What For?

- The first GFlowNet paper [1] explores their use to sample molecular graphs, when given a reward function that corresponds to the estimated binding affinity of the molecule with a protein target. More generally, GFlowNets can be used to learn an experimental design policy, where the reward estimates information gain [6].
- GFlowNets could be used more generally in the MCMC and variational arsenal, including for learning to sample from expressive posterior distributions, either over input space, latent variables or parameters, or both. See [4] for an example of the use of GFlowNets to sample negative examples from an energy function being learned to form an energy-based model.
- GFlowNets could be used more generally to sample over graphs (like causal graphs or explanatory graphs) or sets or compute probabilities, marginalized probabilities, entropies or mutual information over such compositional data structures, and avoid the requirement to work with explicitly normalized probabilities.
- We plan to use GFlowNet to learn how to reason and think in a way similar to humans: each reasoning or each plan or each explanation for some given context can be described by a graph obtained by reusing building blocks (causal mechanisms or relations between entities), and conditional GFlowNets can be trained to sample them or provide probabilistic quantities of interest (conditional probabilities, entropies, marginalized quantities such as free energies, etc).

FAQ

See also the following frequently asked questions:

GFlowNet FAQ