Generalization and Distributed Learning of GFlowNets

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TL;DR

- we introduce the first non-vacuous generalization bounds for GFlowNets,
- we develop the first Azuma-type PAC-Bayesian bounds for understanding the generalization of GFlowNets under the light of Martingale theory,
- we demonstrate the harmful effect of the trajectory length on the proven learnability of a generalizable policy for GFlowNets,
- we introduce the first distributed algorithm for learning GFlowNets, Subgraph Asynchronous Learning, and show that it drastically accelerates learning convergence and mode discovery when compared against a centralized approach for relevant benchmark tasks

I. Background: GFlowNets

GFlowNets are amortized algorithms for sampling from distributions over discrete and compositional objects (such as graphs).

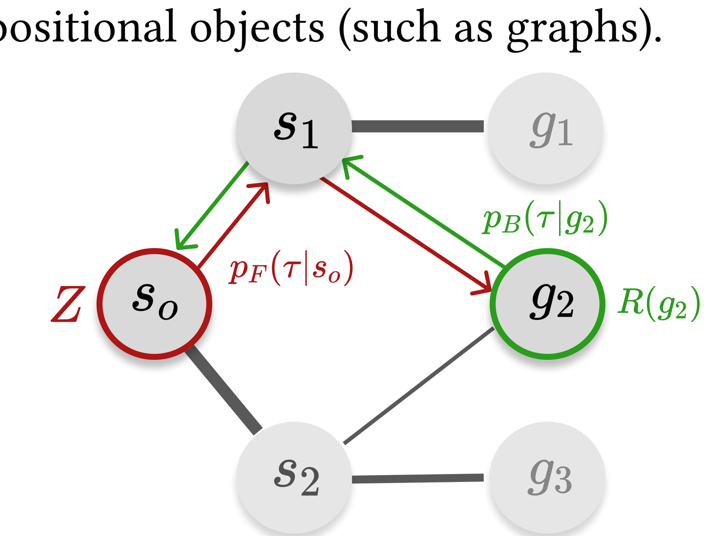

Figure 1: A GFlowNet learns a forward policy on a state graph.

Briefly, a **flow network** is defined over an extension $\mathcal{S}$ of $\mathcal{G}$, which then represents the sink nodes. To navigate within this network and sample from $\mathcal{G}$ proportionally to a **reward function** $R : \mathcal{G} \to \mathbb{R}_+$, a forward (resp. backward) policy $p_F(\tau)$ ($p_B(\tau|x)$) is used.

$$p_F(\tau) = \prod_{(s,s')\in\tau} p_{F(s' \mid s)} \text{ and} \sum_{\tau \rightsquigarrow g} p_F(\tau) = R(g). \quad (1)$$

To achieve this, we parameterize $p_F(\tau)$ as a neural network trained by minimizing

$$\mathcal{L}_{TB}(p_F) = \mathbb{E}\left[\left(\log \frac{p_F(\tau)Z}{p_B(\tau \mid x)R(x)}\right)^2\right]. \quad (2)$$

for a given $p_B(\tau|x)$. GFlowNets can be trained in an **off-policy** fashion and the above expectation can be under any full-support distribution over trajectories.

II. Background: Probably Approximate Correct Bayesian Bounds

Let $\mathcal{L}$ be a loss function on a parameter space Θ, e.g., the squared loss. Also, let $\hat{\mathcal{L}}(\theta, \boldsymbol{X})$ be its empirical counterpart evaluated on a dataset $\boldsymbol{X}$.

PAC-Bayesian bounds. Given "prior" Q (independent of $\boldsymbol{X}$) and posterior P distributions over Θ, a PAC-Bayesian bound establishes an upper limit for the expectation of (unobserved) $\mathcal{L}$ based on the (observed) $\hat{\mathcal{L}}$ and a complexity term φ and a confidence level δ,

$$\mathbb{E}_{\theta\sim P}[\mathcal{L}(\theta)] \leq \mathbb{E}_{\theta\sim P}\left[\hat{\mathcal{L}}(\theta, \boldsymbol{X})\right] + \varphi(\delta, P, Q, |\boldsymbol{X}|). \quad (3)$$

When $\mathcal{L}(\theta) \leq B$ a.e., we refer to a bound as *vacuous* if

$$\mathbb{E}_{\theta\sim P}\left[\hat{\mathcal{L}}(\theta, \boldsymbol{X})\right] + \varphi(\delta, P, Q, |\boldsymbol{X}|) \geq B. \quad (4)$$

Otherwise, the bound is *non-vacuous*. Historically, the search for non-vacuous PAC-Bayesian bounds has been associated to the search for provably generalizable learning algorithms. In this regard, recent works have built upon the basic PAC-Bayesian inequalities to obtain theoretical guarantees for GANs, transformers, armed bandits, and variational autoencoders.

Data-dependent priors for PAC-Bayesian bounds. Given "prior" Q (independent of $\boldsymbol{X}$) and posterior P distributions over Θ, a PAC-Bayesian bound establishes an upper limit for the expectation of (unobserved) $\mathcal{L}$ based on the (observed) $\hat{\mathcal{L}}$ and a complexity term φ and a confidence level δ,

$$\mathbb{E}_{\theta\sim P}[\mathcal{L}(\theta)] \leq \mathbb{E}_{\theta\sim P}\left[\hat{\mathcal{L}}(\theta, \boldsymbol{X})\right] + \varphi(\delta, P, Q, |\boldsymbol{X}|). \quad (5)$$