A contrastive objective for training GFlowNets

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Summary

1. Problem: Sampling from an unnormalized distribution
2. Generative Flow Networks (GFlowNets)
3. Contrastive balance and contrastive loss
4. Experiments
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Problem: Sampling from an unnormalized distribution

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Let $(\mathcal{X}, \Sigma, \mu)$ be a measurable **state space** with σ-algebra Σ.

Let $r \colon \mathcal{X} \to \mathbb{R}_+$ be a **target probability density** (target density for short) and $R(A) = \int_A r(x)\mu(\mathrm{d}x)$ be the associated measure.

We are interested in the problem of drawing $x \in \mathcal{X}$ s.t. $\mathbb{P}[x \in A] \propto R(A)$ for every $A \in \Sigma$.

This problem could be addressed from the perspective of MCMC, normalizing flows, diffusion models, etc. Here we consider **Generative Flow Networks**.

Problem: Sampling from an unnormalized distribution

It will be useful to think about the discrete case in which

1. $\mathcal{X}$ is finite (but potentially intractably large);
2. Σ is the discrete σ-algebra; and
3. R is an unnormalized probability mass function.

Generative Flow Networks (GFlowNets)

GFlowNets

A GFlowNet casts the sampling problem on $\mathcal{X}$ as a planning problem over an extension $\mathcal{S} \supseteq \mathcal{X}$ of $\mathcal{X}$.

Core principle

A GFlowNet learns a (Markovian) **policy network** $p_F : \mathcal{S} \times \mathcal{S} \to \mathbb{R}_+$ on $\mathcal{S}$ such that, for a prescribed **initial state** s_o, the marginal of $p_F(\cdot|s_o)$ matches R up to a normalizing constant.

GFlowNets

In practice, p_F's support is defined on a **state graph** that dictates how the states in $\mathcal{S}$ are interconnected.

Core definition

A **state graph** is a directed acyclic graph (DAG) $(\mathcal{S}, \mathcal{E})$ defined on $\mathcal{S}$ with edges $\mathcal{E}$.
We let s_o be a special element of $\mathcal{S}$ called the **initial state**; it is the only state without incoming edges.

We refer to p_F as a **forward policy** on $\mathcal{X}$ if $p_F(s, \cdot)$ is supported on $\{u \colon (s, u) \in \mathcal{E}\}$.

Learning a GFlowNet

To learn a GFlowNet, we introduce a **backward policy**[1] p_B.

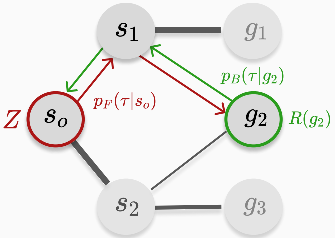
Then, we seek for a p_F satisfying the **trajectory balance** (TB) condition.

$$Zp_F(\tau|s_o) = p_B(\tau|x)r(x), \qquad (1)$$

in which Z is an unknown constant represent the partition function of r, $Z := \int r(x)\mu(\mathrm{d}x)$ and

$$p_F(\tau|s_o) = \prod_{(s,s')\in\tau} p_F(s'|s)$$

for every trajectory τ (please see the figure on the right).



[1] A forward policy on the transposed (edge-direction-switched) state graph.

Learning a GFlowNet

$$Zp_F(\tau|s_o) = p_B(\tau|x)r(x),$$

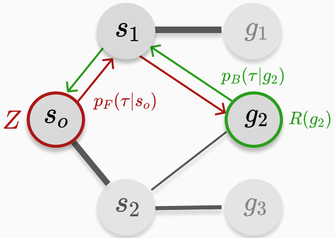
If the TB condition above is satisfied, we can immediately conclude that

$$\underbrace{p_\top(x)}_{\text{Marginal of } x \text{ wrt } p_F(\cdot|s_o)} = \sum_{\tau \to x} p_F(\tau|s_o)$$

$$= \sum_{\tau \rightsquigarrow x} \frac{r(x)p_B(\tau|x)}{Z}$$

$$\propto r(x) \underbrace{\sum_{\tau \rightsquigarrow x} p_B(\tau|x)}_{=1}$$

$$= r(x).$$



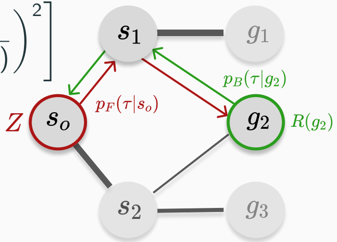
Thus, $p_F(\cdot|s_o)$ samples correctly from $r(x)/Z$.

Learning a GFlowNet

Neither p_F or Z are known; $p_B(s, \cdot)$ is fixed as an uniform over the parents of s in the state graph.

As such, we parameterize $p_F(s, \cdot)$ as a neural network with parameters θ. We then enforce the TB via the loss

$$\mathcal{L}_{TB}(p_F, p_B, Z) = \mathbb{E}_{\tau \sim p_E}\left[\left(\log \frac{Z p_F(\tau|s_o)}{r(x) p_B(\tau|x)}\right)^2\right]$$



in which p_E is a *exploratory policy* that might depend on p_F. We fix

$$p_E = \epsilon p_U + (1 - \epsilon) p_F$$

as an ϵ-greedy version of p_F; $p_U(s, \cdot)$ is uniform over s's children.

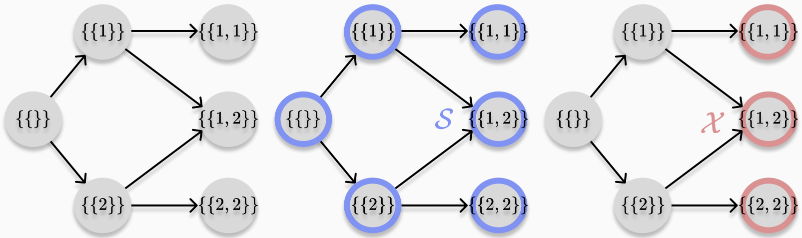
Example: multiset generation

For concreteness, we consider the problem of **multiset generation**.

Illustrative problem

Let $\mathcal{X}$ be the space de m-sized multisubsets of $\mathcal{D} = \{1, \ldots, d\}$. How to sample $x \in \mathcal{X}$ in proportion to a given $R \colon \mathcal{G} \to \mathbb{R}_+$?

The figure below illustrates a state graph for this problem when $m = 2$ and $\mathcal{D} = \{1, 2\}$; $\mathcal{X}$ is the state space and $\mathcal{S}$ is its extension.



s_o represents an empty multiset.

Contrastive balance and contrastive loss

Contrastive balance and contrastive loss

Enforcing the TB condition presents a potentially enormous challenge: estimating the partition function Z[2].

Our objective is to **derive a balance condition** that does not depend on Z.

We will demonstrate that the following **contrastive balance** (CB) condition is equivalent to TB.

Contrastive balance condition

$$\frac{p_F(\tau|s_o)}{p_B(\tau|x)r(x)} = \frac{p_F(\tau'|s_o)}{p_B(\tau'|x')r(x')} \tag{2}$$

for every pair of trajectories (τ, τ') respectively finishing at (x, x').

[2] Exact computation of Z is NP-hard for specific graphical models.

Contrastive balance and contrastive loss

TB $\implies$ CB: We first note that the TB condition entails

$$Zp_F(\tau|s_o) = p_B(\tau|x)r(x) \text{ and } Zp_F(\tau'|s_o) = p_B(\tau'|x)r(x'). \quad (3)$$

Hence,

$$Z = \frac{p_F(\tau|s_o)}{p_B(\tau|x)r(x)} = \frac{p_F(\tau'|s_o)}{p_B(\tau'|x)r(x')}. \quad (4)$$

CB $\implies$ TB: Define

$$Z := \frac{p_F(\tau|s_o)}{p_B(\tau|x)r(x)} = \frac{p_F(\tau'|s_o)}{p_B(\tau'|x)r(x')}. \quad (5)$$

Then,

$$Zp_F(\tau|s_o) = p_B(\tau|x)r(x) \quad (6)$$

for every trajectory τ finishing at x.

Contrastive balance and contrastive loss

To enforce the CB condition, we minimize the following loss.

Contrastive loss

$$\mathcal{L}_{\mathrm{CB}}(p_F, p_B) = \mathop{\mathbb{E}}_{\tau,\tau' \sim p_E} \left[\left(\log \frac{p_F(\tau|s_o)}{p_B(\tau|x)r(x)} - \log \frac{p_F(\tau'|s_o)}{p_B(\tau'|x')r(x')} \right)^2 \right].$$

Experiments

Sampling from a MoG

Does $\mathcal{L}_{\mathrm{CB}}$ leads to faster learning convergence than $\mathcal{L}_{\mathrm{TB}}$?

Task. Train a GFlowNet to sample from a 2-dimensional sparse mixture of Gaussian (MoG) distributions with pdf

$$r(x) = \frac{1}{9} \sum_{1 \le i \le 9} \mathcal{N}(x | \mu_i, \sigma_i I). \qquad (7)$$

Samples from r are depicted on the right.

GFlowNet design. The iterative generative process starts at $s_o = (0, 0)$ and fills up one coordinate at a time with a sample from a learned MoG.

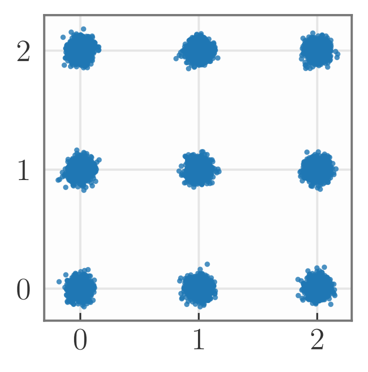
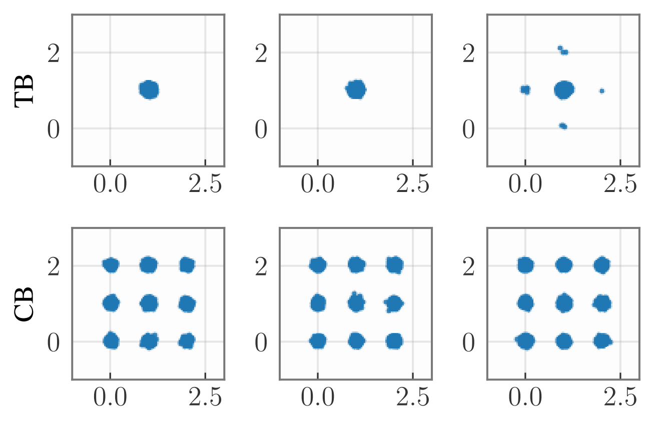


Figure 2: Target distribution.

Sampling from a MoG



$\mathcal{L}_{\mathrm{CB}}$ leads to a drastically better distributional approximation than $\mathcal{L}_{\mathrm{TB}}$.

Conclusions

Takeaway message

1. Generative flow networks are an **emerging family** of models for **sampling** from **unnormalized distributions**.
2. Accurately estimating the partition function is **hard**.
3. The **Contrastive Balance** (CB) condition **avoids introducing the partition function** into the training process by **comparing** the alignemnt to the TB condition of **pairs of the trajectories**.

This work is an extension of our ICML 2024 paper "Embarrassingly Parallel GFlowNets", which will also be presented later today in TS10.

Questions?

Thanks!