Streaming Bayes GFlowNets

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Approximate Bayesian Inference

Let $\mathcal{X} = \{x_1, ..., x_N\}$ be a finite, compositional space.

Also, let $\mathcal{D}$ be the data space, $f(\cdot \mid x) : \mathcal{D} \to \mathbb{R}$ be a likelihood function, and $\pi : \mathcal{X} \to \mathbb{R}$ be a prior on $\mathcal{X}$.

Approximate Bayesian inference

Our objective is to approximate the a sequence of posterior distributions,

$$\pi(x \mid D_1, ..., D_i) \propto f(D_1, ..., D_i \mid x)\pi(x) \text{ for } i \geq 1.$$

This is known as the **streaming Bayes problem.**

That is, Bayesian inference over **unbounded data.**

Approximate Bayesian inference

For conciseness, we will let

$$R_i(x) = f(D_1, ..., D_i \mid x)\pi(x)$$

be the **unnormalized posterior distribution.**

Important.

We assume that D_i and D_j are independent.

BUT each D_i may have its own likelihood function.

Approximate Bayesian inference

We approximate

$$\left(R_i\right)_{i\geq 1}$$

with a tractable family $\left(p^{\theta_i}\right)_{i\geq 1}$ parametrized by θ.

Obviously we are only interested in the latest θ_i for each i.

No need to store unboundedly many models!

Approximate Bayesian inference

Traditional techniques (e.g., MFVI) rely on R_i's gradient.

However, $\nabla_x R_i(x)$ does not exist in discrete spaces.

GFlowNets (Bengio, 2021) address this problem.

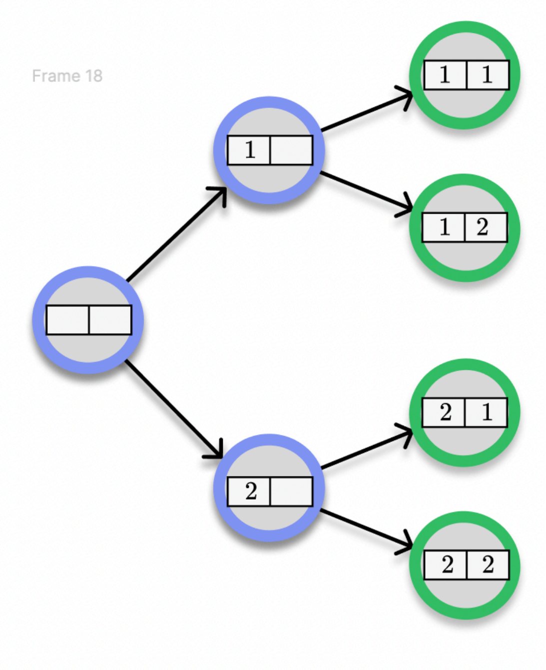
They can also be used for Streaming Bayes, as I will show.

Generative Flow Networks (GFlowNets)

Compositional objects are uniquely characterized by:

1. A **state space,** $\mathcal{S}$, with both incomplete and complete objects. $\mathcal{S}$ also contains the **simplest of states** s_o.
2. A **terminal state space,** $\mathcal{X}$, which is our original parameter space. Clearly, $\mathcal{X} \subseteq \mathcal{S}$.
3. A **state graph** dictating how to navigate between states.

Generative Flow Networks (GFlowNets)



State graph (SG).

A GFlowNet learns a **policy** $p_F(\cdot \mid s)$.

$p_F(\cdot \mid s)$ is a distribution over s's children on the SG.

$p_F(\cdot \mid s)$ is a **neural network**

$$h_\theta : \mathcal{S} \to \Delta_{A-1}$$

with parameter θ. Δ_{A-1} is a simplex, and A is the SG's maximum outdegree.

GFlowNets

Our objective is to find a θ_i such that

$$\sum_{\tau \rightsquigarrow x} \underbrace{\prod_{1 \leq t \leq |\tau|} p_F^{\theta_i}(\tau_{t+1} \mid \tau_t)}_{p_F(\tau \mid s_o)} \propto R_i(x)$$

($\tau \rightsquigarrow x$ is a state-sequence from s_o to $x \in \mathcal{X}$).

For this, we introduce a **backward policy** $p_B(\cdot \mid s)$.

$p_B(\cdot \mid s)$ is an **uniform distribution** over s's parents.

We solve this problem by minimizing

$$\theta_i^\star, Z_i^\star = \min_{\theta_i, Z_i} \mathbb{E}_\tau \left[\left(\log \frac{R_i(\tau_{-1}) p_B(\tau \mid \tau_{-1})}{Z_i \cdot p_F^{\theta_i}(\tau \mid \tau_o)} \right)^2 \right]$$

τ_{-1} is the last element of the trajectory τ (which is on $\mathcal{X}$).
$\tau_o = s_o$ is the first.

Z_i is an auxiliary parameter.

We can demonstrate that the unconstrained global optima solves our sampling problem (Bengio, 2021).

Streaming Bayes GFlowNets

Our prior approach results in a policy $p_F^{\theta_i}$.

This policy **generates approximate samples** from $R_i(x)$.

Research question.

How to update $p_F^{\theta_i}$ when novel data D_{i+1} are observed?

Or: how to sample from R_{i+1} given a model for R_i?

(Recall that $R_i(x) = f(D_1, ..., D_i \mid x)\pi(x)$).

Streaming Bayes GFlowNets

We use the ith model as a **prior** for the $(i+1)$th model.

To understand this, notice that

$$
\begin{aligned}
R_{i+1}(x) &= f(D_1, ..., D_{i+1} \mid x)\pi(x) \\
&= \underbrace{f(D_1, ..., D_i \mid x)\pi(x)}_{R_i(x)} f(D_{i+1} \mid x) \\
&= R_i(x) f(D_{i+1} \mid x).
\end{aligned}
$$

Streaming Bayes GFlowNets

$$R_{i+1}(x) = R_i(x) f(D_{i+1} \mid x).$$

Let τ_x be any trajectory from s_o to x. Since

$$R_i(x) = \frac{Z_i^\star \cdot p_F^{\theta_i^\star}(\tau_x \mid s_o)}{p_B(\tau_x \mid x)},$$

then

$$R_{i+1}(x) = \frac{Z_i^\star \cdot p_F^{\theta_i^\star}(\tau_x \mid s_o)}{p_B(\tau_x \mid x)} \cdot f(D_{i+1} \mid x)$$

Streaming Bayes GFlowNets

Our learning objective then becomes

$$\theta^\star_{i+1}, Z^\star_{i+1} = \min_{\theta_{i+1}, Z_{i+1}} \mathbb{E}_\tau \left[\left(\log \frac{R_{i+1}(\tau_{-1}) p_B(\tau \mid \tau_{-1})}{Z_{i+1} \cdot p_F^{\theta_{i+1}}(\tau \mid \tau_o)} \right)^2 \right]$$

$$= \min_{\theta_{i+1}, Z_{i+1}} \mathbb{E}_\tau \left[\left(\log \frac{p_B(\tau \mid \tau_{-1})}{Z_{i+1} \cdot p_F^{\theta_{i+1}}(\tau \mid \tau_o)} + \log \frac{Z_i^\star \cdot p_F^{\theta_i^\star}(\tau \mid \tau_o)}{p_B(\tau \mid \tau_{-1})} \cdot f(D_{i+1} \mid \tau_{-1}) \right)^2 \right]$$

This is the **streaming Bayes** objective (L_{SB}).

Streaming Bayes GFlowNets (catch-up)

1. A sequence of independent data sets, $(D_i)_{i \geq 1}$.
2. A likelihood function, $f(\cdot \mid x)$, indexed by $x \in \mathcal{X}$.

Algorithm:

1. We first learn a policy $p_F^{\theta_1^\star}$ that approximates $\pi(\cdot \mid D_1)$.
2. We iteratively update $p_F^{\theta_i^\star}$ by minimizing L_{SB}.

$$\theta_{i+1}^\star, Z_{i+1}^\star = \min_{\theta_{i+1}, Z_{i+1}} L_{\mathrm{SB}}\left(D_{i+1}, \theta_i^\star, Z_i^\star, f, \pi\right)$$

Streaming Bayes GFlowNets

Important.

Streaming Bayes GFlowNets do not require

1. **likelihood evaluation** on the **entire data history**;
2. unbounded storage for **model snapshots**.

Empirical illustration

Example: Linear preference learning with integer-valued features (Cole, 1993).

Data. $(d_{i1}, d_{i2}, p_i) \in \{1,0\}^k \times \{1,0\}^k \times \{1,0\}$.

$p_i = 1$ means that $d_{i2} \succeq d_{i1}$.

$p_i = 0$ means that $d_{i1} \succeq d_{i2}$.

d_{i1} and d_{i2} are binary feature vectors.

Model. We use a simple logistic model,

$$p(d_{i1} \succeq d_{i2} \mid x) = \sigma\left(x^T(y_{i1} - y_{i2})\right).$$

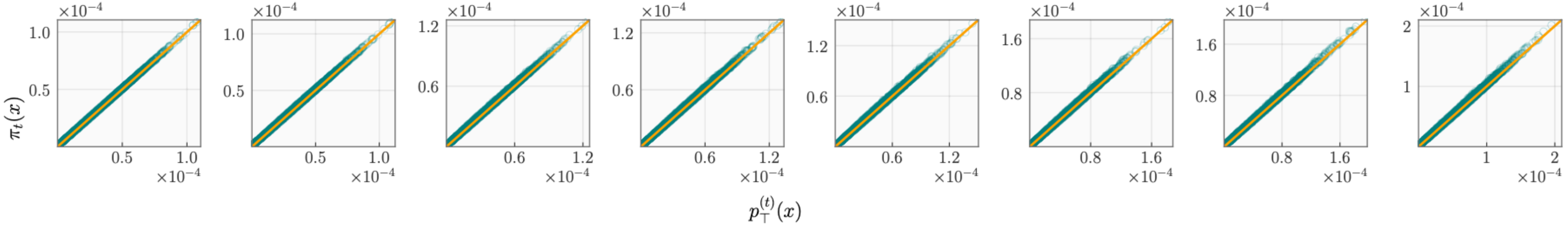
$x \in [[0, u]]^{\{k\}}$ is an integer vector.

We choose a **factorized truncated Poisson prior** for x.

We observe a (simulated) stream $(D_i)_{i \geq 1}$ of tuples (d_1, d_2, p).

Empirical illustration

We compare the true posterior (y axis) with our approximation (x axis) for $1 \leq i \leq 8$.



As we can see, Streaming Bayes GFlowNet accurately approximates the streaming posterior.

Take home message

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

Traditional approaches to streaming Bayesian inference fail on discrete parameter spaces.

Streaming Bayes GFlowNets are a scalable solution for Bayesian inference in the face of continual data streams.

SB-GFlowNets pave the road for reduced environmental footprint for GFlowNet training via model reuse.

References

Bengio, Y., et al. GFlowNet Foundations. JMLR, 2021.

Cole, T.. Scaling and rounding regression coefficients to integers. Applied Statistics, 1993.