Generalization and Distributed Learning of GFlowNets

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Approximate Discrete Bayesian Inference

Let $\mathcal{X} = \{x_1, ..., x_n\}$ be a finite and large space.

Let $\mathcal{D}$ be the **data space** and $f : \mathcal{D} \times \mathcal{X} \to \mathbb{R}$ be a probabilistic model indexed by $\mathcal{X}$.

Let $\pi : \mathcal{X} \to \mathbb{R}$ be a prior over $\mathcal{X}$. Examples:

1. $\mathcal{X}$ = phylogenetic trees, $\mathcal{D}$ = nucleotide sequences.
2. $\mathcal{X}$ = drugs, $\mathcal{D}$ = pharmacological properties.
3. $\mathcal{X}$ = sentences, $\mathcal{D}$ = answers (for a given question).

Our objective is to estimate the **posterior** $\pi(\cdot \mid D)$ over $\mathcal{X}$ given a subset $D \subset \mathcal{D}$.

$$\pi(x \mid D) = f(D \mid x)\pi(x)\left(\sum_{y \in \mathcal{X}} \pi(y \mid D)\right)^{-1}$$

Due to $\mathcal{X}$'s intractable size, the **partition function**

$$Z = \sum_{y \in \mathcal{X}} \pi(y \mid D)$$

cannot be directly computed.

In doing so, our goal is to both compute expectations over and estimate the modes of $\pi(x \mid D)$. That is,

$$\mathbb{E}_{x \sim \pi(\cdot \mid D)}[\kappa(x)]$$

for a **decision function** $\kappa : \mathcal{X} \to \mathbb{R}$, and

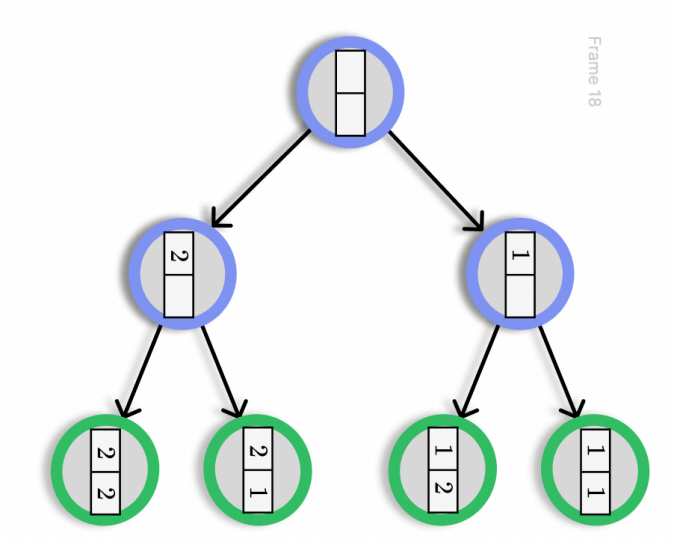
$$\max_{x \in \mathcal{X}} \pi(x \mid D).$$

Owing to $\mathcal{X}$'s lack of a differential structure, traditional approaches (e.g., HMC) often fail to properly approximate $\pi(\cdot \mid D)$. This is the problem we will address.

Generative Flow Networks (GFlowNets)

GFlowNets cast the problem of approximating $\pi(\cdot \mid D)$ as that of **learning** a stochastic inductive process on an **extended space** $\mathcal{S}$ of **sub-instances** of $\mathcal{X}$.

When perfectly learned, this process reaches each $x \in \mathcal{X}$ proportionally to $f(x \mid D)\pi(x)$. That is, it generates **exact samples** from the **posterior**. We refer to $\mathcal{X}$ as the set of **terminal states**.



2-sized sentence-generation over the vocabulary $\{1, 2\}$.

$\mathcal{X}$ = terminal states, $\mathcal{S} \setminus \mathcal{X}$ = extended states. We call this is a **state graph**, which is a **pointed directed acyclic graph**.

Generative Flow Networks (GFlowNets)

From a learning perspective, we define parametric models

1. for a **forward policy**, $p_F : \mathcal{S} \times \mathcal{S} \to [0, 1]$, and
2. for a **backward policy**, $p_B : \mathcal{S} \times \mathcal{S} \to [0, 1]$.

$p_F(s_2 \mid s_1)$ measures the probability of going from s_1 to s_2.

$p_B(s_1 \mid s_2)$ measures the probability of reverting the above action (when traversing the state graph backwards).

We parameterize both p_F and p_B with neural networks.

Generative Flow Networks (GFlowNets)

Recall that our objective is for p_F to satisfy

$$\sum_{\tau : s_o \rightsquigarrow x} \underbrace{\prod_{(s_i, s_{i+1}) \in \tau} p_F(s_{i+1} \mid s_i)}_{p_F(\tau \mid s_o)} \propto f(x \mid D)\pi(x)$$

(s_o is the **source** of the state graph). This is satisfied when

$$\mathcal{V}_{p_E}\left(\frac{p_F(\tau \mid s_o)}{p_B(\tau \mid x) f(x \mid D)\pi(x)}\right) = 0$$

for a distribution p_E such that $p_E(\tau) > 0$ for every τ.

Generative Flow Networks (GFlowNets)

We remark on two facts from this setting.

1. p_B is an **artifact** that enables tractable learning of p_F.
2. Learning is based on adaptive stochastic gradient-based estimates of $\mathcal{V}_{p_E}$, i.e.,

$$p_F^{(t+1)} \leftarrow p_F^{(t)} - \gamma_t \nabla \mathcal{V}_{p_E}^K,$$

in which $\mathcal{V}_{p_E}^K$ is a Monte Carlo estimate of $\mathcal{V}_{p_E}$ based on samples $\{\tau_1, ..., \tau_K\} \sim p_E$ and a **learning rate** schedule $\{\gamma_t\}$.

Learning & Generalization of GFlowNets

In conclusion, a GFlowNet learns a stochastic policy over a fixed state graph via stochastic gradient descent.

1. Learning is based on **partial observations** of the state graph. Does the learned policy **provably generalize** beyond the observed states?
2. Which **algorithmic improvements** can speed up the learning of a **generalizable policy**?

Crash course on PAC-Bayes bounds

Probably Approximately Correct (PAC) Bayes techniques provide a principled approach for obtaining non-vacuous statistical bounds on the generalization of a model.

1. Let $L : \Theta \times \mathcal{X} \to \mathbb{R}$ be a loss function and $\hat{L}$ be its empirical estimate of $\mathbb{E}_x[L]$. The **generalization gap** is

$$g(\theta) = \mathbb{E}_x[L(\theta, x)] - \hat{L} \text{ for each } \theta \in \Theta.$$

2. **PAC-Bayes bounds** limit the expected gap,

$$\mathbb{E}_{\theta \sim Q}[g(\theta)] \leq \varphi(L, \Theta, P, Q) \text{ for a functional } \varphi \text{ and distributions } P, Q.$$

3. Assumptions: boundedness of L and stationarily distributed observations.
   - The former can be **relaxed** by redefining L as $L'(\theta, x) = \min(L(\theta, x), B)$ for a sufficiently large $B \in \mathbb{R}$.
   - Stationarity is a good **first approximation** when dealing with **static** datasets.

Important: our bound does not take into account the learning algorithm. This is the reason we bound $\mathbb{E}_\theta[g(\theta)]$ instead of $g\left(\hat{\theta}\right)$ for the learned $\hat{\theta}$.

PAC-Bayes for GFlowNets

- As explained earlier, GFlowNet learning is based on a sequence $\{S_t\}_{t=1}^{N}$ of b-sized trajectory datasets, $S_t = \left\{\tau_1^{(t)}, ..., \tau_b^{(t)}\right\}$. We assume $\{S_t\}_{t=1}^{N}$ is stationary.
- Based on the PAC-Bayes framework, our understanding of GFlowNet generalization should be grounded on:

  1. A bounded loss fuction, L.
  2. Distributions $P, Q : \Theta \to \mathbb{R}$ over the parameters Θ of the neural network parameterizing p_F.

PAC-Bayes for GFlowNets

- We adopt FCS as a performance metric for GFlowNets, which we have introduced in an earlier work.
- In a nutshell, for $S = \{\tau_1, ..., \tau_K\}$,

$$\text{FCS}\ (p_F, S) = \frac{1}{2} \sum_{\tau \in S} |\ p_T(x) - \hat{p}_T(x)\ |,$$

1. x is the terminal state associated with $\tau \in S$ and
2. p_T (resp. $\hat{p}_T$) is the true (resp. estimated) marginal distribution of $x \in S$.

PAC-Bayes for GFlowNets

- Both p_T and $\hat{p}_T$ can be efficiently computed on S:

$$p_T(y) = \frac{f(y \mid D)\pi(y)}{\sum_{\tau \in S} f(x \mid D)\pi(x)} \text{ and } \hat{p}_T(y) = \mathbb{E}_{p_B}\left[\frac{p_F(\tau \mid s_o)}{p_B(\tau \mid y)}\right].$$

- FCS is clearly bounded by $[0, 1]$ (it is a total variation distance restricted to S).
- We define the **generalization gap** of a GFlowNet as

$$g(p_F) := \mathbb{E}_{S \sim p_E}[\text{FCS }(p_F, S)] - \frac{1}{N} \sum_{1 \leq t \leq N} \text{FCS }(p_F, S_t).$$

PAC-Bayes for GFlowNets

- Building upon this, a PAC-Bayes bound for g is:

$$\mathbb{E}_P[g(p_F)] \leq \mathcal{O}\left(\frac{K}{N^{\frac{1}{2}}}\right) + \mathrm{KL}\ (P\|Q),$$

with $\mathrm{KL}\ (P\|Q) = \mathbb{E}_P\left[\log \frac{dP}{dQ}\right]$ as the Kullback-Leibler divergence between P and Q.

(we will skip the technical details)

- When the right-hand side of the above formula is larger than 1, the bound is said to be **vacuous**.

PAC-Bayes for GFlowNets

- Building upon this, a PAC-Bayes bound for g is:

$$\mathbb{E}_P[g(p_F)] \leq \mathcal{O}\left(\sqrt{\frac{\mathrm{KL}\ (P\|Q)}{N}}\right),$$

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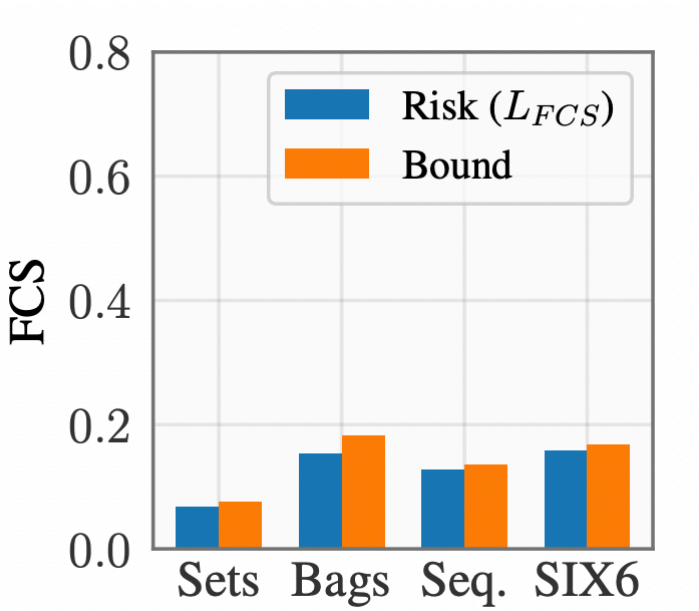
PAC-Bayes for GFlowNets

- Remaining ingredients: P and Q.
- As per traditional work, we let both P and Q be isotropic Gaussian distributions with fixed variance.
- We also split $\{S_t\}_{t=1}^{N}$ into two datasets, $\mathcal{S}_1$ and $\mathcal{S}_2$.
  - P is learned by minimizing the variance loss, $\mathcal{V}_{p_E}$, defined above (smooth proxy for FCS) on $\mathcal{S}_1$.
  - Q is learned by minimizing the upper bound for the learned P on $\mathcal{S}_2$.

PAC-Bayes for GFlowNets



This approach consistently produces non-vacuous bounds on consolidated benchmark tasks.

PAC-Bayes and Distributed Learning

- We show that, for an adequate loss function $L : \Theta \to \mathbb{R}$,

$$\mathbb{E}_P[L(p_F)] \lesssim \mathbb{E}_P\left[\hat{L}(p_F)\right] + \mathcal{O}\left(\frac{\mathrm{KL}\ (P \parallel Q) + \log M}{N}\right),$$

in which M is the maximum trajectory length within the state graph. Examples:

1. Phylogenetic inference: M is the tree size.
2. Sentence generation: M is the maximum sentence size.

PAC-Bayes and Distributed Learning

$$\mathbb{E}_P[L(p_F)] \lesssim \mathbb{E}_P\left[\hat{L}(p_F)\right] + \mathcal{O}\left(\frac{\mathrm{KL}\ (P \parallel Q) + \log M}{N}\right).$$

This formula provides two actionable solutions for improving generalization.

1. By **reducing model size**, we reduce $\mathrm{KL}\ (P\|Q)$ (larger for high-dimensional P, Q).
2. By **shrinking the state graph**, we reduce $\log M$.

PAC-Bayes and Distributed Learning

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Distributed Learning of GFlowNets

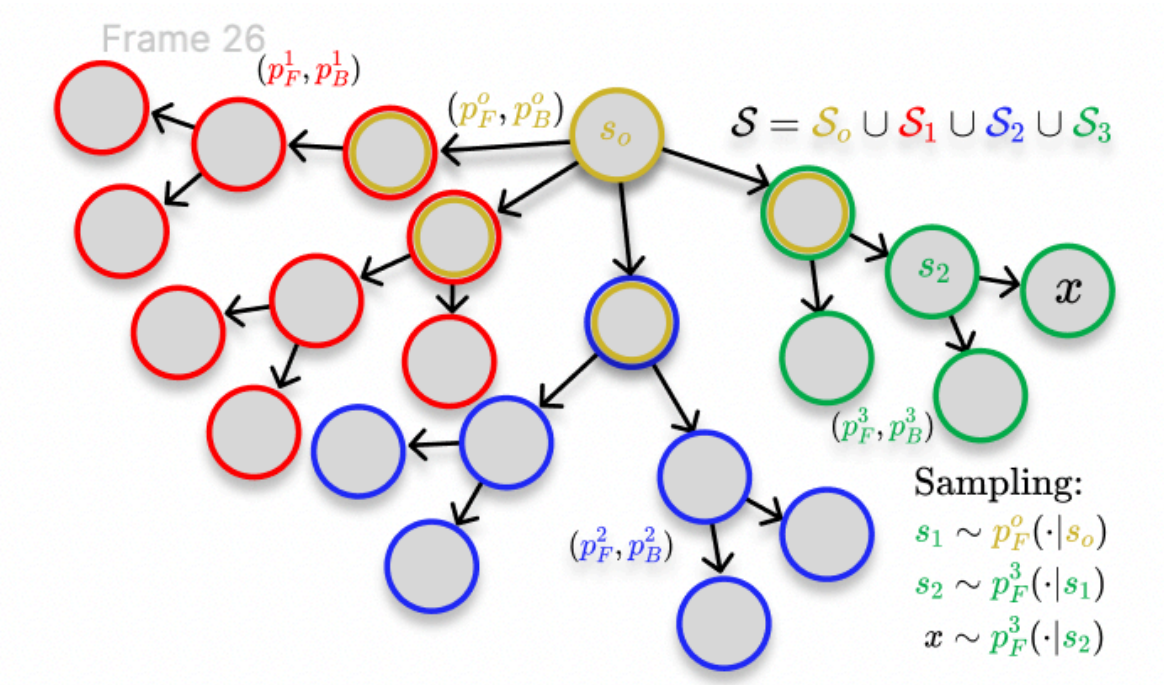
We propose a distributed algorithm that **breaks up the state graph** into pieces learned by **smaller GFlowNets**.

Each GFlowNet parallely addresses a simpler problem: $\downarrow \mathrm{KL}\ (P \| Q)$ and $\downarrow M$.

The trained GFlowNets are then be efficiently aggregated.

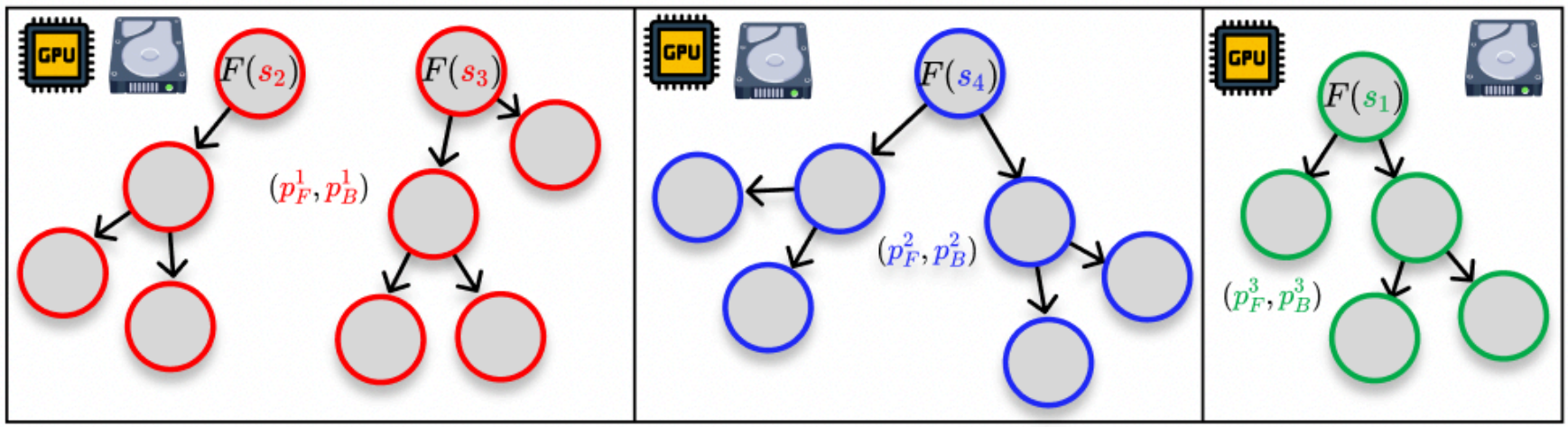
Our algorithm, Subgraph Asynchronous Learning (SAL), can be easily implemented in **computer clusters**.

Subgraph Asynchronous Learning



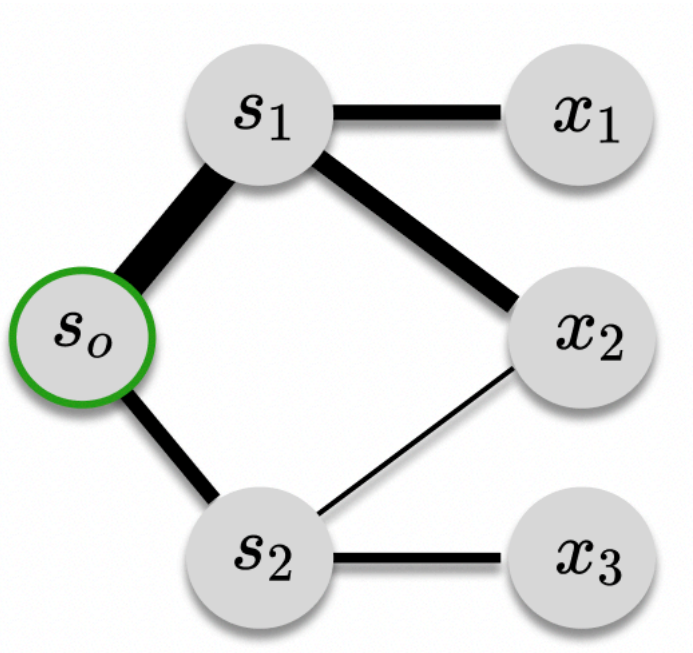
State graph.

Frame 31



State graph divided into independent chunks.
A GFlowNet is parallelly learned for each chunk.

SAL: Intuition & Flow Assignment

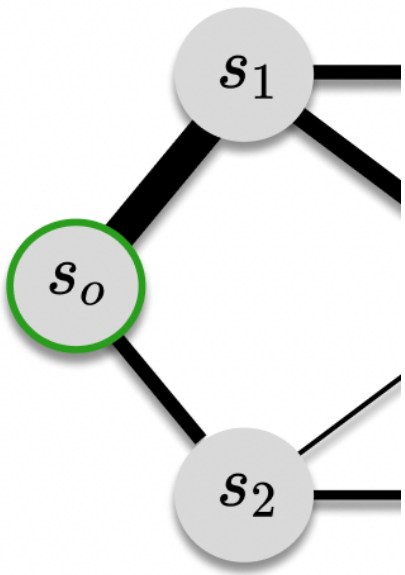


Analogy: A GFlowNet learns a flow assignment in a flow network (this is the reason for the model's name).

SAL: Intuition & Flow Assignment

From this viewpoint, SAL learns a flow assignment for **subnetworks** in parallel.
When a subnetwork has **multiple initial states**, we learn an **amortized solution**.

SAL: Intuition & Flow Assignment



In a final step, a centralized model assings the **appropriate amount of flow** to **each subnetwork**.

SAL: Empirical Analysis

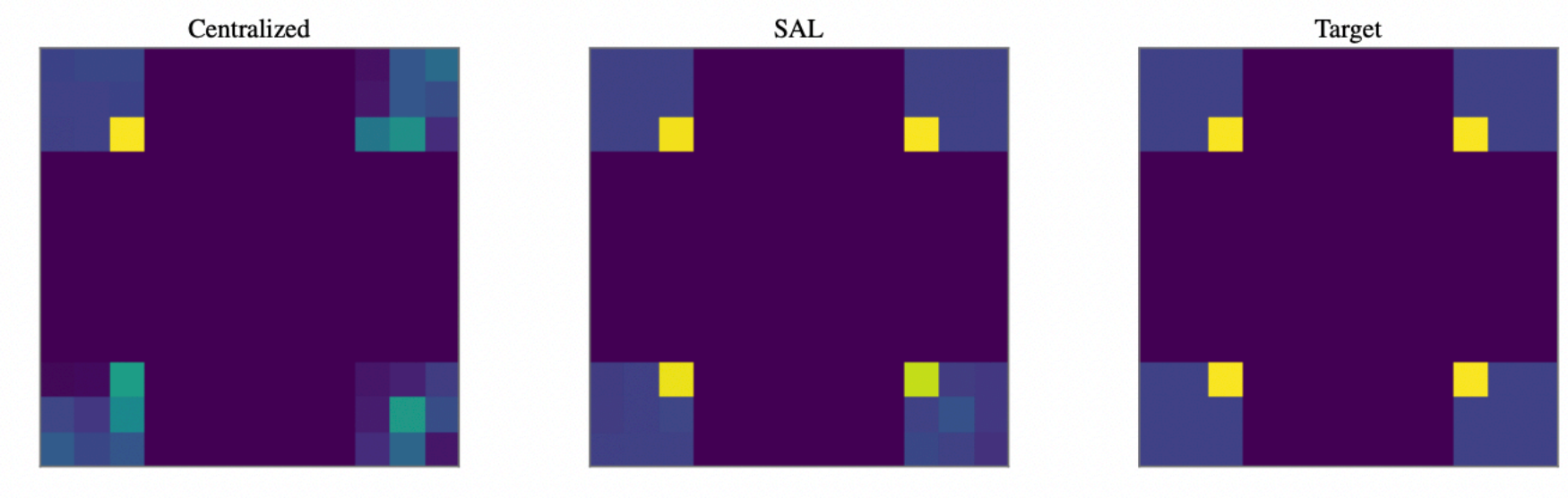
Recall our initial objectives:

1. Estimate posterior expectations.
2. Approximately find posterior modes.

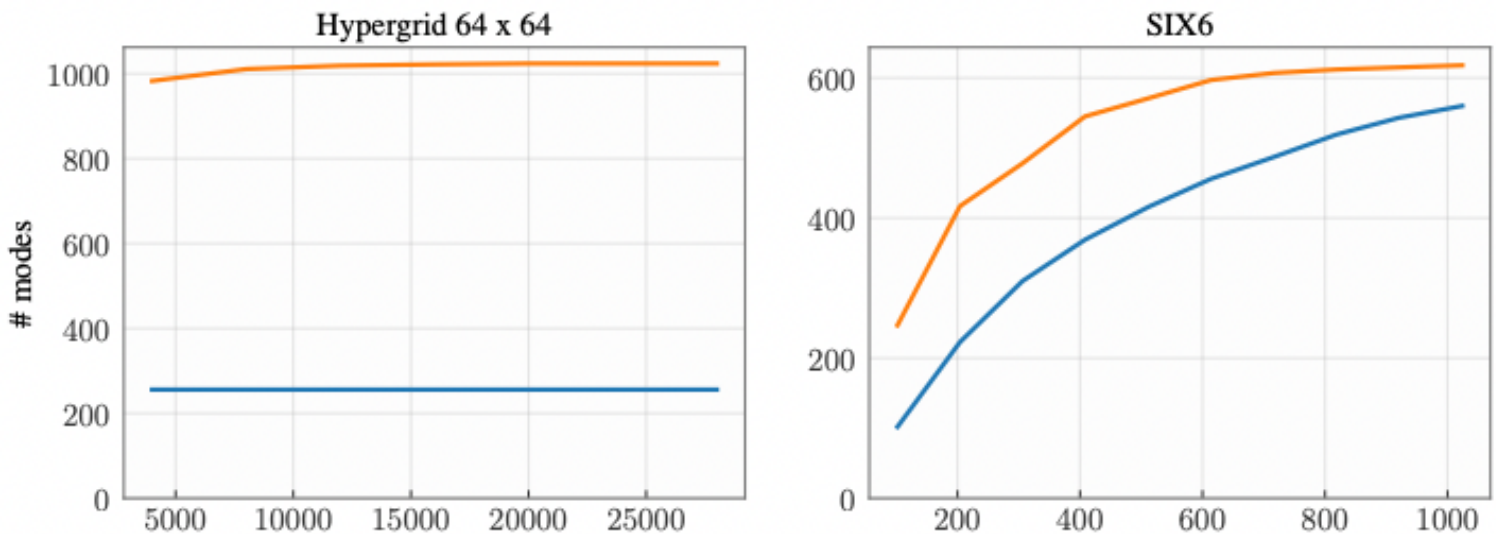
When assessing the former, we evaluate the **goodness-of-fit** of the learned distribution to the posterior.

When assessing the latter, we evaluate the value of $\max_{x \in X} \pi(x) f(D \mid x)$ for a **sampled set** $X \subseteq \mathcal{X}$.

SAL **performs best** in both cases, as we illustrate next.



SAL finds a better approximation to the target distribution than a monolithic model.



SAL finds high-valued states faster than a monolithic model for benchmark tasks.

(A **mode** is defined as a terminal state $x \in \mathcal{X}$ with $\pi(x)f(D|x) > \rho$ for a prescribed ρ)

Take home message

GFlowNets are state-of-the-art models for approximate inference over discrete and compositional distributions.

Our PAC-Bayes bounds rigorously demonstrate that a GFlowNet learns a generalizable policy function.

Our distributed algorithm (SAL) improves generalization by reducing both the model and problem complexities.

SAL also leads to faster mode discovery and better posterior approximations than a centralized model.