Bayesian Inference with GFlowNets

When do GFlowNets learn the right distribution?

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The sampling problem

Let

1. $\mathcal{X}$ be a set and
2. $R\colon \mathcal{X} \to \mathbb{R}_+$ be a positive function on $\mathcal{X}$.

The sampling problem

How to generate samples from

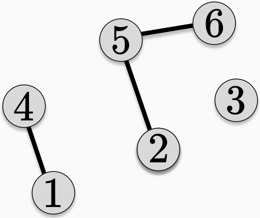
$$\pi(x) \propto R(x)?$$

For Bayesian inference: $R(x) = f(\mathcal{D}|x)p(x)$ (unnormalized posterior)

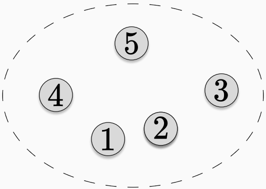
Usual solutions: MCMC, diffusion models, normalizing flows, etc.

Generative Flow Networks (GFlowNets)

GFlowNets solve the sampling problem for a **compositional space**.



Graphs



Sets

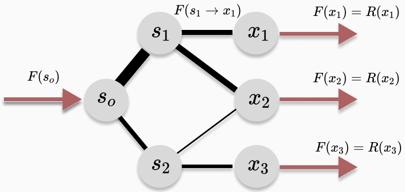
A natural language sentence has a compositional structure

Sentences

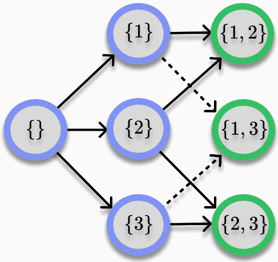
Compositional space

A space $\mathcal{X}$ is **compositional** if its elements can be sequentially constructed from a single **initial state**.

Generative Flow Networks (GFlowNets)



State graph (SG)

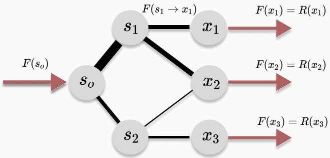


SG for generating 2-sized subsets of $\{1, 2, 3\}$

Central idea

Reframe the state graph as a **flow network** and the sampling problem as a **flow assignment problem**.

GFlowNets: Learning a flow



State graph (SG)

1. Incoming flow = outgoing flow.

$$\sum_{s' \in \mathrm{Ch}(s)} F(s \to s') = \sum_{s' \in \mathrm{Pa}(s)} F(s' \to s).$$

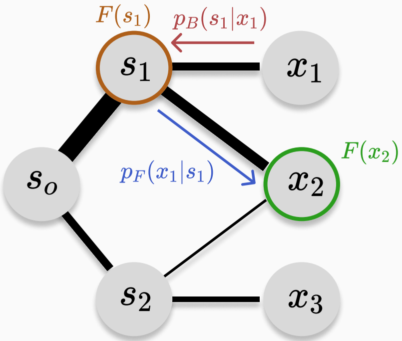
2. Terminal flow = $R(x)$.

$$\sum_{s' \in \mathrm{Pa}(x)} F(s' \to x) = R(x).$$

An ideal setup for Machine Learning

We have a clear goal (finding F) with a simple set of constraints.

GFlowNets: Learning a flow



1. We reparameterize

$$F(s \to s') = F(s) \quad \underbrace{p_F(s'|s)}_{\text{Markovian kernel}}$$

$$F(s' \to s) = F(s') \quad \underbrace{p_B(s|s')}_{\text{Markovian kernel}}$$

2. The constraints become

$$F(s)p_F(s'|s) = F(s')p_B(s|s')$$

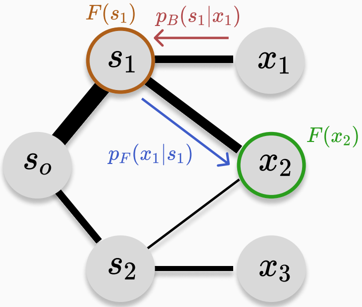
and $F(x) = R(x)$.

Transform the hard constraints into loss functions

$$\mathcal{L}_{DB}(s, s') = \left(\log \frac{F(s)p_F(s'|s)}{F(s')p_B(s|s')}\right)^2$$

This is the **detailed balance** loss. We hardcode $F := R$ for $x \in \mathcal{X}$.

GFlowNets: Learning a flow with neural networks



1. We define

$$F(s) = \underbrace{\mathrm{NN_F}}_{\text{Neural network}}(s)$$

2. Also,

$$p_F(s'|s) = \mathrm{Softmax}(\mathrm{NN_{PF}}(s))[s'],$$

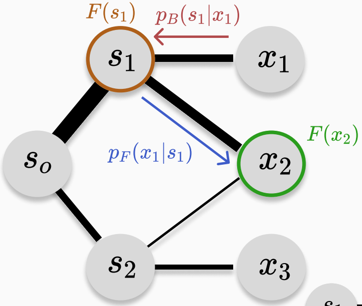
$$p_B(s|s') = \mathrm{Softmax}(\mathrm{NN_{PB}}(s'))[s].$$

A stochastic objective for learning the neural networks

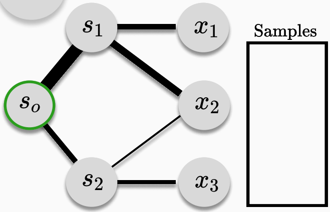
$$\mathcal{L}(F, p_F, p_B) = \mathbb{E}_{\tau \sim p_E}\left[\frac{1}{\#\tau}\sum_{(s,s')\in\tau}\mathcal{L}_{DB}(s,s')\right]$$

p_E is a policy. τ is a trajectory starting at s_o and finishing on $\mathcal{X}$ (e.g., x_2), and $\#\tau$ represents the number of transitions in τ.

GFlowNets: What should you keep in mind?



$$F^\star, {p_F}^\star, {p_B}^\star = \underbrace{\arg\min_{F, p_F, p_B} \mathcal{L}_{\mathrm{DB}}(F, p_F, p_B)}_{\text{Stochastic gradient descent}}$$



Sampling from ${p_F}^\star$

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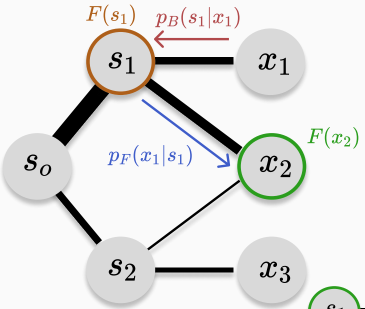

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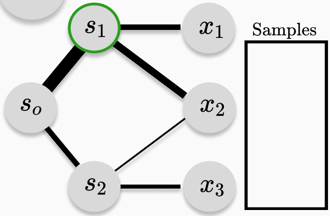

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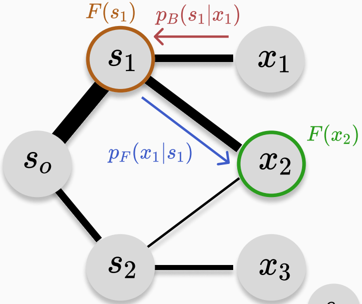
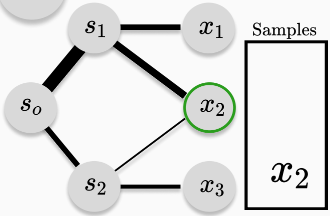


$$\color{green}{F}^\star, \color{blue}{p_F}^\star, \color{red}{p_B}^\star = \underbrace{\arg\min_{F, p_F, p_B} \mathcal{L}_{\mathrm{DB}}(F, p_F, p_B)}_{\text{Stochastic gradient descent}}$$



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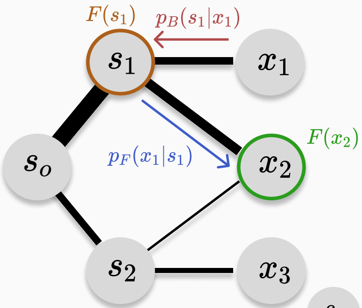

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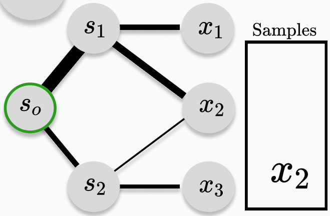

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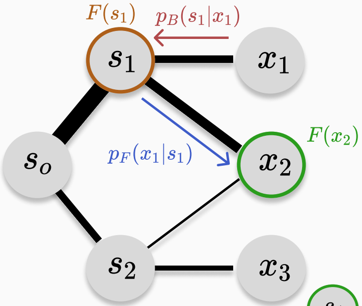

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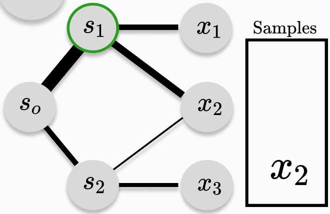

Sampling from ${p_F}^\star$

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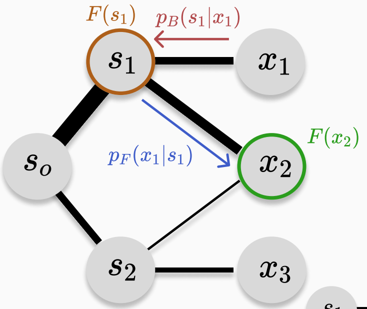

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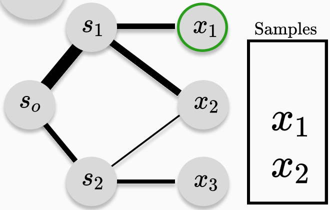

Independent samples with **non-asymptotic** guarantees ($\neq$ MCMC)!

What do GFlowNets promise?

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GFlowNets for AI-driven scientific discovery

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Review

Scientific discovery in the age of artificial intelligence

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Hanchen Wang[1,2,37,38,39], Tianfan Fu[3,39], Yuanqi Du[4,39], Wenhao Gao[5], Kexin Huang[6], Ziming Liu[7], Payal Chandak[8], Shengchao Liu[9,10], Peter Van Katwyk[11,12], Andreea Deac[9,10], Anima Anandkumar[2,13], Karianne Bergen[11,12], Carla P. Gomes[4], Shirley Ho[14,15,16,17], Pushmeet Kohli[18], Joan Lasenby[1], Jure Leskovec[6], Tie-Yan Liu[19], Arjun Manrai[20], Debora Marks[21,22], Bharath Ramsundar[23], Le Song[24,25], Jimeng Sun[26], Jian Tang[9,27,28], Petar Veličković[18,29], Max Welling[30,31], Linfeng Zhang[32,33], Connor W. Coley[5,34], Yoshua Bengio[9,10] & Marinka Zitnik[20,22,35,36]

Bayesian Structure Learning with Generative Flow Networks

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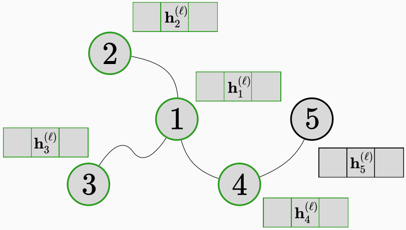
When do GFlowNets learn the right distribution?

What are the limits of GFlowNets?

How to assess a trained GFlowNet?

What are the limits of GFlowNets? A review of GNNs

GFlowNets use Graph Neural Networks (GNNs) to parameterize the flow functions for graph-structured objects. We review what a GNN is below.



1. Aggregate the the features of each node's neighbors.

$$\mathbf{h}_n^{(\ell),\mathrm{agg}} = \sum_{m \in \underbrace{\mathcal{N}(n)}_{\text{Neighborhood of } n} \cup \{n\}} \mathbf{h}_m^{(\ell)}.$$

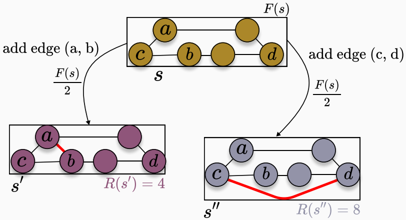
2. Update the node's feature.

$$\mathbf{h}_n^{(\ell+1)} = \mathrm{NN_G}(\mathbf{h}_n^{(\ell),\mathrm{agg}}).$$

Repeat this a few times.

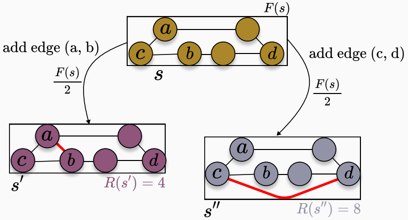
Result: $\mathbf{H} = \left[\mathbf{h}_n^{(L)}\right]_n \in \mathbb{R}^{\#\text{nodes} \times d}$ used as input for downstream tasks.

What are the limits of GNN-based GFlowNets?



1. GNNs cannot distinguish edges (a, b) and (c, d) in s.
2. A GFlowNet always assigns the same flow to s's children — regardless of R.

What are the limits of GNN-based GFlowNets?



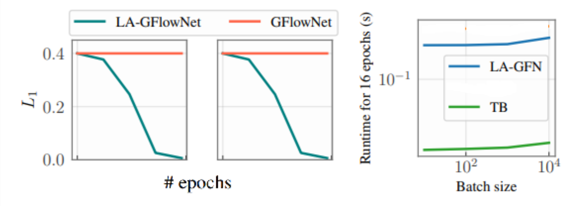
Solution: Look-Ahead (LA) GFlowNets.

$$p_F(s'|s) \propto \exp\left(\mathbf{w}^T \left[\phi^{(s')}_{(a,b)} || \phi^{(s)}_{(a,b)}\right]\right),$$

$$\phi^{(s)} = \mathrm{GNN}(s),\ \phi^{(s')} = \mathrm{GNN}(s').$$

LA-GFlowNets boost the expressiveness GNN-based GFlowNets

LA-GFlowNets incorporate **future embeddings** into the **current policy** to compute the transition probabilities.



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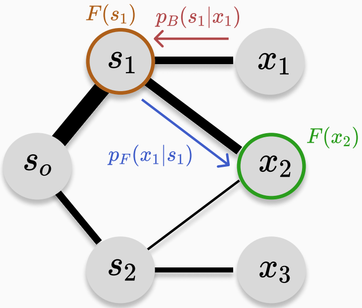


$$\underbrace{p_\top(x)}_{\text{Marginal over } \mathcal{X}} := \sum_{\tau \rightsquigarrow x} p_F(\tau)$$

$$= \underbrace{\mathbb{E}_{\tau \sim p_B(\tau|x)}\left[\frac{p_F(\tau)}{p_B(\tau|x)}\right]}_{\text{Importance sampling}}$$

$$= \frac{1}{T} \sum_{1 \leq i \leq T} \frac{p_F(\tau_i)}{p_B(p_B|x)},$$

$$\{\tau_1, \ldots, \tau_T\} \sim p_B(\cdot|x).$$

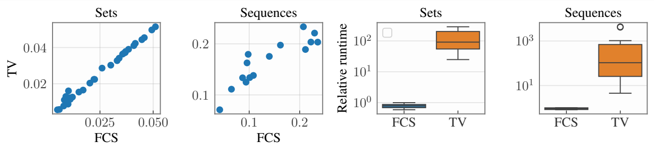
Flow Consistency in Subgraphs (FCS)

FCS consists of the expected total variation in random $\mathcal{X}$-subsets.

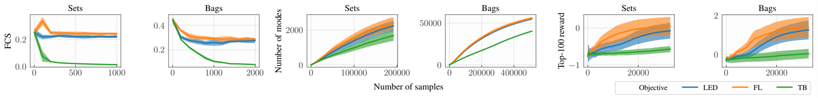
$$\mathbb{E}_{S(\subseteq \mathcal{X}) \sim P}\left[\mathrm{TV}(p_\top^{(S)}, R^{(S)}\right] = \frac{1}{2}\mathbb{E}_{S(\subseteq \mathcal{X}) \sim P}\left[\sum_{x \in S}\left|p_\top^{(S)}(x) - R^{(S)}(x)\right|\right],$$

with $R^{(S)}(x) = {}^{R(x)}/_{\sum_{y \in S} R(y)}$ and $p_\top^{(S)}(x) = {}^{p_\top(x)}/_{\sum_{y \in S} p_\top(y)}$.

How to assess a trained GFlowNet?



FCS is highly correlated and drastically faster-to-compute than TV.



Mode-coverage is not a reliable indicator of correctness.

Conclusions

Take-home message

GFlowNets are excellent samplers for compositional spaces

GFlowNets cast the sampling problem as a flow assignment problem in a flow network. This network describes the sequential construction of complex objects from a single initial state.

GNN-based GFlowNets have fundamentally limited expressiveness.

GNN-based flow functions explicitly constraint the range of distributions realizable by the corresponding GFlowNet. Designing efficient solutions to this problem remains an open issue.

FCS is a reliable measurement of GFlowNet's accuracy.

As such, FCS stands as the best available diagnostic for this family of models. It is a computationally amenable and theoretically sound proxy for the distributional accuracy of GFlowNets.

Questions?

Thank you!