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Improving Generative Flow Networks with Path Regularization

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Outline

- Introduction
- Background: GFlowNets & Optimal Transport Distance
- Method: Path Regularization via Optimal Transport
- Experiment
- Conclusion

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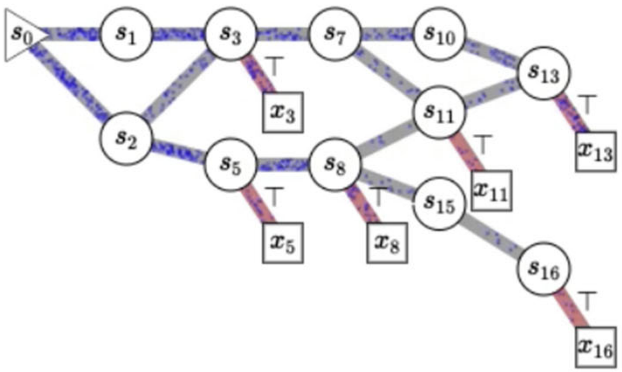
Introduction

➢ **Generative Flow Networks** (GFlowNets) are recently proposed models for learning stochastic policies that generate **compositional objects** by sequences of actions with the probability proportional to a given reward function.

➢ The central problems of GFlowNets are how to improve **exploration** and **generalization.**

➢ In this paper, we propose to train the GFlowNets with an additional **path regularization** via OT to deal with above problems.



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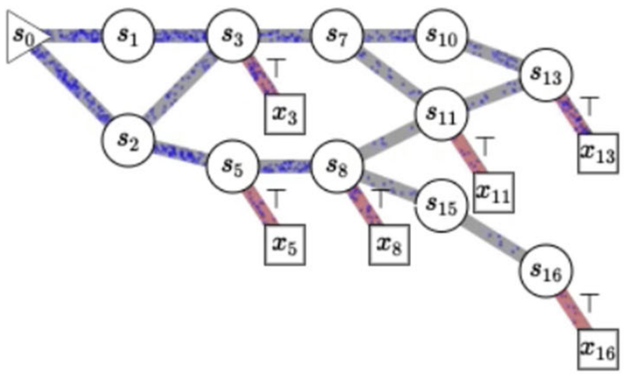
Background

- **GFlowNets: some basic concepts**
  - **Compositional Space *X***, where each object $x \in X$ can be constructed from the source state s_0 and ends in the final state s_f by taking a sequence of discrete actions from the action space A (e.g. a molecule can generated fragment by fragment).



A directed acyclic graph G

node -> state

edge -> action

  - A **complete trajectory τ**, which is a sequence of transitions from s_0 to s_f.

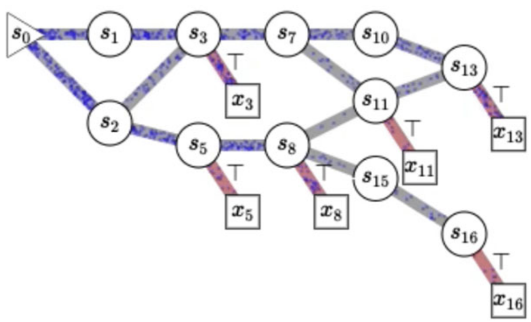
$$\tau = (s_0 \to s_1 \to \ldots \to s_n = x \to s_f)$$

* Bengio E, Jain M, Korablyov M, et al. Flow network based generative models for non-iterative diverse candidate generation[J]. Advances in Neural Information Processing Systems, 2021, 34: 27381-27394.

Background

GFlowNets: Flows

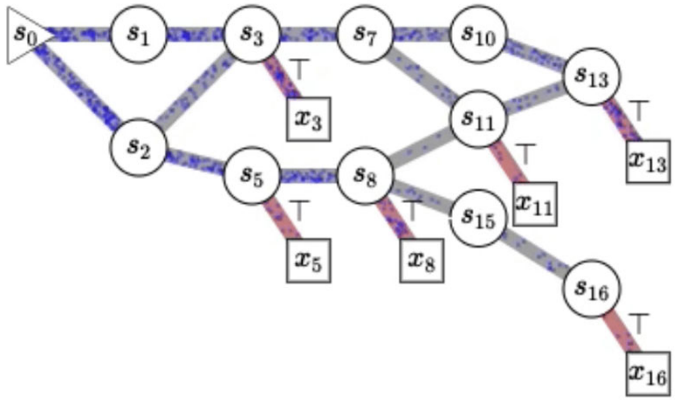
- A **trajectory flow** is a nonnegative function, which represents the probability mass of each complete trajectory τ
- The flow through each state: $F(s) = \sum_{\tau \in \mathcal{T}, s \in \tau} F(\tau)$
- The flow through each edge: $F(s \to s') = \sum_{\tau \in \mathcal{T}, s \to s' \in \tau} F(\tau)$
- The forward transition probabilities(forward policy): $P_F(s'|s) := F(s \to s')/F(s)$
- The backward transition probabilities (backward policy): $P_B(s|s') := F(s \to s')/F(s')$



Background

■ GFlowNets: Learning Objective

- ➢ A GFlowNet can perfectly generate objects proportional to their rewards.
- ➢ In other words, the probability from the source state s_0 to the final state s_f is proportional to the given reward.



Background

■ Optimal Transport Distance

For two discrete probability measures α and β over some space X

- The set of **transportation plans** or **joint probability distributions** can be defined as:

$$\Pi(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \left\{\pi \in \mathbb{R}_+^{k \times l} : \pi \mathbb{1}_l = \boldsymbol{\alpha}, \pi^\top \mathbb{1}_k = \boldsymbol{\beta}\right\}$$

- The Kantorovich **optimal transport** between α and β is defined as follows:

$$\mathrm{OT}_{\mathbf{C}}(\boldsymbol{\alpha}, \boldsymbol{\beta}) := \min_{\pi \in \Pi(\boldsymbol{\alpha}, \boldsymbol{\beta})} \langle \mathbf{C}, \pi \rangle$$

where C is given cost matrix

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Method

Discrete distance -> OT distance -> Path Regularization

■ Directed distance in the GFlowNet

- We define a new **directed distance** between two arbitrary states in the GFlowNet, which is used as **transportation cost** to compute OT distance.
- Note: the directed distance from a state s to another state s' is designed to be **inversely proportional** to the probability of going from s to s'
- Let τ = (s = s0 → s1 → ... → sn = s′) be the sequence of transitions from s to s′ where $s_t \rightarrow s_{t+1}$ can be a **forward or backward transition** (i.e., the given DAG can be considered an undirected connected graph), the **directed distance** from s to s' is defined as follows:

$$d(s, s') := \min_{\tau=(s\rightarrow\ldots\rightarrow s')} \boxed{-\log(P(\tau \mid s))}$$

i.e., the shortest path from s to s′

The length of the trajectory τ

Method

Discrete distance -> OT distance -> Path Regularization

■ Optimal transport formulation of the path regularization

Give **two neighbor states** s and s′ in trajectory τ , **the forward policy** $P_F(\cdot|\mathrm{s})$ is a discrete probability measure supported by Child(s) = $\{u_1, \ldots, u_k\}$ and $P_F(\cdot|\mathrm{s}')$ is a discrete probability measure supported by Child(s′) = $\{v_1, \ldots, v_l\}$.

➢ The **OT distance** between $P_F(\cdot|\mathrm{s})$ and $P_F(\cdot|\mathrm{s}')$ can be defined as:

$$\mathrm{OT}_{\mathbf{C}}\left(P_F(\cdot|s), P_F(\cdot|s')\right) := \min_{\pi \in \prod(P_F(\cdot|s), P_F(\cdot|s'))} \langle \mathbf{C}, \pi \rangle$$

$$\Pi(P_F(\cdot|s), P_F(\cdot|s')) := \{\pi \in \mathbb{R}_+^{k \times l} : \pi \mathbb{1}_l = P_F(\cdot|s), \pi^\top \mathbb{1}_k = P_F(\cdot|s')\}$$

$$\mathbf{C}_{ij} = c(u_i, v_j) := d(u_i, v_j) = \min_{\tau=(u_i \to \ldots \to v_j)} -\log(P(\tau \mid u_i))$$

➢ The cost matrix C can be calculated in practice by approximating as follows:

$$\begin{tikzcd} s \arrow[r] \arrow[d] & s' \arrow[d] \\ u_i \arrow[r] & v_j \end{tikzcd}$$

$$\mathbf{C}_{ij} = \begin{cases} 0, & \text{if} \quad u_i \equiv v_j \\ \min\left(-\log(P_B(s \mid u_i) P_F(s' \mid s) P_F(v_j \mid s')), -\log(P(v_j \mid u_i))\right), & \text{else if} \quad u_i \to v_j \in \mathcal{A} \\ -\log(P_B(s \mid u_i) P_F(s' \mid s) P_F(v_j \mid s')), & \text{otherwise.} \end{cases}$$

Method

Discrete distance -> OT distance -> Path Regularization

■ Optimal transport formulation of the path regularization

Give **two neighbor states** s and s′ in trajectory τ , **the forward policy** $P_F(\cdot|s)$ is a discrete probability measure supported by Child(s) = $\{u_1, \ldots, u_k\}$ and $P_F(\cdot|s')$ is a discrete probability measure supported by Child(s′) = $\{v_1, \ldots, v_l\}$.

- For any complete trajectory τ , we define the path regularization via OT as follows:

$$\mathcal{L}_{OT}(\tau) := \sum_{t=0}^{n-1} OT_{\mathbf{C}_{t;\theta}}\left(P_F(\cdot|s_t;\theta), P_F(\cdot|s_{t+1};\theta)\right)$$

- If π_θ is the training policy, then **the trajectory loss** is updated:

$$\mathbb{E}_{\tau\sim\pi_\theta}\nabla_\theta(\mathcal{L}_{\mathrm{TB}}(\tau)+\lambda\mathcal{L}_{\mathrm{OT}}(\tau))$$

where λ ∈ R, λ > 0 indicates that we want to **minimize** the path regularization to to improve the generalization and , λ < 0 indicates that we want to **maximize** the path regularization to generate more diverse and novel candidates.

Method

Discrete distance -> OT distance -> Path Regularization

■ Upper bound of optimal transport distance

- Our path regularization's definition requires computing the OT distances for all edges in the trajectory τ , which imposes a heavy burden on the computing
- To overcome this problem, we propose the **upper bound** of the OT distance:

$$
\begin{aligned}
\mathrm{OT}_{\mathbf{C}}\left(P_F(\cdot|s_t), P_F(\cdot|s_{t+1})\right) &:= \min_{\pi \in \prod(P_F(\cdot|s_t), P_F(\cdot|s_{t+1}))} \langle \mathbf{C}, \pi \rangle \\
&\leq \sum_i \sum_j \pi_{ij} \mathbf{C}_{ij} \\
&\leq -\sum_i \sum_j \pi_{ij} \log\left(P_B(s_t|u_i) P_F(s_{t+1}|s_t) P_F(v_j|s_{t+1})\right) \\
&= -\sum_i \sum_j \pi_{ij} \log\left(P_B(s_t|u_i)\right) - \sum_i \sum_j \pi_{ij} \log\left(P_F(s_{t+1}|s_t)\right) - \sum_i \sum_j \pi_{ij} \log\left(P_F(v_j|s_{t+1})\right) \\
&= -\sum_i \log\left(P_B(s_t|u_i)\right) \sum_j \pi_{ij} - \log\left(P_F(s_{t+1}|s_t)\right) \sum_i \sum_j \pi_{ij} - \sum_i \log\left(P_F(v_j|s_{t+1})\right) \sum_j \pi_{ij} \\
&= -\sum_i \log\left(P_B(s_t|u_i)\right) P_F(u_i|s_t) - \log\left(P_F(s_{t+1}|s_t)\right) - \sum_j \log\left(P_F(v_j|s_{t+1})\right) P_F(v_j|s_{t+1}) \\
&= \sum_{u \in \mathrm{Child}(s_t)} P_F(u|s_t) \log(P_B(s_t|u)) - \log(P_F(s_{t+1}|s_t)) + \mathbf{H}(P_F(.|s_{t+1}).
\end{aligned}
$$

Method

Discrete distance -> OT distance -> Path Regularization

■ Upper bound of optimal transport distance

➢ Since the path regularization via OT can be difined as follows:

$$\mathcal{L}_{OT}(\tau) := \sum_{t=0}^{n-1} OT_{\mathbf{C}_{t;\theta}}\left(P_F(\cdot|s_t;\theta), P_F(\cdot|s_{t+1};\theta)\right).$$

➢ The path regularization via OT can be upper bound by:

$$\mathcal{L}_{UB}(\tau) := \sum_{t=0}^{n-1} \left[\sum_{u \in Child(s_t)} P_F(u|s_t) \log(P_B(s_t|u)) - \log(P_F(s_{t+1}|s_t)) + \mathbf{H}(P_F(\cdot|s_{t+1})) \right].$$

$$\sum_{t=0}^{n-1} -\log(P_F(s_{t+1}|s_t)) = -\log\left(\prod_{t=0}^{n-1} P_F(s_{t+1}|s_t)\right) = -\log(P(\tau))$$

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Experiment

■ Hyper-grid Environment

This task aims to evaluates the **generalization ability** of the GFlowNet to guess and sample unvisited modes of the interested distribution.

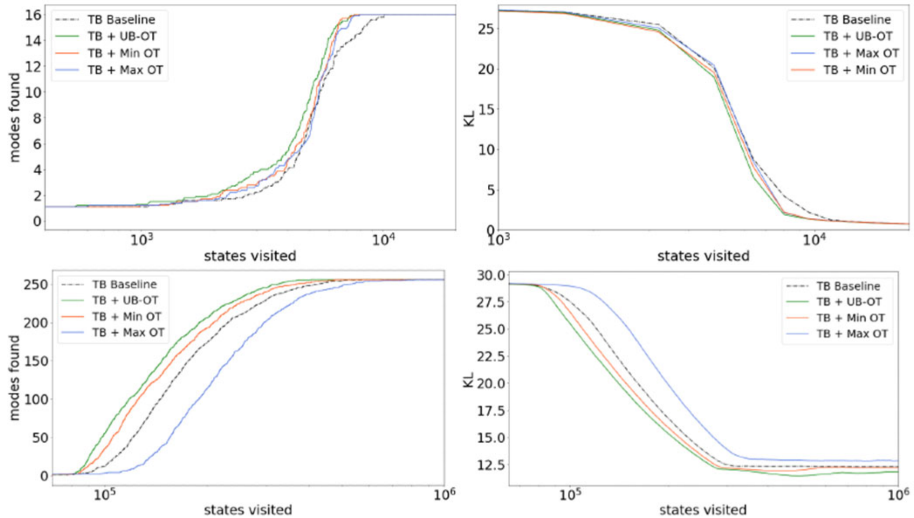

Figure 2: Results on the $4-D$ (upper) and $8-D$ (lower) hyper-grid environment. Left: Number of modes found during training. Right: KL divergence between the true and empirical distribution.

➢ The GFlowNet model trained by **minimizing the path regularization via OT** and **the upper bound** both performer well in improving generalization ability.

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Experiment

■ Synthetic Discrete Probabilistic Modeling tasks

➢ Training the GFlowNet with either **minimizing** the path regularization via OT (Min OT) or via the **upper bound** (UB OT) gains the better **NLL** and **MMD** scores than the baseline and Max OT.

Metrix	Method	2spirals	8gaussians	circles	moons	pinwheel	swissroll	checkerboard
NLL ↓	PCD	20.094	19.991	20.565	19.763	19.593	20.172	21.214
	ALOE	20.295	20.350	20.565	19.287	19.821	20.160	54.653
	ALOE +	20.062	19.984	20.570	19.743	19.576	20.170	21.142
	EB-GFN (paper)	20.050	19.982	20.546	19.732	19.554	20.146	20.696
	EB-GFN	20.0679	19.9862	**20.5598**	19.7324	19.5735	20.1599	20.6839
	EB-GFN + Max OT	20.0673	19.9857	20.5599	19.7319	19.5714	20.1597	20.6837
	EB-GFN + UB OT	20.0651	**19.9854**	20.5600	**19.7305**	19.5707	20.1596	20.6836
	EB-GFN + Min OT	**20.0640**	19.9855	**20.5598**	19.7308	**19.5699**	**20.1595**	**20.6831**
MMD ↓	PCD	2.160	0.954	0.188	0.962	0.505	1.382	2.831
	ALOE	21.926	107.320	0.497	26.894	39.091	0.471	61.562
	ALOE +	0.149	0.078	0.636	0.516	1.746	0.718	12.138
	EB-GFN (paper)	0.583	0.531	0.305	0.121	0.492	0.274	1.206
	EB-GFN	0.3012	0.0408	−0.1724	−0.1744	0.2056	0.1555	−0.0986
	EB-GFN + Max OT	0.3258	0.0197	−0.1919	−0.0456	0.1377	0.0763	−0.0903
	EB-GFN + UB OT	0.2902	**0.0102**	**−0.2819**	−0.1253	0.1561	**0.0257**	−0.0923
	EB-GFN + Min OT	**0.1816**	0.0343	−0.2775	**−0.1966**	**0.1220**	0.1334	**−0.1071**

Table 4: Results on the Synthetic EB-GFN tasks. The negative log-likelihood (NLL) and MMD are displayed in units of 1×10^{-4}. ALOE+ uses a 30 larger parametrization than ALOE and EB-GFN. We only take into account the the reproduce results of EB-GFN when comparing with our methods (Min OT, Max OT, and UB OT).

* Zhang D, Malkin N, Liu Z, et al. Generative flow networks for discrete probabilistic modeling[C]//International Conference on Machine Learning. PMLR, 2022: 26412-26428.

Experiment

■ Biological Sequences Design

- The experiments are conducted in the multi-round active learning setting, with the goal of **generating a diverse set of useful candidates** after evaluation rounds.

	Performance	Diversity	Novelty
DynaPPO	0.938 ± 0.009	12.12 ± 1.71	9.31 ± 0.69
COMs	0.761 ± 0.009	19.38 ± 0.14	26.47 ± 1.30
GFlowNet-AL (paper)	0.932 ± 0.002	22.34 ± 1.24	28.44 ± 1.32
GFlowNet-AL	0.874 ± 0.022	$\mathbf{31.98 \pm 2.27}$	23.91 ± 1.87
GFlowNet+Min OT-AL	0.847 ± 0.033	20.32 ± 7.38	23.63 ± 1.66
GFlowNet+UB OT-AL	0.828 ± 0.022	29.89 ± 2.80	24.16 ± 1.75
GFlowNet+Max OT-AL	0.917 ± 0.003	31.56 ± 2.43	$\mathbf{28.86 \pm 0.96}$

Table 1: Results on the AMP task with $K = 100$.

	Performance	Diversity	Novelty
DynaPPO	0.58 ± 0.02	5.18 ± 0.04	0.83 ± 0.03
COMs	0.74 ± 0.04	4.36 ± 0.24	1.16 ± 0.11
BO-qEI	0.44 ± 0.05	4.78 ± 0.17	0.62 ± 0.23
CbAS	0.45 ± 0.14	5.35 ± 0.16	0.46 ± 0.04
MINs	0.40 ± 0.14	$\mathbf{5.57 \pm 0.15}$	0.36 ± 0.00
CMA-ES	0.47 ± 0.12	4.89 ± 0.01	0.64 ± 0.21
AmortizedBO	0.62 ± 0.01	4.97 ± 0.06	1.00 ± 0.57
GFlowNet-AL (paper)	0.84 ± 0.05	4.53 ± 0.46	2.12 ± 0.04
GFlowNet-AL	0.83 ± 0.01	4.66 ± 0.08	1.14 ± 0.03
GFlowNet+Min OT-AL	0.82 ± 0.01	4.72 ± 0.10	1.13 ± 0.04
GFlowNet+UB OT-AL	0.83 ± 0.01	4.68 ± 0.10	1.14 ± 0.05
GFlowNet+Max OT-AL	$\mathbf{0.85 \pm 0.02}$	4.52 ± 0.18	$\mathbf{1.21 \pm 0.10}$

Table 2: Results on the TF Bind 8 task with $K = 128$.

* Jain M, Bengio E, Hernandez-Garcia A, et al. Biological sequence design with gflownets[C]//International Conference on Machine Learning. PMLR, 2022: 9786-9801.

Experiment

■ Biological Sequences Design

- The experiments are conducted in the multi-round active learning setting, with the goal of **generating a diverse set of useful candidates** after evaluation rounds.

	Performance	Diversity	Novelty
DynaPPO	0.794 ± 0.002	206.19 ± 0.19	203.20 ± 0.47
COMs	$\mathbf{0.831 \pm 0.003}$	204.14 ± 0.14	201.64 ± 0.42
BO-qEI	0.045 ± 0.003	139.89 ± 0.18	203.60 ± 0.06
CbAS	0.817 ± 0.012	5.42 ± 0.18	1.81 ± 0.16
MINs	0.761 ± 0.007	5.39 ± 0.00	2.42 ± 0.00
CMA-ES	0.063 ± 0.003	201.43 ± 0.12	203.82 ± 0.09
AmortizedBO	0.051 ± 0.001	205.32 ± 0.12	202.34 ± 0.25
GFlowNet-AL (paper)	0.853 ± 0.004	211.51 ± 0.73	210.56 ± 0.82
GFlowNet-AL	0.8232 ± 0.0001	218.54 ± 7.88	222.05 ± 5.49
GFlowNet+Min OT-AL	0.8231 ± 0.0001	182.03 ± 0.25	220.56 ± 2.02
GFlowNet+UB OT-AL	0.8232 ± 0.0001	221.64 ± 0.11	218.02 ± 0.79
GFlowNet+Max OT-AL	0.8233 ± 0.0001	$\mathbf{225.00 \pm 3.76}$	$\mathbf{242.11 \pm 1.44}$

Table 3: Results on the GFP task with $K = 128$.

- The GFlowNet-AL model trained by **maximizing the path regularization via OT** performs well in generating more diverse and novel candidates.

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Conclusion

- We propose to train the GFlowNet with **an additional path regularization via Optimal Transport** that places prior constraints on the underlying structure of the GFlowNet.
- We derive **an efficient implementation** of the regularization by finding its **closed-form solutions** in specific cases and a meaningful **upper bound** that can be used as an approximation when we want to minimize the regularization term.
- Experiments have shown that **minimizing the path regularization** via OT improves the GFlowNet's **generalization** while **maximizing the path regularization** via OT enhances the **exploration ability** of the GFlowNet.

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Thank You for listening!

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