDD w/o guidance	99.2%
RRN (Palm)	100%
Recurrent Transformer (Yang)	100%

With the results we see that discrete diffusion models have yet to outperform other networks, such as the transformer. However, the recent score entropy discrete diffusion models (SEDD) which have rivaled GPT-2 on textual tasks seem to show great promise. Though masked language discrete diffusion models struggle, we see that by adding constraint guidance, model performance improves. We hope this encourages future work in adding classifier guidance to models such as SEDD.

Methods (Guided Sampling)

Our method adapts the MLM diffusion model and adds guidance. It is most similar to (Gruver et al.) which apply MLM to protein sequences. However unlike (Gruver et al.) we do not train the value function on diffusion model logits and instead on real data sequences.

Our constraint value function $v_\theta(w)$ is trained on one-hot encodings of discrete sudoku board sequences w. Similar to (Gruver et al.), we use the langevin-dynamics inspired update step

$$h'_t \leftarrow h'_t - \eta \nabla_{h'_t}[\lambda \mathrm{KL}(p_\theta(\hat{w}|h'_t) || p_\theta(\hat{w}|h_t)) - v_\theta(h'_t)], \tag{1}$$

where h_t is the original diffusion logits and h'_t is the guided perturbed logits.
We trade off moving towards regions of higher value and staying close to the diffusion data distribution.

To calculate the gradient of $v_\theta(\cdot)$, we use the gumbel-max trick to generate categorical discrete samples from logits, $w \sim gum(h'_t)$ while allowing for gradient calculation.

We apply multiple $K = 25$ langevin-dynamics update steps for each diffusion reverse step to allow for more stable gradient guidance.

Algorithm 1: Guided Discrete Diffusion Sampling

Input: Denoiser $p_\theta(\hat{w}|x_t, t) = [T_\theta, H_\theta]$, constraint function v_θ, noise schedule noising $q(w_t, t)$
Output: Generated discrete sample w_0

```
w_T ← [MASK]^L ;
/* diffusion sampling steps */
for t = T, ..., 1 do
    h^0 ← T_θ(w_t) ;
    /* guidance sampling steps */
    for i = 0, ..., K − 1 do
        h^{i+1} ← h^i + ∇_h v_θ(gum(h^i)) + λ∇_h KL(π(H_θ(h_0)) || π(H_θ(h^i)))
    end
    w_{t−1} ∼ H_θ(h^K)
    /* renoise according to noise schedule */
    w_{t−1} = q(w_{t−1}, t − 1)
end
/* returns sampled discrete sequence */
return w_0
```

Optionally we also consider the returning the perturbed h_t* of maximal value $v_\theta(Gum(h_t*))$.

Conclusion

Though highly constrained CSPs like Sudoku may seem difficult for generative models, we show that discrete diffusion models are able to perform reasonably well, albeit still requiring improvement to rival the performance of autoregressive transformers.

5	3	4	6	7	8	9	1	2
6	7	2	1	9	5	3	4	8
1	9	8	3	4	2	5	6	7
8	5	9	7	6	1	4	2	3
4	2	6	8	5	3	7	9	1
7	1	3	9	2	4	8	5	6
9	6	1	5	3	7	2	8	4
2	8	7	4	1	9	6	3	5
3	4	5	2	8	6	1	7	9

In summary:

- Discrete diffusion models show promise on CSP settings such as Sudoku
- Constraint guidance improves discrete diffusion model output
- SEDD outperforms MLM discrete diffusion
- However, discrete diffusion fails to outperform against transformers
- Opens up further research on constraint guidance for discrete diffusion models

References

[1] Nate Gruver et al. Protein design with guided discrete diffusion, 2023.

[2] Aaron Lou et al. Discrete diffusion modeling by estimating the ratios of the data distribution, 2024.

Future Research

Future directions include: applying constraint guidance to Score Entropy Discrete Diffusion (SEDD); investigating other notions of guidance (e.g classifier-free guidance); more rigorous experimentation on various CSP benchmarks

Contact Information

Web https://www.springtail.ai/
Author Email justin,tim@springtail.ai
Organization Email info@springtail.ai