# Analyzing GFlowNets: Stability, Expressiveness, and Assessment

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TL;DR

- we analyze GFlowNets from three fundamental perspectives: **stability**, **expressiveness**, and **assessment**,
- for stability, we quantify the impact of node-level balance violations over the learned distribution to derive a novel transition-decomposable learning objective,
- for expressiveness, we establish the distributional limits of GFlowNets parameterized by 1-WL GNNs and propose **LA-GFlowNets**, a provably more expressive extension of GFNs,
- for assessment, we develop a theoretically sound metric for measuring the accuracy of GFlowNets based on distributional errors on subsets of the state space.

## I. Background: GFlowNets

GFlowNets are **amortized samplers** for distributions on a set $\mathcal{X}$ of **compositional objects** (e.g., graphs) defined by three ingredients.

1. a state graph $\mathcal{G} = (\{s_o\} \cup \mathcal{S} \cup \mathcal{X}, \mathcal{E})$, which is a DAG on $\mathcal{S} \supseteq \mathcal{X}$,
2. forward and backward policies, $p_F$ and $p_B$, on $\mathcal{G}$,
3. a flow function, $F$, representing the flow within each state.

A GFlowNet is trained to ensure the marginal over $\mathcal{X}$ induced by $p_{F(\cdot \mid s_o)}$ matches a **reward function** $R : \mathcal{X} \to \mathbb{R}_+$. Often, this is done by

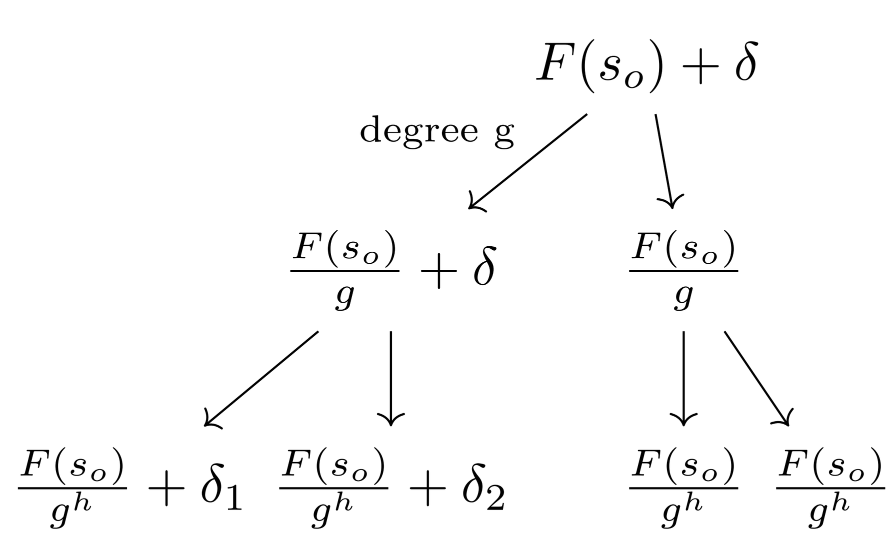
$$p_F = \operatorname{argmin}_{p_F} \mathcal{L}_{DB}(p_F) = \mathbb{E}_{\tau \sim p_F(\cdot \mid s_o)}\left[\frac{1}{\#}\tau \sum_{(s,s') \in \tau} \left(\log \frac{F(s) p_F(s' \mid s)}{F(s') p_B(s \mid s')}\right)^2\right] \quad (1)$$

## II. Bounds on the TV of GFlowNets

**[Stability to local balance violations.]** Let $(\mathcal{G}, p_F, p_B, F)$ be a GFlowNet wrt $R$. Define $(\mathcal{G}, \tilde{p}_F, p_B, \tilde{F})$ by increasing the flow $F(s)$ in some $s$ by $\delta$ and redirecting the extra flow to a child $s^\star$ of $s$. Also, let $\mathcal{D}_{s^\star} \subset \mathcal{X}$ be the terminal descendants of $s^\star$. Then,

$$\frac{\delta}{F(s_0) + \delta}\left(1 - \sum_{x \in \mathcal{D}_{s^\star}} \pi(x)\right) \leq |\tilde{p}_T - \pi|_{TV} \leq \frac{\delta}{F(s_0) + \delta}\left(1 - \min_{x \in \mathcal{D}_{s^\star}} \pi(x)\right).$$

The figure below illustrates the above result for a tree-structured state graph when the extra flow is added to the initial state.




Our analysis suggest that errors at earlier nodes, associated to smaller $\min_{x \in \mathcal{D}_{s^\star}} \pi(x)$, dominate the loss function of GFlowNets in (1).

**[Empirical illustration.]** Figure 2 confirms that, for the initial training epochs, the DB loss is mostly dominated by violations to the balance of shallow — and rewardless — states.

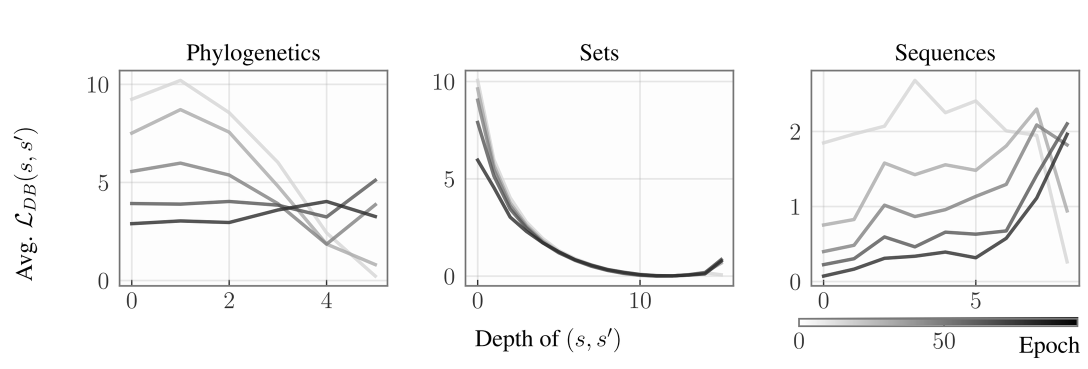



Figure 2: DB loss is dominated by imbalances at early states.

Experiments showed that, by weighting each transition in the DB loss proportionally to the inverse of the incoming node's number of terminal descendants, convergence is often significantly sped up.

## III. Distributional limits of 1-WL GFlowNets

Forward policies are frequently parameterized by 1-WL GNNs. We show that this parameterization **limits the expressivity** of GFlowNets.

Let $\mathcal{G}$ be a tree-structured state graph with reward $R$. Let $T(s) \subseteq \mathcal{X}$ for $s \in \mathcal{S}$ be the terminal descendants of $s$. If there is a $s = (V, E) \in \mathcal{S}$ with $(a, b) \neq (b, c) \in V^2 \setminus E$ indistinguishable by 1-WL s.t.

$$\sum_{x \in T(s')} R(x) \neq \sum_{x in T(s'')} R(x) \quad (2)$$

with $s' = (V, E \cup \{(a, b)\})$ and $s^{\{''\}} = (V, E \cup \{(c, d)\})$, then there is no 1-WL GFlowNet capable of approximating $\pi \propto R$ with TV zero.

On the positive side, we also prove that a GFlowNet equipped with a 1-WL GNN for $p_F$ can learn arbitrary distributions over trees.

If $\mathcal{S}$ is a set of trees such that $(s, s') \in \mathcal{E}$ implies that $s \subset s'$ with $\#E(s') = \#E(s) + 1$, then there is a GFlowNet equipped with 1-WL GNNs that can approximate any distribution $\pi$ over $\mathcal{X} \subseteq \mathcal{S}$.

To boost expressivity, we incorporate the embeddings of $s'$ when evaluating $p_F(s' \mid s)$. The resulting algorithm is called LA-GFlowNet.

**[Empirical illustration]**. To exemplify the results above, we consider the task of learning a distribution over regular graphs by employing the conventional edge-adding generative process in a state graph satisfying (2). Results are laid out in Figure 3.

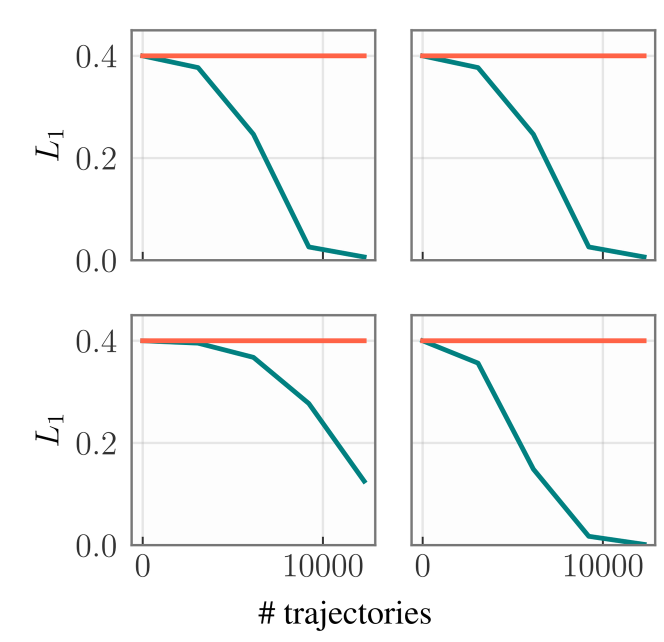



Figure 3: Cases in which, in contrast to LA-GFNs, GNN-based GFNs are unable to sample from the target due to limited expressivity.

## IV. Diagnosing GFlowNets

We design a sound and tractable metric for assessing the goodness-of-fit of a GFlowNet, called **flow-consistency in subnetworks**.

**[FCS]**. For $S \subseteq \mathcal{X}$, let $p_T^{(S)}$ and $\pi^{(S)}$ be the restrictions of the learned and target measures to $S$. Also, let $P_S$ be a distribution over subsets of $\mathcal{X}$ and $\theta$ be the model's parameters. Then,

$$\mathrm{FCS}(p_T, \pi) = \mathbb{E}_{S \sim P_S}[e(S, \theta)] := \mathbb{E}_{S \sim P_S}\left[\frac{1}{2}\sum_{x \in S} |p_T^{(S)}(x; \theta) - \pi^{(S)}(x)|\right]. \quad (3)$$

For FCS, $p_T(x; \theta)$ can be easily computed by $\sum_{\tau \rightsquigarrow x} p_F(\tau \mid s_o)$ for a small subset $S$ of $x$. We also show that FCS and TV are roughly equivalent.

Let $P_S$ be a distribution over $(S \subseteq \mathcal{X} : \#S = \beta)$ for a $\beta \geq 2$. Also, let $d_{TV} = e(\mathcal{X}, \theta)$ be the TV between $p_T$ and $\pi$ for a GFlowNet parameterized by $\theta$. Then, $d_{TV} = 0$ if and only if $\mathbb{E}_{S \sim P_S}[e(S, \theta)] = 0$.

We consider the prototypical task of set generation to illustrate the correspondence between FCS and TV in the examples below.

**[Empirical illustration]**. Figure at side shows that TV and FCS are highly correlated for the task of set generation. Results correspond to 20 different runs with varying rewards and set sizes.