Embarrassingly Parallel GFlowNets

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TL;DR
- we introduce the **contrastive balance condition (CBC)** as a provably sufficient criterion for sampling correctness in GFlowNets,
- we develop the **first general-purpose algorithm**, called **Embarrassingly Parallel GFlowNets** (EP-GFlowNets), enabling minimum-communication parallel inference for probabilistic models supported on discrete and compositional spaces,
- 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. GFlowNets

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

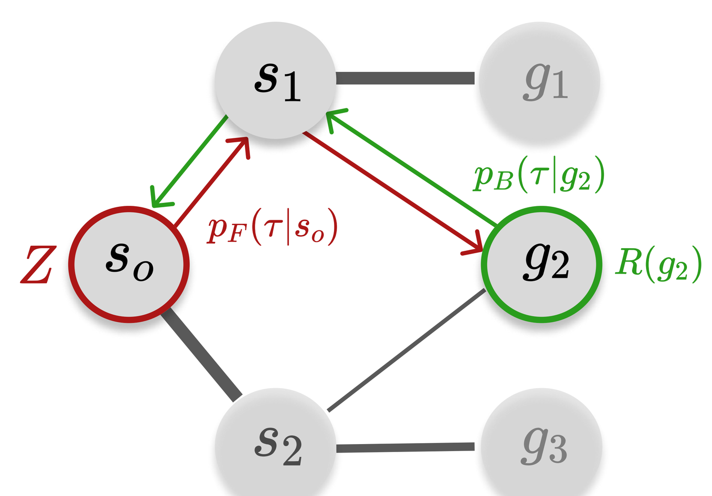

Figure 1: A GFlowNet learns a forward policy on a state graph.

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.

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

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

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

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. Embarrassingly Parallel Inference

Reward functions can often be multiplicatively decomposed in simpler primitives,

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

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.

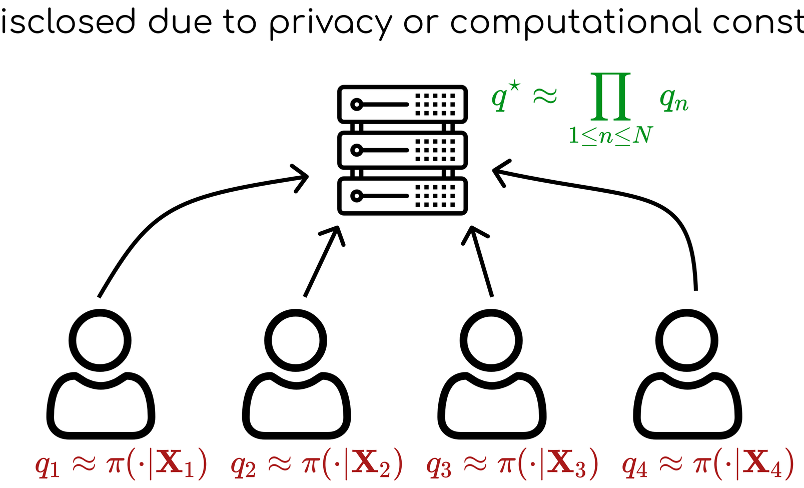

Figure 2: Approximated and embarrassingly parallel Bayesian inference.

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

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

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,

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

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

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

Then, $p_F^\star = \text{argmin } \mathcal{L}_{CB}(p_F)$ 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.

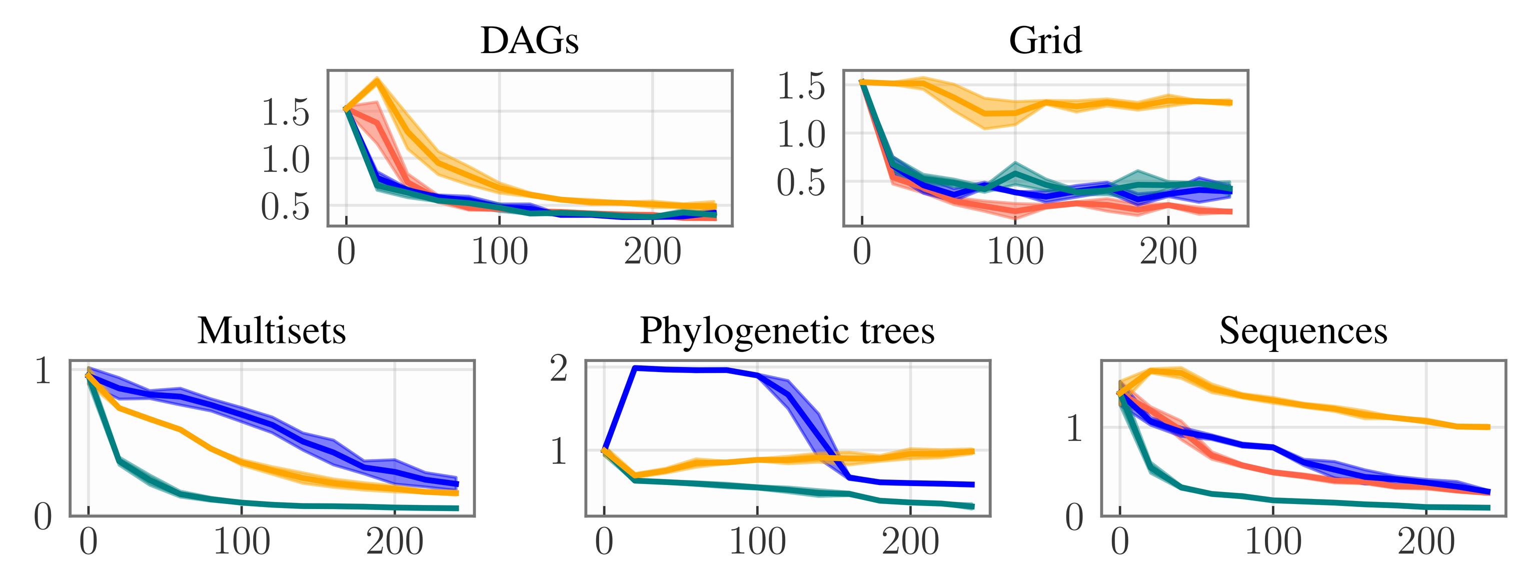

Figure 3: $\mathcal{L}_{CB}$ often outperforms $\mathcal{L}_{TB}$, $\mathcal{L}_{DB}$, and $\mathcal{L}_{DB\text{mod}}$ in terms of convergence speed.

IV. EP-GFlowNets and Aggregating Balance Condition

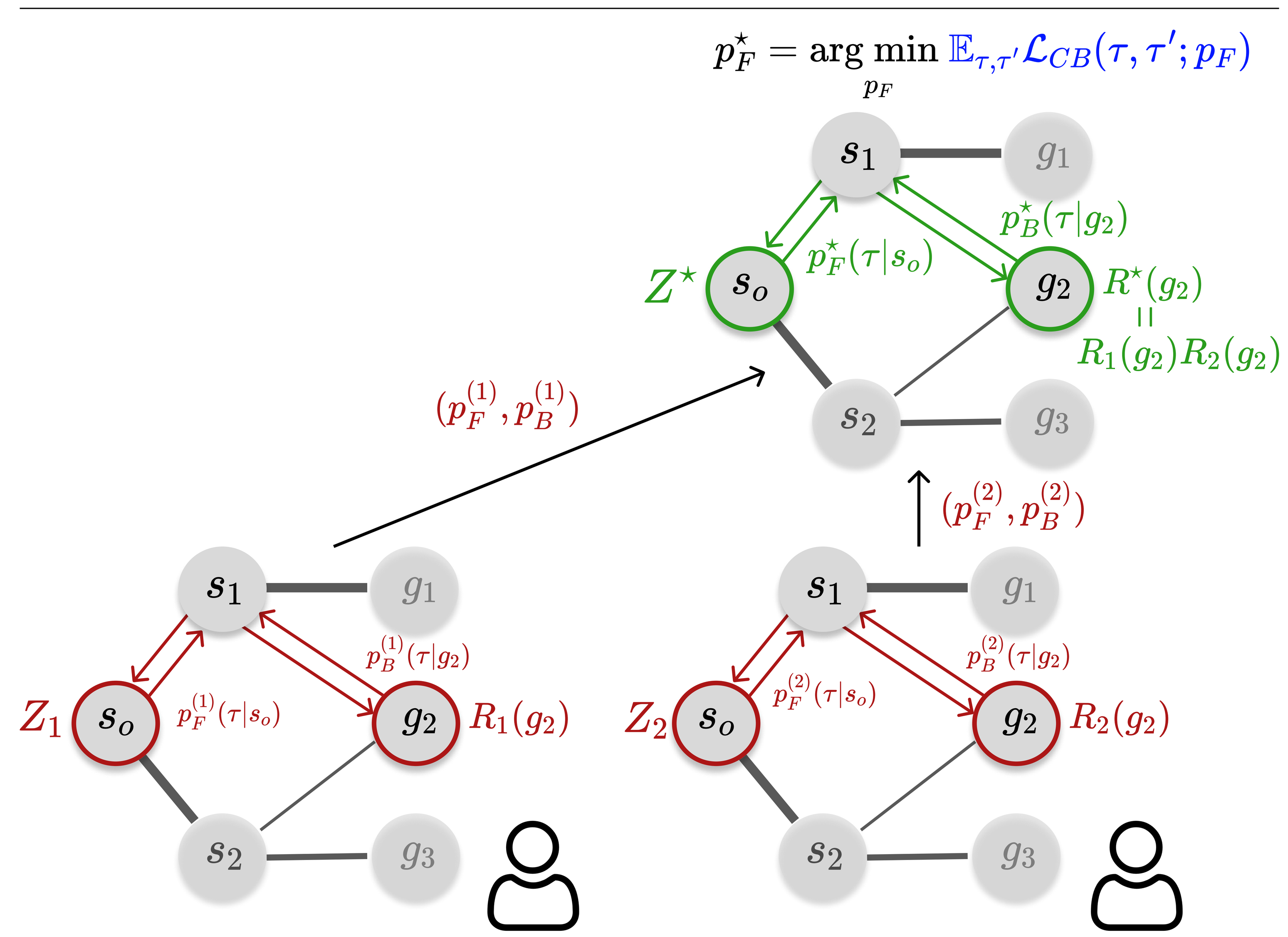

Figure 4: Comparison between learning objectives in terms of convergence speed.

Aggregating balance condition.

a (7)

Aggregating balance loss.

a (8)

V. Empirical results on benchmark tasks

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