Human-aided Discovery of Ancestral Graphs

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TL;DR

- we introduce the **contrastive balance condition (CBC)** as a provably sufficient and minimally parameterized criterion for sampling correctness in GFlowNets,
- we develop the **first general-purpose algorithm**, called **Embarrassingly Parallel GFlowNets** (EP-GFlowNets), enabling minimum-communication parallel and federated inference for probabilistic models with compositional and finite supports,
- we show that EP-GFlowNets can accurately and efficiently learn to sample from a target in a distributed setting in many benchmark tasks, including phylogenetic inference and Bayesian structure learning,
- we verify that minimizing the **CB loss**, derived from the CBC, often leads to faster convergence than alternative learning objectives.

I. Background: GFlowNets

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

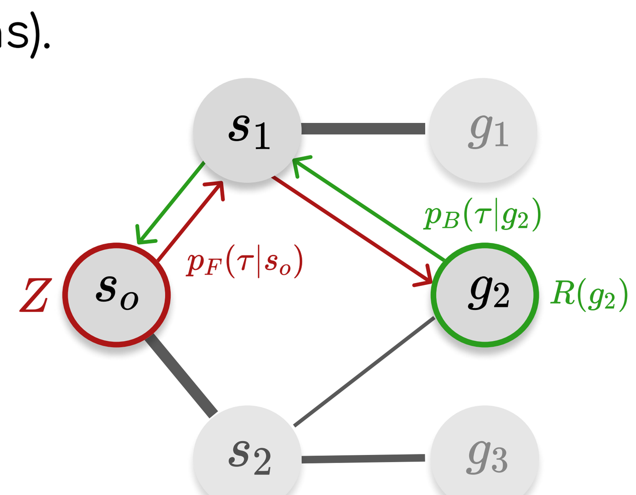

Figure 1: A GFlowNet learns a forward policy on a state graph.

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: Embarrassingly Parallel Inference

Reward functions can often be multiplicatively decomposed in simpler primitives,

$$R(g) = \prod_{1\le i\le N} R_i(g). \quad (3)$$

Each R_i may be a **subposterior** conditioned on a subsample of the data (Figure 2). Often, the R_i's cannot be disclosed due to privacy or computational constraints.

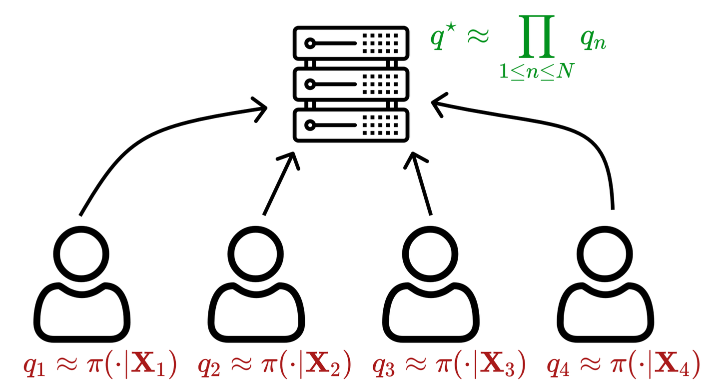

Figure 2: Approximated and embarrassingly parallel Bayesian inference.

Commonly, an approximation q_i to each R_i is locally learned and publicly shared to a centralizing server. An approximation to R, then, is obtained by approximating

$$q(g) \approx \prod_{1\le i\le n} q_i(g). \quad (4)$$

III. Contrastive Balance Condition

Our objective is to solve the approximation problem in Equation 4 when each q_i is a trained GFlowNet. To achieve this, we develop the **CB condition**.

Contrastive balance condition. Let p_F and p_B be the policies of a GFlowNet. Then,

$$\frac{p_F(\tau)}{R(x)p_B(\tau|x)} = \frac{p_F(\tau')}{R(x')p_B(\tau'|x')} \quad (5)$$

for all trajectories τ, τ' finishing at x, x' is a sufficient condition for ensuring that a GFlowNet samples sink nodes from $\mathcal{G}$ proportionally to R.

Differently from alternative balance conditions, the CB **does not rely** on auxiliary quantities such as Z. Clearly, enforcing CB is a sound learning objective for training GFlowNets.

Contrastive balance loss. Let p_F and p_B be the policies of a GFlowNet. Define

$$\mathcal{L}_{CB}(p_F) = \mathbb{E}\left[\left(\log \frac{p_F(\tau)}{R(x)p_B(\tau|x)} - \log \frac{p_F(\tau')}{R(x')p_B(\tau'|x')}\right)^2\right]. \quad (6)$$

Then, $p_F^* = \text{argmin } \mathcal{L}_{CB}(p_F)$ samples from $\mathcal{G}$ proportionally to R.

Our empirical analysis shows that minimizing $\mathcal{L}_{CB}$, which has minimal parameterization, often leads to faster convergence relatively to previously proposed methods.

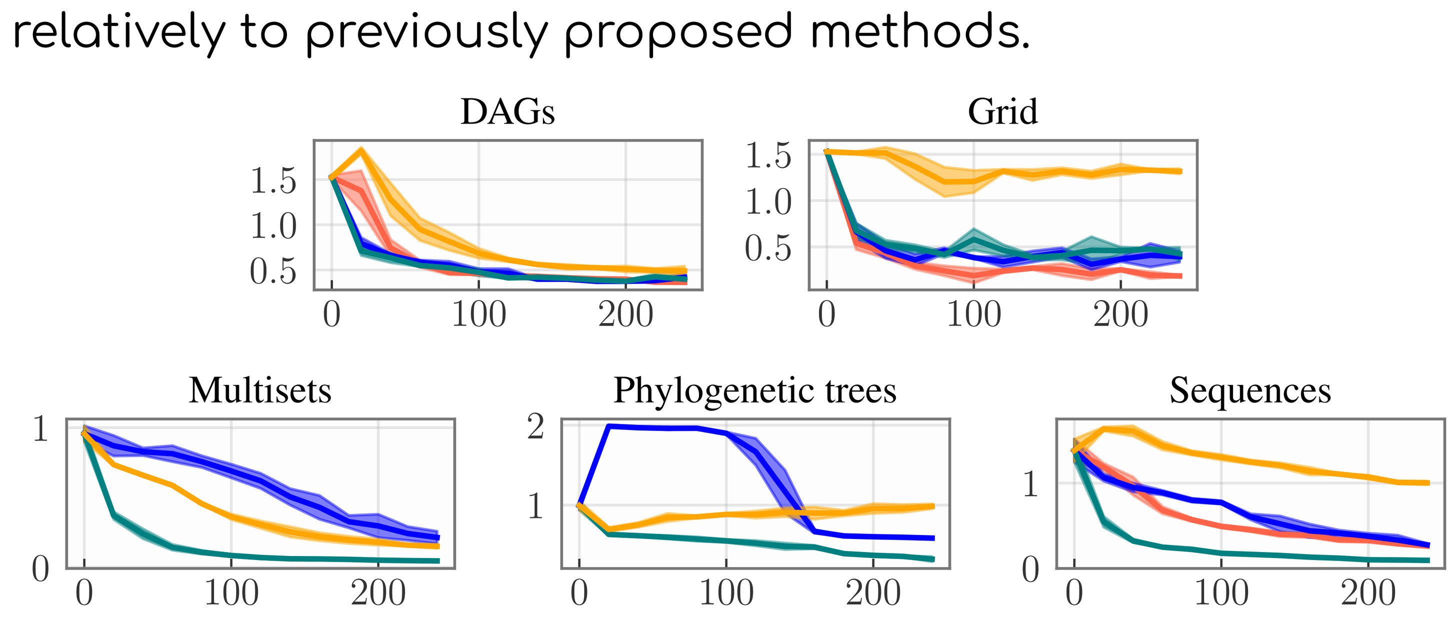

Figure 3: $\mathcal{L}_{CB}$ often outperforms $\mathcal{L}_{TB}$, $\mathcal{L}_{DB}$, and $\mathcal{L}_{DB\text{mod}}$ in terms of convergence speed.

IV. EP-GFlowNets and Aggregating Balance Condition

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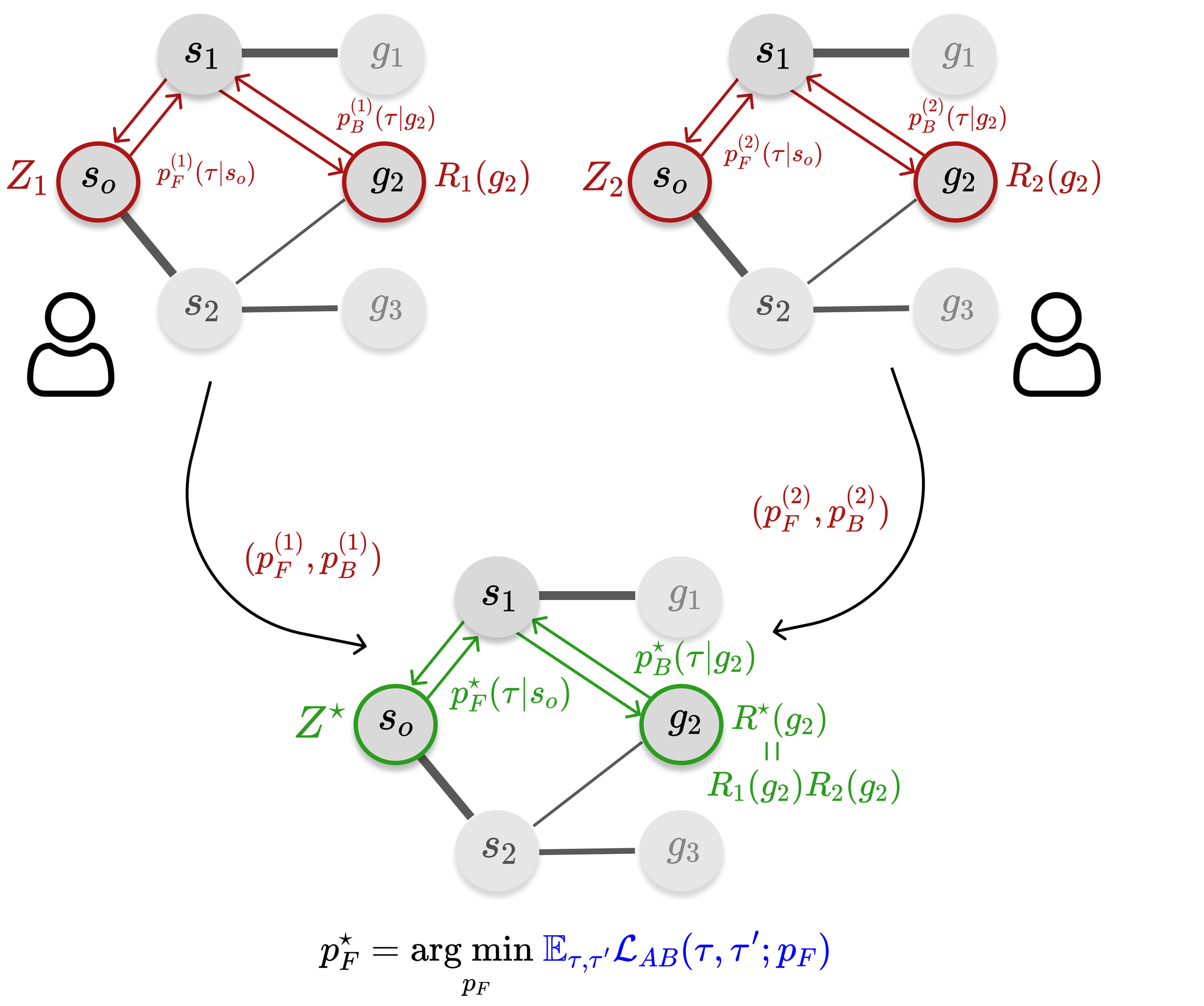

Figure 4: An overview of EP-GFlowNets for learning GFlowNets in a distributed setting.

We develop a **divide-and-conquer** algorithm to train GFlowNets in a parallel.

The condition below shows how to aggregate locally trained GFlowNets in a **single communication step** without directly evaluating the individual reward functions in the server.

Aggregating balance condition. Let $\left(p_F^{(1)}, p_B^{(1)}\right), \ldots, \left(p_F^{(N)}, p_B^{(N)}\right)$ be the policies of N independently trained GFlowNets. Assume each $\left(p_F^{(i)}, p_B^{(i)}\right)$ samples proportionally to R_i. If

$$\frac{\left(\prod_{1 \le i \le N} p_F^{(i)}(\tau)\right)}{\left(\prod_{1 \le i \le N} p_B^{(i)}(\tau \mid x)\right)} p_F(\tau') p_B(\tau \mid x) = \frac{\left(\prod_{1 \le i \le N} p_F^{(i)}(\tau')\right)}{\left(\prod_{1 \le i \le N} p_B^{(i)}(\tau' \mid x')\right)} p_F(\tau) p_B(\tau' \mid x'), \quad (7)$$

then the GFlowNet (p_F, p_B) samples from $\mathcal{G}$ proportionally to $\prod_{1 \le i \le N} R_i$.

Similarly to the CB condition, we enforce the condition above by minimizing the expected log-squared difference between the left- and right-hand sides.

Aggregating balance loss. Under the conditions of Equation 7, define

$$\mathcal{L}_{AB}(p_F) = \mathbb{E}\left[\left(\log \frac{\left(\prod_{1 \le i \le N} p_F^{(i)}(\tau)\right)}{\left(\prod_{1 \le i \le N} p_B^{(i)}(\tau \mid x)\right)} \frac{p_F(\tau')}{p_B(\tau' \mid x')} - \log \frac{\left(\prod_{1 \le i \le N} p_F^{(i)}(\tau')\right)}{\left(\prod_{1 \le i \le N} p_B^{(i)}(\tau' \mid x')\right)} \frac{p_F(\tau)}{p_B(\tau \mid x)}\right)^2\right]. \quad (8)$$

Then, $\mathcal{L}_{AB}$ is globally minimized at a policy p_F sampling proportionally to $\prod_{1 \le i \le N} R_i$.

Realistically, each GFlowNet will **only partially satisfy** their local balance conditions. Yet, we show the aggregated model can be **accurate** even under such **imperfect conditions**.

Influence of local failures. Under the notations of Equation 7, assume that

$$1 - \alpha_n \le \min_{x \in \mathcal{G}, \tau \rightsquigarrow x} \frac{p_F^{(n)}(\tau)}{p_B^{(n)}(\tau \mid x) R_n(x)} \le \max_{x \in \text{cal}\{X\}, \tau \rightsquigarrow x} \frac{p_F^{(n)}(\tau)}{p_B^{(n)}(\tau \mid x) R_n(x)} \le 1 + \beta_n \quad (9)$$

for each $n \in [[1, N]]$. Also, assume that the aggregated model satisfies Equation 7. Then, the Jeffrey divergence between the learned $\hat{R}$ and target R distributions is bounded by

$$\mathcal{D}_J\left(R, \hat{R}\right) \le \sum_{n=1}^{N} \log\left(\frac{1 + \beta_n}{1 - \alpha_n}\right). \quad (10)$$

V. Empirical results on benchmark tasks

We assess the performance of EP-GFlowNets in distributed versions of set and sequence generation, grid exploration, Bayesian phylogenetic inference and structure learning.

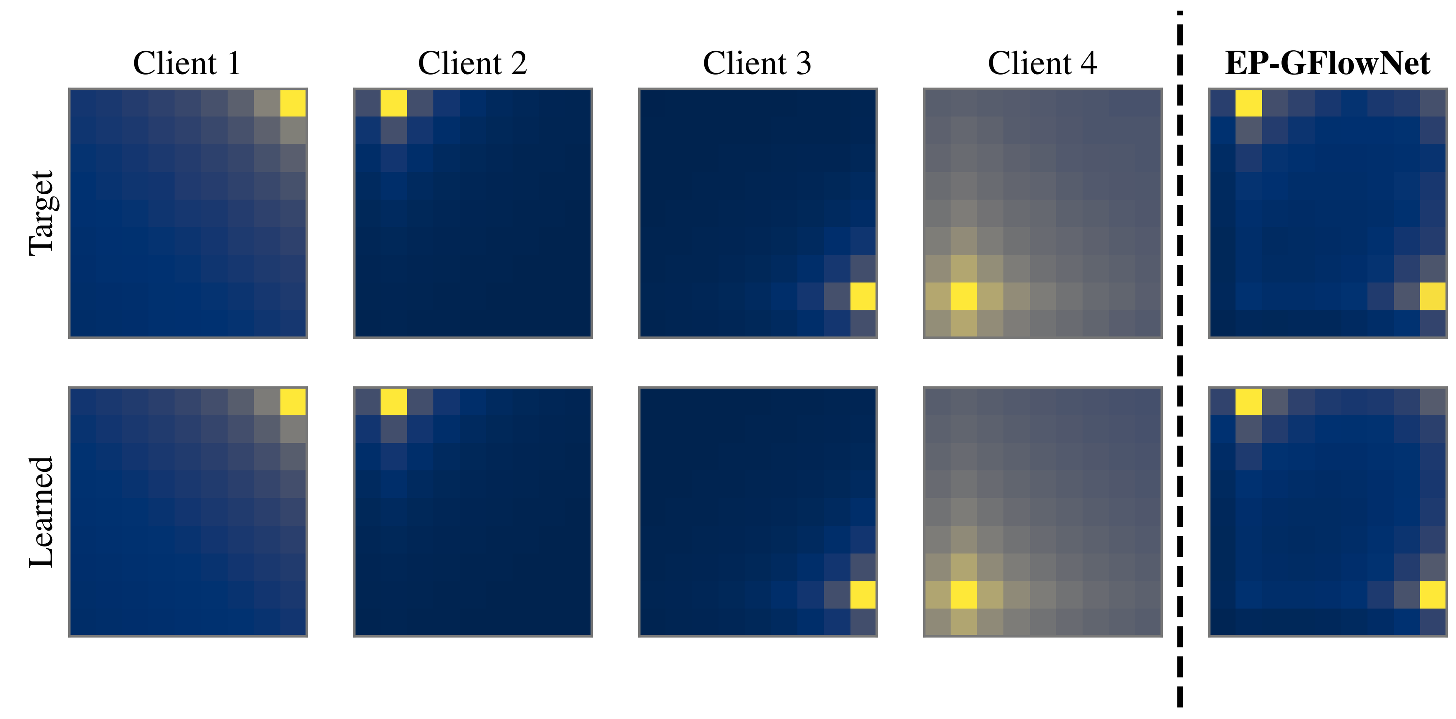

Figure 5: Results for the Grid environment showcasing the correctness of EP-GFlowNets.

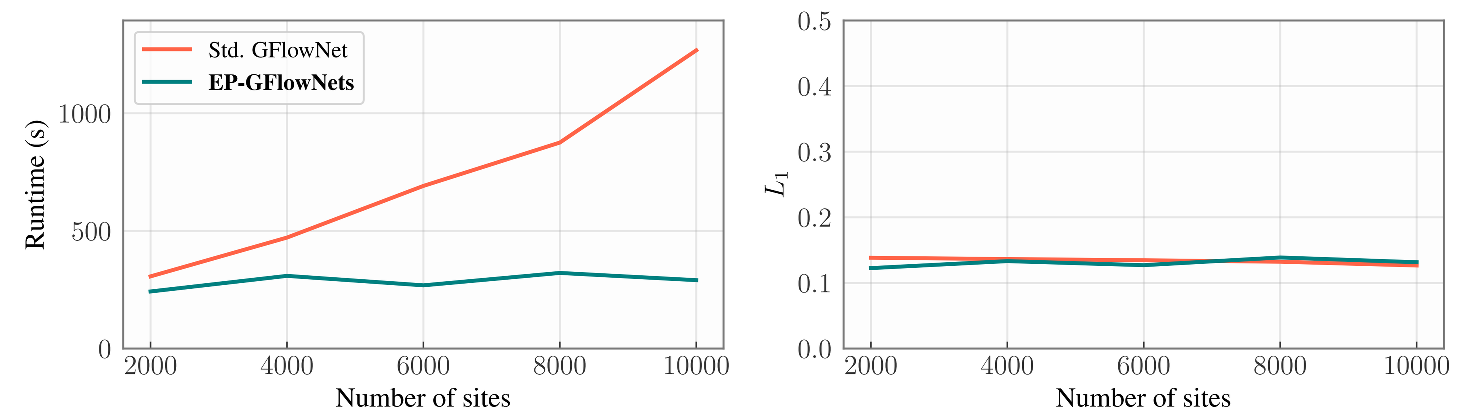

Figure 6: Results for Bayesian phylogenetic inference highlight that EP-GFlowNets can achieve a significant speed-up in learning while incurring a negligible accuracy loss.

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