
A Theory of Multi-Agent Generative Flow Networks

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Abstract

1 Generative flow networks utilize a flow-matching loss to learn a stochastic pol-
2 icy for generating objects from a sequence of actions, such that the probability
3 of generating a pattern can be proportional to the corresponding given reward.
4 However, a theoretical framework for multi-agent generative flow networks (MA-
5 GFlowNets) has not yet been proposed. In this paper, we propose the theory
6 framework of MA-GFlowNets, which can be applied to multiple agents to generate
7 objects collaboratively through a series of joint actions. We further propose four
8 algorithms: a centralized flow network for centralized training of MA-GFlowNets,
9 an independent flow network for decentralized execution, a joint flow network for
10 achieving centralized training with decentralized execution, and its updated condi-
11 tional version. Joint Flow training is based on a local-global principle allowing to
12 train a collection of (local) GFN as a unique (global) GFN. This principle provides
13 a loss of reasonable complexity and allows to leverage usual results on GFN to
14 provide theoretical guarantees that the independent policies generate samples with
15 probability proportional to the reward function. Experimental results demonstrate
16 the superiority of the proposed framework compared to reinforcement learning and
17 MCMC-based methods.

18

1 Introduction

19 Generative flow networks (GFlowNets) [1] can sample a diverse set of candidates in an active learning
20 setting, where the training objective is to approximate sampling of the candidates proportionally to a
21 given reward function. Compared to reinforcement learning (RL), where the learned policy is more
22 inclined to sample action sequences with higher rewards, GFlowNets can perform exploration tasks
23 better. The goal of GFlowNets is not to generate a single highest-reward action sequence, but rather
24 is to sample a sequence of actions from the leading modes of the reward function [2]. However, based
25 on current theoretical results, GFlowNets cannot support multi-agent systems.

26 A multi-agent system is a set of autonomous interacting entities that share a typical environment,
27 perceive through sensors, and act in conjunction with actuators [3]. Multi-agent reinforcement
28 learning (MARL), especially cooperative MARL, is widely used in robot teams, distributed control,
29 resource management, data mining, etc [4, 5, 6]. There two major challenges for cooperative MARL:
30 scalability and partial observability [7, 8]. Since the joint state-action space grows exponentially
31 with the number of agents, coupled with the environment’s partial observability and communication
32 constraints, each agent needs to make individual decisions based on the local action observation
33 history with guaranteed performance [9, 10, 11]. In MARL, to address these challenges, a popular
34 centralized training with decentralized execution (CTDE) paradigm [12, 13] is proposed, in which
35 the agent’s policy is trained in a centralized manner by accessing global information and executed
36 in a decentralized manner based only on the local history. However, extending these techniques to
37 GFlowNets is not straightforward, especially in constructing CTDE-architecture flow networks and
38 finding IGM conditions for flow networks need investigating.

39 In this paper, we propose the multi-agent generative flow networks (MA-GFlowNets) framework for
40 cooperative decision-making tasks. Our framework can generate more diverse patterns through se-
41 quential joint actions with probabilities proportional to the reward function. Unlike vanilla GFlowNets,
42 the proposed method analyzes the interaction of multiple agent actions and shows how to sample
43 actions from multi-flow functions. Our approach consists of building a virtual global GFN capturing
44 the policies of all agents and ensuring consistency of local (agent) policies. Variations of this approach
45 yield different flow-matching losses and training algorithms.

46 Furthermore, we propose the Centralized Flow Network (CFN), Independent Flow Network (IFN),
47 Joint Flow Network (JFN), and Conditioned Joint Flow Network (CJFN) algorithms for multi-agent
48 GFlowNets framework. CFN considers multi-agent dynamics as a whole for policy optimization
49 regardless of the combinatorial complexity and demand for independent execution, so it is slower;
50 while IFN is faster, but suffers from the flow non-stationary problem. In contrast, JFN and CJFN,
51 which are trained based on the local-global principle, takes full advantage of CFN and IFN. They can
52 reduce the complexity of flow estimation and support decentralized execution, which are beneficial to
53 solving practical cooperative decision-making problems.

54 **Main Contributions:** 1) We first generalize the measure GFlowNets framework to the multi-agent
55 setting, and propose a theory of multi-agent generative flow networks for cooperative decision-making
56 tasks; 2) We propose four algorithms under the measure framework, namely CFN, IFN, JFN and
57 CJFN, for training multi-agent GFlowNets, which are respectively based on centralized training,
58 independent execution, and the latter two algorithms are based on the CTDE paradigm; 3) We propose
59 a local-global principle and then prove that the joint state-action flow function can be decomposed
60 into the product form of multiple independent flows, and that a unique Markovian flow can be trained
61 based on the flow matching condition; 4) Control tasks experiments demonstrate that the proposed
62 algorithms can outperform current cooperative MARL algorithms in terms of exploration capabilities.

63 1.1 Preliminaries and Notations

64 **Measurable GFlowNets** [14, 15, 16], extending the original definition of GFlowNets [17, 1]
65 to non-acyclic continuous and mixed continuous-discrete statespaces, are defined by a tuple
66 $(\mathcal{S}, \mathcal{A}, S, T, R, F_{\text{out}})$ in the single-agent setting, where \mathcal{S} and \mathcal{A} denote the state and action space, S
67 and T are the state and transition map, π and F_{out} are the forward policy and outflow respectively.
68

69 More precisely, the state space \mathcal{S} and the state-dependent action spaces
70 \mathcal{A}_s are measurable spaces; for each state $s \in \mathcal{S}$, the environment comes
71 with a stochastic transition map¹ $\mathcal{A}_s \xrightarrow{T_s} \mathcal{S}$. We formalize this dependency
72 on state by bundling (packing) state and action together into a bundle
73 $\{(s, a) \mid s \in \mathcal{S}, a \in \mathcal{A}_s\} = \mathcal{A} \xrightarrow{S, T} \mathcal{S}$ where $S(s, a) := s$ and $T(s, a) := T_s(a)$. For graphs, a
74 bundled action is an edge $s \rightarrow s'$; the state map S returns the origin s while the transition map returns
75 the destination s' . The forward policy π is a section of S , i.e., a kernel $\mathcal{S} \xrightarrow{\pi} \mathcal{A}$ such that $S \circ \pi$ is
76 identity on \mathcal{S} . The outflow (or state-flow) F_{out} and the reward R are non-negative finite measure on
77 \mathcal{S} . The state space \mathcal{S} has two special states s_0 and s_f such that $T(s_0, a) \neq s_0$ and $T(s_f, a) = s_f$ for
78 all actions a ; furthermore, there is a special action STOP such that $T(s, \text{STOP}) = s_f$ for all state s .
79 The reward R is generally non-trainable and unknown but implicitly a component of F_{out} and π ; since
80 the reward may not be tractable in the multi-agent setting, we favor a reward-free parameterization
81 of GFlowNets, ie we restrict all objects to $\mathcal{S}^* := \mathcal{S} \setminus \{s_0, s_f\}$. Therefore, we parameterize them
82 by triplets $\mathbb{F} = (\pi^*, F_{\text{out}}^*, F_{\text{init}})$ where $\pi^*(a|s) = \pi(a|s, a \neq \text{STOP})$, $F_{\text{out}}^* := F_{\text{out}} - R$ and
83 $F_{\text{init}} = F_{\text{out}}(s_0)T \circ \pi(s_0)$. We define a Markov chain $(s_t)_{t \geq 1}$ by sampling a first state s_1 from
84 F_{init} , then $a_t = \pi(s_t)$ and $s_{t+1} = T(a_t)$. The sample generated by the GFlowNet is the last position
85 before hitting s_f . The sampling time τ is then the first t such that $a_t = \text{STOP}$. The distribution of
86 s_τ is controlled by the so-called flow-matching constraint

$$\mathcal{A} \xrightarrow{\substack{S \\ \pi \\ T}} \mathcal{S} \xrightarrow{\substack{R \\ F_{\text{out}}}} \mathbb{R}_+$$

$$F_{\text{out}} = F_{\text{in}} := F_{\text{init}} + F_{\text{out}}^* \pi^* T, \quad (1)$$

87 as measures on \mathcal{S} , and the sampling Theorem first proved in [1]:

¹We adopt the naming convention of [18]. The kernel $K : \mathcal{X} \rightarrow \mathcal{Y}$ is a stochastic map which is formalized as follows: for all $x \in \mathcal{X}$, $K(x \rightarrow \cdot)$ is a probability distribution on \mathcal{Y} . In addition, $K(x \rightarrow \cdot)$ varies measurably with x in the sense that for all measurable set $A \subset \mathcal{Y}$, the real valued map $x \mapsto K(x \rightarrow A)$ is measurable.

88 **Theorem 1** ([15] Theorem 2). *Let $\mathbb{F} := (\pi, F_{\text{out}}^*, F_{\text{init}})$ be a GFlowNets on $(\mathcal{S}, \mathcal{A}, S, T, R)$. If the
89 reward R is non-zero and \mathbb{F} satisfies the flow-matching constraint, then its sampling time is almost
90 surely finite and the sampling distribution is proportional to R . More precisely:*

$$\mathbb{P}(\tau < +\infty) = 1, \mathbb{E}(\tau) \leq \frac{F_{\text{out}}(\mathcal{S})}{R(\mathcal{S})} - 1, \text{ and } s_\tau \sim \frac{1}{R(\mathcal{S})} R. \quad (2)$$

91 In passing we introduce $\hat{R} := F_{\text{in}} - F_{\text{out}}^*$, $F_{\text{in}}^* := F_{\text{out}}^* \pi^* T$ and $F_{\text{action}} := F_{\text{out}} \otimes \pi$.

92 **Flow-matching losses (FM)**, denoted by \mathcal{L}_{FM} , are used to enforce the flow-matching constraint
93 1. They compare the outflow F_{out} with the inflow $F_{\text{in}} := F_{\text{init}} + F_{\text{out}}^* \pi^* T$; and are minimized
94 when $F_{\text{in}} = F_{\text{out}}$ so that a gradient descent on GFlowNets parameters may enforce equation 1. The
95 previous works [2, 19] used divergence-based FM losses valid as long as the state space is acyclic
96 while [15, 20, 14] introduced stable FM losses and regularization allowing training in the presence of
97 cycles:

$$\mathcal{L}_{\text{FM}}^{\text{div}}(\mathbb{F}^\theta) = \mathbb{E}_{s \sim \nu_{\text{state}}} g \circ \log \left(\frac{dF_{\text{in}}^\theta}{dF_{\text{out}}^\theta}(s) \right) \quad \mathcal{L}_{\text{FM}}^{\text{stable}}(\mathbb{F}^\theta) = \mathbb{E}_{s \sim \nu_{\text{state}}} g \left(\frac{dF_{\text{in}}^\theta}{d\lambda}(s) - \frac{dF_{\text{out}}^\theta}{d\lambda}(s) \right), \quad (3)$$

98 where g is some positive function, decreasing on $]-\infty, 0]$, $g(0) = 0$ and increasing on $[0, +\infty[$. The
99 simplest choices are $g(x) = x^2$ or $g(x) = \log(1 + \alpha|x|^\beta)$.

100 1.2 Multi-agent Problem Formulation

101 The **multi-agent setting** formalizes the data of state, actions, and transitions for multiple agents.
102 Each agent $i \in I$ in the finite agent set I has its own observation
103 $\mathcal{O}^{(i)}$ in its observation space $\mathcal{O}^{(i)}$; it depends on the state via
104 the projection $\mathcal{S} \xrightarrow{p^{(i)}} \mathcal{O}^{(i)}$. For simplicity sake, we identify
105 $\mathcal{S} = \prod_{i \in I} \mathcal{O}^{(i)}$. Each agent has its own action space $\mathcal{A}^{(i)}$ and
106 each of the agent observation-dependent action space \mathcal{A}_o contains
107 a special action STOP; the environment is such that once an
108 agent chooses STOP, it is put on hold until all agents do as well.
109 The game finishes when all agents have chosen STOP; a reward
110 is given based on the last state. The reward received is formalized
111 by a non-negative function $r : \mathcal{S} \rightarrow \mathbb{R}_+$. We assume that each agent may freely choose its own action
112 independently from the actions chosen by other agents: this is formalized via $\mathcal{A}_s = \prod_{i \in I} \mathcal{A}_{o^{(i)}} / \sim$ ie
113 the Cartesian product of agent actions space up to the identification of the STOP actions. A trajectory
114 of the system of agents is a, possibly infinite, sequence of states $(s_t)_{t < \tau+1}$ with $\tau \in \mathbb{N} \cup \{\infty\}$ starting
115 at the source state $s_0 \in \mathcal{S}$ and may eventually calling STOP; the space of trajectories is \mathcal{T} . A policy
116 on \mathcal{S} induces a Markov chain hence a distribution on trajectories.

117 MA-GFlowNets are tuples $((\mathbb{F}^{(i)})_{i \in I}, \mathbb{F})$, where each *local* GFlowNets $\mathbb{F}^{(i)}$ is defined on
118 $(\mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)}, T^{(i)}, R^{(i)})$ for $i \in I$ and the *global* GFlowNets \mathbb{F} is defined on $(\mathcal{S}, \mathcal{A}, S, T, R)$.
119 **The objective of MA-GFlowNets**, similarly to GFlowNets, is to build a policy π so that the induced
120 trajectories are finite and s_τ is distributed proportionally to $R := r\lambda$ where λ is some fixed measure
121 on \mathcal{S} and $\int_{s \in \mathcal{S}} r(s) d\lambda(s)$ is finite. In general, some GFlowNets (local or global) may be virtual, i.e.
122 not implemented.

123 2 Multi-Agent GFlowNets

124 This section is devoted to details and theory regarding the variations of algorithms for MA-GFlowNets
125 training. If resources allow, the most direct approach is included in the training of the global model
126 directly, leading to a centralized training algorithm in which the local GFlowNets are virtual. As
127 expected, such an algorithm suffers from high computational complexity, hence, demanding decentral-
128 ized algorithms. Decentralized algorithms require the agents to collaborate to some extent. We
129 achieve such a collaboration by enforcing consistency rules between the local and global GFlowNets.
130 The global GFlowNets is virtual and is used to build a training loss for the local models ensuring the
131 global model is GFlowNets, so that the sampling Theorem applies. The sampling properties of the
132 MA-GFlowNets are then deduced from the flow-matching property of the virtual global model.

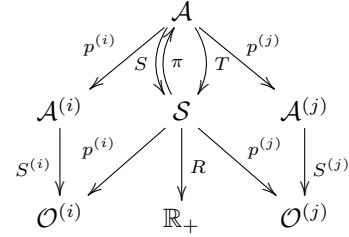


Figure 1: Multi-agent formalism

133 **2.1 Centralized Training**

134 Centralized training consists in training of the global flow directly. Here, the local flows are virtual: they are theoretically recovered from the global flow as image by the observation maps but
135 not implemented. We use FM-losses as given in equations 3 applied to the flow on $(\mathcal{S}, \mathcal{A})$. See
136 Algorithm 1. Implicitly, F_{out} contains a parameterizable component from F_{out}^* , while F_{in} contains
137 the parameterization of π^* and F_{init} .

Algorithm 1 Centralized Flow Network Training Algorithm for MA-GFlowNets

Require: A multi-agent environment $(\mathcal{S}, \mathcal{A}, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, p_i, S, T, R)$, a parameterized GFlowNets $\mathbb{F} := (\pi, F_{\text{out}}^*, F_{\text{init}})$ on $(\mathcal{S}, \mathcal{A})$.
while not converged **do**
 Sample and add trajectories $(s_t)_{t \geq 0} \in \mathcal{T}$ to replay buffer with policy $\pi(s_t \rightarrow a_t)$.
 Generate training distribution ν_{state} .
 Apply minimization step of the FM loss $\mathcal{L}_{\text{FM}}^{\text{stable}}(\mathbb{F}^\theta)$.
end while

139 From the algorithmic viewpoint, the CFN algorithm is identical to a single GFlowNets. As a
140 consequence, the usual results on the measurable GFlowNets apply as is. There are, however, a
141 number of key difficulties: 1) even on graphs, the computational complexity increases as $O(|\mathcal{A}_s|^N)$
142 at any given explored state; 2) centralized training requires all agents to share observations, which is
143 impractical since in many applications the agents only have access to their own observations.

144 **2.2 Local Training: Independent**

145 The dual training method is embodied in the training of local GFlowNets instead of the global one.
146 In this case, the local flows $\mathbb{F}^{(i)}$ are parameterized and the global flow is virtual. In the same way, a
147 local FM loss is used for each client. In order to have well-defined local GFlowNets, we need a local
148 reward, for which a natural definition is $R^{(i)}(o_t^{(i)}) := \mathbb{E}(R(s_t|o_t^{(i)})$. The local training loss function
149 can be written as: $\mathcal{L}(\mathbb{F}^{(i)}) = \mathbb{E} \sum_{t=1}^{\tau} g\left(F_{\text{in}}^{\theta_i}(o_t^{(i)}) - F_{\text{out}}^{\theta_i}(o_t^{(i)})\right)$.

150 The algorithm 3 in Appendix B describes the simplest
151 training method, which solves the issue of exponential
152 action complexity with an increasing number of
153 agents. In this formulation, however, two issues arise:
154 the evaluation of ingoing flow $F_{\text{in}}^{(i)}(o^{(i)})$ becomes
155 harder as we need to find all transitions leading to
156 a given local observation (and not to a given global
157 state). This problem may be non-trivial as it is also
158 related to the actions of other agents. More impor-
159 tantly, in this case, the local reward is intractable, so
160 we cannot accurately estimate the reward $R^{(i)}(o^{(i)})$
161 of each node. Falling back to using the stochastic
162 reward $R^{(i)}(o^{(i)}) := R(s_t|o_t^{(i)})$ instead leads to transition uncertainty and spurious rewards, which
163 can cause non-stationarity and/or mode collapse as shown in Figure 2.

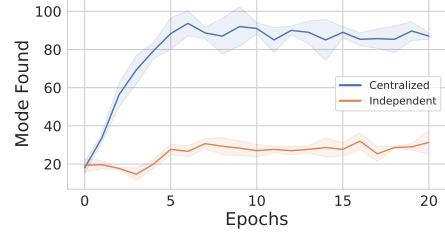


Figure 2: Performance comparison on Hypergrid task.

164 **2.3 Local-Global Training**

165 **2.3.1 Local-Global Principle: Joint Flow Network**

166 Local-global training is based upon the following local-global principle, which combined with
167 Theorem 1 ensures that the MA-GFlowNet has sampling distribution proportional to the reward R .

168 **Theorem 2** (Joint MA-GFlowNets). *Given local GFlowNets $\mathbb{F}^{(i)}$ on some environments
169 $(\mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)}, T^{(i)})$ there exists a global GFlowNets $\mathbb{F}^{\text{joint}}$ on a multi-agent environment
170 $(\prod_{i \in I} \mathcal{O}^{(i)}, \mathcal{A}, S, T)$ consistent with the local GFlowNets $\mathbb{F}^{(i)}$, such that*

$$F_{\text{out}}^* = \prod_{i \in I} F_{\text{out}}^{(i)*}, \quad F_{\text{in}} = \prod_{i \in I} F_{\text{in}}^{(i)}. \quad (4)$$

171 Moreover, if $\mathbb{F}^{\text{joint}}$ satisfies equation 1 for a reward R and each $\hat{R}^{(i)} \geq 0$ then $R = \prod_{i \in I} \hat{R}^{(i)}$.
172 Theorem 2 states that if the \tilde{T} guided by the local transition map $T^{(i)}$ is consistent with the true
173 transition map T , and the global reward R is the product of the local rewards, then the local and global
174 flow function satisfies the (4). Based on this conclusion, our Joint Flow Network (JFN) algorithm
175 leverages Theorem 2 by sampling trajectories with policy

$$o_t^{(i)} = p_i(s_t^{(i)}) \text{ and } \pi^{(i)}(o_t^{(i)} \rightarrow a_t^{(i)}), \quad i \in I \quad (5)$$

176 with $a_t = (a_t^{(i)} : i \in I)$ and $s_{t+1} = T(s_t, a_t)$, build formally the (global) joint GFlowNet from
177 local GFlowNets and train the collection of agent via the FM-loss of the joint GFlowNet. Equation 4
178 ensures that the inflow and outflow of the (global) joint GFlowNet are both easily computable from
179 the local inflows and outflows provided by agents. See algorithm 2.

Algorithm 2 Joint Flow Network Training Algorithm for MA-GFlowNets

Require: Number of agents N , A multi-agent environment $(\mathcal{S}, \mathcal{A}, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, p_i, S, T, R)$.

Require: Local GFlowNets $(\pi^{(i),*}, F_{\text{out}}^{(i)*}, F_{\text{init}}^{(i)})_{i \in I}$.

while not converged **do**

 Sample and add trajectories $(s_t)_{t \geq 0} \in \mathcal{T}$ to replay buffer with policy according to (5).

 Generate training distribution ν_{state} from replay buffer

 Apply minimization step of $\mathcal{L}_{\text{FM}}^{\text{stable}}(\mathbb{F}^{\theta, \text{joint}})$ for R

end while

180 This training regimen presents two key advantages: over centralized training, the action complexity
181 is linear w.r.t. the number of agents and local actions as in the independent training; over independent
182 training, the reward is not spurious. Indeed, in $\mathcal{L}_{\text{FM}}^{\text{stable}}(\mathbb{F}^{\theta, \text{joint}})$, by equation 4, the computation of
183 F_{in} and F_{out}^* reduces to computing the inflow and star-outflow for each local GFlowNets. Also,
184 only the global reward R appears. The remaining, possibly difficult, challenge is the estimation of
185 local ingoing flows from the local observations as it depends on the local transitions $T^{(i)}$, see first
186 point below. At this stage, the relations between the global/joint/local flow-matching constraints
187 are unclear, and furthermore, the induced policy of the local GFlowNets still depends on the yet
188 undefined local rewards. The following point clarify those links.

189 First, the collection of local GFlowNets induces local transitions kernels $T^{(i)} : \mathcal{O}^{(i)} \rightarrow \mathcal{O}^{(i)}$
190 which are not uniquely determined in general by a single GFlowNets. Indeed, the local policies
191 induce a global policy $\pi(s_t \rightarrow a_t) := \prod_{i \in I} \pi(o_t^{(i)} \rightarrow a_t^{(i)})$. Then, the (virtual) transition kernel
192 $T^{(i)}(a_t^{(i)}) = p^{(i)}(T(a_t) | a_t^{(i)})$ of the GFlowNets i depends on the distribution of states and the
193 corresponding actions of **all** local GFlowNets. See appendix A.5 for details. Note that $T^{(i)}$ are
194 derived from the actual environment T and the joint GFlowNets on the multi-agent environment with
195 the true transition T , while the Theorem above ensures splitting of star-inflows and virtual rewards
196 only for the approximated \tilde{T} . Furthermore, local rewards may be formalized as stochastic rewards to
197 take into account the lack of information of a single agent, but they are never used during training:
198 the allocation of rewards across agents is irrelevant. Only the virtual rewards $\hat{R}^{(i)} = F_{\text{out}}^{(i)*} - F_{\text{in}}^{(i)}$
199 are relevant but they are effectively free. As a consequence, Algorithm 2 effectively trains both the
200 joint flow as well as a product environment model. But since in general $T \neq \tilde{T}$ Algorithm 2 may fail
201 to reach satisfactory convergence.

202 Second, beware that in our construction of the joint MA-GFlowNets, there is no guarantee that the
203 global initial flow is split as the product of the local initial flows. In fact, we favor a construction in
204 which F_{init} is non-trivial to account for the inability of local agents to assess synchronization with
205 another agent. See Appendix A.8 for formalization details.

206 Third, we may partially link local and global flow-matching properties.

207 **Theorem 3.** Let $(\mathbb{F}^{(i)})_{i \in I}$ be local GFlowNets and let \mathbb{F} be their joint GFlowNets. Assume that none
208 of the local GFlowNets are zero and that each $\hat{R}^{(i)} \geq 0$. If \mathbb{F} satisfies equation 1, then there exists an
209 “essential” subdomain of each $\mathcal{O}^{(i)}$ on which local GFlowNets satisfy the flow-matching constraint.

210 The restriction regarding the domain on which local GFlowNets satisfy the flow-matching constraint
211 is detailed in Appendix A.8, this sophistication arises because of the stopping condition of the

212 multi-agent system. The essential domain may be informally formulated as “where the local agent
213 is still playing”: an agent may decide (or be forced) to stop playing, letting other agents continue
214 playing, the forfeited player is then on hold until the game stops and rewards are actually awarded.

215 To conclude, the joint GFlowNets provides an approximation of the target global GFlowNets, this
216 approximation may fail if the transition kernel T is highly coupled or if the reward is not a product.

217 2.3.2 Conditioned Joint Flow Network

218 Training of MA-GFlowNets via training of the virtual joint GFlowNets is an approximation of
219 the centralized training. In fact, the space of joint GFlowNets is smaller than that of the general
220 MA-GFlowNets, as only rewards that splits into the product $R(s) = \prod_{i \in I} R^{(i)}(o^{(i)})$ may be exactly
221 sampled. If the rewards are not of this form, the training may still be subject to a spurious reward or
222 mode collapse. One may easily build more sophisticated counter-examples based on this one.

223 Our proposed solution is to build a conditioned JFN inspired by augmented flows [21, 22] methods,
224 which allow the bypass of architectural constraints for Normalization flows [23]. The trick is to
225 add a shared “hidden” state to the joint MA-GFlowNets allowing the agent to synchronize. This
226 hidden state is constant across a given episode and may be understood as a cooperative strategy
227 chosen beforehand by the agents. Formally, this simply consist in augmenting the state space and the
228 observation spaces by a strategy space Ω to get $\tilde{\mathcal{S}} = \mathcal{S} \times \Omega$ and $\tilde{\mathcal{O}}^{(i)} = \mathcal{O}^{(i)} \times \Omega$, F_{init} is augmented
229 by a distribution \mathbb{P} on Ω , the observation projections as well as transition kernel act trivially on Ω
230 ie $T(s; \omega) = T(s)$ and $p^{(i)}(s; \omega) = (p^{(i)}(s), \omega)$. The joint MA-GFlowNets theorem applies the
231 same way, beware that the observation part of $T^{(i)}$ now have a dependency on Ω even though T
232 does not. In theory, Ω may be big enough to parameterize the whole trajectory space \mathcal{T} , in which
233 case it is possible to have decoupled conditioned local transition kernels $T^{(i)}(\cdot; \omega)$ so that $\tilde{T} = T$
234 on a relevant domain. Furthermore, the limitation on the reward is also lifted if the flow-matching
235 property is enforced on the expected joint flow $\mathbb{E}_\omega \mathbb{F}^{\text{joint}}$. Two possible losses may be considered:
236 $\mathbb{E}_\omega \mathcal{L}_{\text{FM}}^{\text{stable}}(\mathbb{F}^{\theta, \text{joint}}(\cdot; \omega))$ or $\mathcal{L}_{\text{FM}}^{\text{stable}}(\mathbb{E}_\omega \mathbb{F}^{\theta, \text{joint}}(\cdot; \omega))$. The former, which we use in our experiments, is
237 simpler to implement but does not a priori lift the constraint on the reward.

238 The training phase of the Conditioned Joint Flow Network (CJFN) is shown in Algorithm 4 in the
239 appendix. We first sample trajectories with policy $o_t^{(i)} = p_i(s_t^{(i)})$ and $\pi_\omega^{(i)}(o_t^{(i)} \rightarrow a_t^{(i)})$, $i \in I$ with
240 $a_t = (a_t^{(i)} : i \in I)$ and $s_{t+1} = T(s_t, a_t)$. Then we train the sampling policy by minimizing the FM
241 loss $\mathbb{E}_\omega \mathcal{L}_{\text{FM}}^{\text{stable}}(\mathbb{F}^{\theta, \text{joint}}(\cdot; \omega))$.

242 3 Related Works

243 Generative Flow Networks:

244 Nowadays, GFlowNets has achieved promising performance in many fields, such as molecule genera-
245 tion [2, 19, 24], discrete probabilistic modeling [25], structure learning [26], domain adaptation [27],
246 graph neural networks training [28, 29], and large language model training [30, 31, 32]. This network
247 could sample the distribution of trajectories with high rewards and can be useful in tasks where
248 the reward distribution is more diverse. GFlowNets is similar to reinforcement learning (RL) [33].
249 However, RL aims to maximize the expected reward favoring mode collapse onto the single highest
250 reward yielding action sequence, while GFlowNets favor diversity. Tiapkin et al. [34] bridged
251 GFlowNets to entropy-RL.

252 Comprehensive distributed GFlowNets framework is still lacking. Previously, the meta GFlowNets
253 algorithm [35] was proposed to solve the problem of GFlowNets distributed training but it requires
254 the observation state and task objectives of each agent to be the same, which is not suitable for
255 multi-agent problems. Later, a multi-agent GFlowNets algorithm was proposed in [36], but lacked
256 theoretical support and general framework. Connections between MA-GFlowNets and multi-agent
257 RL are discussed in Appendix C.

258 **Cooperative Multi-agent Reinforcement Learning:** There exist many MARL algorithms to solve
259 collaborative tasks. Two extreme algorithms for this purpose are independent learning [37] and
260 centralized training. Independent training methods regard the influence of other agents as part of the



Figure 3: The performance comparison results on the 3m map of StarCraft

261 environment, but the team reward function often has difficulty in measuring the contribution of each
 262 agent, resulting in the agent facing a non-stationary environment [9].

263 On the contrary, centralized training treats the multi-agent problem as a single-agent counterpart.
 264 However, this method has high combinatorial complexity and is difficult to scale beyond dozens of
 265 agents [7]. Therefore, the most popular paradigm is centralized training and decentralized execution
 266 (CTDE), including value-based [9, 11, 38, 10] and policy-based [39, 40, 41] methods. The goal of
 267 value-based methods is to decompose the joint value function among the agents for decentralized
 268 execution. This requires satisfying the condition that the local maximum of each agent’s value
 269 function should be equal to the global maximum of the joint value function.

270 The methods, VDN [9] and QMIX [11] employ two classic and efficient factorization structures,
 271 additivity and monotonicity, respectively, despite their strict factorization method. In QTRAN [38]
 272 and QPLEX [10], extra design features are introduced for decomposition, such as the factorization
 273 structure and advantage function. The policy-based methods extend the single-agent TRPO [42] and
 274 PPO [43] into the multi-agent setting, such as MAPPO [40], which has shown surprising effectiveness
 275 in cooperative multi-agent games. These algorithms maximize the long-term reward, however, it is
 276 difficult for them to learn more diverse policies in order to generate more promising results.

277 4 Experiments

278 We first verify the performance of CFN on a multi-agent hyper-grid domain where partition functions
 279 can be accurately computed. We then compare the performance of CFN and CJFN with standard
 280 MCMC and some RL methods to show that our proposed sampling distributions better match
 281 normalized rewards. All our code is done using the PyTorch [44] library. We re-implemented the
 282 multi-agent RL algorithms and other baselines.

283 4.1 Hyper-grid Environment

284 We consider a multi-agent MDP where states are the cells of a N -dimensional hypercubic grid of
 285 side length H . In this environment, all agents start from the initialization point $x = (0, 0, \dots)$, and
 286 are only allowed to increase coordinate i with action a_i . In addition, each agent has a stop action.
 287 When all agents choose the stop action or reach the maximum H of the episode length, the entire
 288 system resets for the next round of sampling. The reward function is designed as

$$R(x) = R_0 + R_1 \prod_i \mathbb{I}(0.25 < |x_i/H - 0.5|) + R_2 \prod_i \mathbb{I}(0.3 < |x_i/H - 0.5| < 0.4), \quad (6)$$

289 where $x = [x_1, \dots, x_I]$ includes all agent states and the reward term $0 < R_0 \ll R_1 < R_2$ leads a
 290 distribution of modes. The specific details about the environments and experiments can be found in
 291 the appendix.

292 We compare CFN and CJFN with a modified MCMC and RL methods. In the modified MCMC
 293 method [45], we allow iterative reduction of coordinates on the basis of joint action space and cancel
 294 the setting of stop actions to form an ergodic chain. As for the RL methods, we consider the maximum
 295 entropy algorithm, i.e., multi-agent SAC [46], and a previous cooperative multi-agent algorithm, i.e.,

296 MAPPO, [40]. To measure the performance of these methods, we use the normalized L1 error as
 297 $\mathbb{E}[|p(s_f) - \pi(s_f)| \times N]$ with $p(s_f) = R(s_f)/Z$ being the sample distribution computed by the true
 298 reward, where N is cardinality of the space of s_f .

299 Moreover, we can consider the mode found
 300 theme to demonstrate the superiority of the
 301 proposed algorithm.

302 Figure 4 illustrates the performance superiority
 303 of our proposed algorithm compared to other methods in the L1 error and Mode
 304 Found. We find that on small-scale environ-
 305 ments shown in Figure 4-Left, CFN can
 306 achieve the best performance because CFN
 307 can accurately estimate the flow of joint ac-
 308 tions when the joint action space dimension
 309 is small. There are two main reasons for the
 310 large L1-error index. First, we normalized
 311 the standard L1 error and multiplied it by a
 312 constant to avoid the inconvenience of visu-
 313 alization of a smaller magnitude. Secondly,
 314 when evaluating L1-error, we only sampled
 315 20 rounds for calculation, and with the in-
 316 crease of the number of samples, L1-error
 317 will further decrease. As the complexity
 318 of the estimation of action flow increases,
 319 we find that the performance of CFN de-
 320 grades while the joint-flow-based methods
 321 still achieve good estimation and maintain
 322 the speed of convergence, as shown in Fig-
 324 ure 4-Middle.

325 4.2 StarCraft

326 Figure 3 shows the performance of the proposed algorithm on the StarCraft 3m map [47], where (a)
 327 shows the win rate comparison with different algorithms, and (b) and (c) show the decision results
 328 sampled using the proposed algorithm. In the experiment, the outflow flow is calculated when the flow
 329 function is large, and the maximum flow is used to calculate the win rate when sampling. It can be
 330 found that since the experimental environment is not a sampling environment with diversified rewards,
 331 although the proposed algorithm is not significantly better than other algorithms, it still illustrates its
 332 potential in large-scale decision-making. In addition, the proposed algorithm can sample results with
 333 more diverse rewards, such as (b) and (c), and the number of units left implies the trajectory reward.

334 5 Conclusion

335 In this paper, we discussed the policy optimization problem when GFlowNets meets the multi-agent
 336 systems. Different from RL, the goal of MA-GFlowNets is to find diverse samples with probability
 337 proportional to the reward function. Since the joint flow is equivalent to the product of independent
 338 flow of each agent, we designed a CTDE method to avoid the flow estimation complexity problem in
 339 a fully centralized algorithm and the non-stationary environment in the independent learning process,
 340 simultaneously. Experimental results on Hyper-Grid environments and StarCraft task demonstrated
 341 the superiority of the proposed algorithms.

342 **Limitation and Future Work:** Our theory is incomplete as it does not apply to non-cooperative
 343 agents and has limited support of different game/agent terminations or initialization. A local-global
 344 principle beyond independent agent policies would also be particularly interesting. Our experiments
 345 do not cover the whole range of the theory in particular regarding continuous tasks and CJFN loss on
 346 projected GFN. An ablation study analyzing the tradeoff of small versus big condition space Ω would
 347 enlighten its importance. Finally, a metrization of the space of global GFlowNet would allow a more
 348 precise functional and optimization analysis of JFN/CJFN and their limitations.

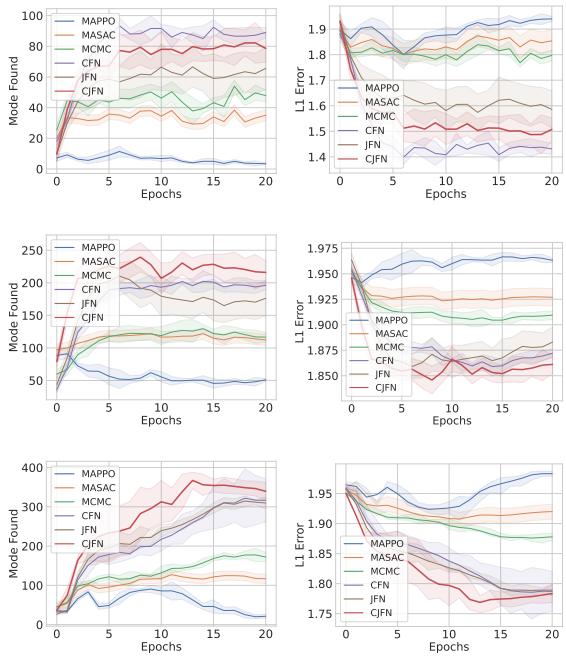


Figure 4: Mode Found (Left, higher is better) and L1 error (Right, lower is better) performance of different algorithms on hyper-grid environments. **Top:** Hyper-Grid v1, **Middle:** Hyper-Grid v2, **Bottom:** Hyper-Grid v3.

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476 **A Joint Flow Theory**

477 The goal of this section is to lay down so elementary points on the measurable theory of MA-
478 GFlowNets as well as prove the main theorem on the joint GFlowNet.

479 **A.1 Notations on Measures and Kernels**

480 We mostly use notations from [18] regarding kernels and measures. The measurable GFlowNet
481 formalism is that of [14] In the whole section, since we deal with technicalities, we use kernel
482 type notations for image by kernels and maps (seen as deterministic kernels). So that for a kernel
483 $K : X \rightarrow Y$ and a measure μ on X we denote by μK the measure on Y defined by $\mu K(B) =$
484 $\int_{x \in X} K(x \rightarrow B) d\mu(x)$ for $B \subset Y$ measurable and $\mu \otimes K$ is the measure on $X \times Y$ so that
485 $\mu \otimes K(A \times B) = \int_{x \in A} K(x \rightarrow B) d\mu(x)$. Recall that a measure ν dominates a measure μ which is
486 denoted $\mu \ll \nu$, if for all measurable A , $\nu(A) = 0 \Rightarrow \mu(A) = 0$. The Radon-Nykodim Theorem
487 ensures that if $\mu \ll \nu$ and μ, ν are finite then there exists $\varphi \in L^1(\nu)$ so that $\mu = \varphi \nu$. This function φ
488 is called the Radon-Nykodim derivative and is denoted $\frac{d\mu}{d\nu}$. We favor notations $\mu(A \rightarrow B)$ when μ is
489 a measure on $X \times Y$ and $A \subset X$ and $B \subset Y$; also $\mu(A \rightarrow \cdot)$ means the measure $B \mapsto \mu(A \rightarrow B)$.
490 We provide the notations in Table 1.

Table 1: The Descriptions of Different Notations

Notation	Descriptions
\mathcal{S}	state space, any measurable space with special elements s_0, s_f
λ	background measure on \mathcal{S} ; usually the counting measure on discrete spaces, or the Lebesgue measure on continuous spaces
\mathcal{A}	action space, a measurable space with special element STOP, it is a bundle over \mathcal{S}
$\mathcal{S}^{(i)} = \mathcal{O}^{(i)}$	state/observation space of agent i , same properties as \mathcal{S}
$\mathcal{A}^{(i)}$	action space of agent i , has a special element $\text{STOP}^{(i)}$, it is a bundle over $\mathcal{S}^{(i)}$
\mathcal{A}_s	action space on state s , ie the fiber above s of the bundle $\mathcal{A} \xrightarrow{s} \mathcal{S}$
$\mathcal{A}_{o^{(i)}}$	action space on observation $o^{(i)}$, ie the fiber above $o^{(i)}$ of the bundle $\mathcal{A}^{(i)} \xrightarrow{S^{(i)}} \mathcal{O}^{(i)}$
S	state map $S(s, a) = s$, i.e., return the current state s
$S^{(i)}$	state map of agent i
T	Transition map $T(s, a) = T_s(a) = s'$, i.e., transfer the current state s into next state s'
$T^{(i)}$	Transition map of agent i , depend in general of the chosen action of all agent and is thus stochastic
R	the reward measure on $\mathcal{S} \setminus \{s_0, s_f\}$, usually known via its density r with respect to the background measure λ
$R^{(i)}$	the perceived reward measure of agent i , usually intractable and stochastic
\hat{R}	the GFlowNet reward measure on $\mathcal{S} \setminus \{s_0, s_f\}$ used at inference time instead of R for stop decision making
$\hat{R}^{(i)}$	the GFlowNet reward measure of agent i on $\mathcal{O}^{(i)} \setminus \{s_0, s_f\}$ used at inference time instead of $R^{(i)}$ for stop decision making
F_{out}	out-flow or state-flow, non-negative measure on $\mathcal{S} \setminus \{s_0, s_f\}$
$F_{\text{out}}^{(i)}$	out-flow or state-flow of agent (i) , non-negative measure on $\mathcal{O}^{(i)} \setminus \{s_0, s_f\}$
F_{out}^*	star out-flow, non-negative measure on the space $\mathcal{S} \setminus \{s_0, s_f\}$ such that $F_{\text{out}}^* := F_{\text{out}} - R$
$F_{\text{out}}^{(i),*}$	star out-flow of agent i , non-negative measure on the space $\mathcal{O}^{(i)} \setminus \{s_0, s_f\}$ such that $F_{\text{out}}^{(i),*} = F_{\text{out}}^{(i)} - R^{(i)}$
π	the forward policy, can call STOP action
π^*	the forward policy defined on the space $\mathcal{S} \setminus \{s_0, s_f\}$, does not call STOP action
$\pi^{(i)}$	the forward policy of agent i , can call STOP action
$\pi^{(i),*}$	the star forward policy of agent i defined on the space $\mathcal{S} \setminus \{s_0, s_f\}$, does not call STOP action
F_{init}	the unnormalized distribution used to sample s_1 while moving $s_0 \rightarrow s_1$
$F_{\text{init}}^{(i)}$	the unnormalized distribution used by agent i to sample $s_1^{(i)}$ while moving $s_0 \rightarrow s_1$
$r(s)$	the density of reward at s on a continuous statespace

491 **A.2 An Introduction for Notations**

492 We understand that our formalism is abstract, this section is devoted justifying our choices and
493 providing examples.

494 **A.2.1 Motivations**

495 To begin with, our motivation to formalize the action space as a measurable bundle $\mathcal{A} := \{(s, a) \mid s \in$
 496 $\mathcal{S}, a \in \mathcal{A}_s\} \xrightarrow{S} \mathcal{S}$ is three fold:

- 497 1. The available actions from a state may depend on the state itself: on a grid, the actions
 498 available while on the boundary of the grid are certainly more limited than while in the
 499 middle. More generally, on a graph, actions are typically formalized by edges $s \xrightarrow{a} s'$ of the
 500 graph, the data of an edge contains both the origin s and the destination s' . In other words,
 501 on graphs, actions are bundled with an origin state. It is thus natural to consider the actions
 502 as bundled with the origin state. When an agent is transiting from a state to another via an
 503 action, the state map tells where it comes from while the transition map tells where it is
 504 going.
- 505 2. We want our formalism to cover as many cases as possible in a unified way: Graphs, vector
 506 spaces with linear group actions or mixture of discrete and continuous state spaces. Measures
 507 and measurable spaces provide a nice formalism to capture the quantity of reward on a given
 508 set or a probability distribution.
- 509 3. We want a well-founded and possibly standardized mathematical formalism. In particular,
 510 the policy takes as input a state and returns a distribution of actions. the actions should
 511 correspond to the input state. To avoid having a cumbersome notion of policy as a family of
 512 distributions π_s each on \mathcal{A}_s , we prefer to consider the union of the state-dependent action
 513 spaces $\mathcal{A} := \bigcup_{s \in \mathcal{S}} \mathcal{A}_s$ and define the policy as Markov kernel $\mathcal{S} \rightarrow \mathcal{A}$. However, we still
 514 need to satisfy the constraint that the distribution $\pi(s)$ is supported by \mathcal{A}_s . Bundles are
 515 usual mathematical objects formalizing such situations and constraints and are thus well
 516 suited for this purpose and the constraint is easily expressed as $S \circ \pi(s) = s, \forall s \in \mathcal{S}$.

517 Our synthetic formalism comes with a few drawbacks due to the level of abstraction:

- 518 1. The notation $\pi(s)$ differs from the more common notation $\pi(s, a)$ as the action already
 519 contains s implicitly.
- 520 2. We need to use Radon-Nikodym derivative. At a given state, on a graph, a GFlowNets has a
 521 probability of stopping

$$\mathbb{P}(\text{STOP}|s) = \frac{R(s)}{F_{\text{out}}(s)}.$$

On a continuous statespace with reference measure λ , the stop probability is

$$\mathbb{P}(\text{STOP}|s) = \frac{r(s)}{f_{\text{out}}(s)}$$

520 where $r(s)$ is the density of reward at s and $f_{\text{out}}(s)$ is the density of outflow at s . A natural
 521 measure-theoretic way of writing these equations as one is via Radon-Nikodym derivation:
 522 given two measures μ, ν ; if $\mu(X) = 0 \Rightarrow \nu(X) = 0$ for any measurable $X \subset \mathcal{S}$ then μ is
 523 said to dominate ν and, by Radon-Nikodym Theorem, there exists a measurable function
 524 $\varphi \in L^1(\mu)$ such that $\nu(X) = \int_{x \in X} \varphi(x) d\nu(x)$ for all measurable $X \subset \mathcal{S}$. This φ is the
 525 Radon-Nikodym derivative $\frac{d\nu}{d\mu}$.

If one has a measure λ dominating both R and F_{out} and if F_{out} dominated R then

$$\mathbb{P}(\text{STOP}|s) := \frac{dR}{dF_{\text{out}}}(s) = \frac{dR}{d\lambda}(s) \times \left(\frac{dF_{\text{out}}}{d\lambda} \right)^{-1}.$$

526 When \mathcal{S} is discrete, we choose λ as the counting measure, and we recover the graph formula
 527 above. When \mathcal{S} is continuous, we choose λ as the Lebesgue measure, and we recover the
 528 second formula.

529 **A.2.2 Example**

Consider the D -dimensional W -width hypergrid case with agent set I , see Figure 5. The state space
 is the finite set $\mathcal{S} = (\{1, \dots, W\}^D)^I$, say each agent only observes its own position on the grid

so that $\mathcal{O}^{(i)} = \{1, \dots, W\}^D$. the observation-dependent action space of the i -th agent $\mathcal{A}_{o^{(i)}}$ is a subset of $H := \{\pm \mathbf{1}_k : 1 \leq k \leq W\}$ where $\mathbf{1}_k$ is the hot-one array $(0, \dots, 0, 1, 0, \dots, 0)$ with a one at the k -th coordinate. The set $\mathcal{A}_{o^{(i)}}$ depends on s : if $1 < s_k < W$ then $\mathcal{A}_{o^{(i)}} = \{\pm \mathbf{1}_k : 1 \leq k \leq W\} \cup \{\text{STOP}\}$ but if $s_k = 1$ then $-\mathbf{1}_k \notin \mathcal{A}_{o^{(i)}}$ and similarly if $s_k = W$. The local total action space is then

$$\mathcal{A}_{o^{(i)}}^{(i)} = \{(s, a) \mid 1 \leq s_k \leq W \text{ and } 1 \leq s_k + a_k \leq W\} \cup \{\text{STOP}\} \subset \{1, \dots, W\}^D \times H \cup \{\text{STOP}\}.$$

530 The local state maps $S^{(i)}$ is $S^{(i)}(o^{(i)}, a) = o^{(i)}$. Since each agent may choose its action freely, for
531 any $s \in \mathcal{S}$, $\mathcal{A}_s = \prod_{i \in I} \mathcal{A}_{o^{(i)}} / \sim$ however, since $\mathcal{A}_{o^{(i)}}$ depends on i and s then $\mathcal{A} \neq \prod_{i \in I} \mathcal{A}_{o^{(i)}} / \sim$.

The local transition kernel $T^{(i)}$ depends both on the global transition kernel and the policies of all the agents. Two possible choices of transitions depend on whether the agent interacts or not. In the non-interacting case $T_1(s, a) = s + a$. If agents may not occupy the same position then the transition rejects the action if the agent moving would put them in the same position; so $T_2(s, a) = s + a$ if $s + a$ is legal, otherwise $p^{(i)} \circ T_2(s, a) = o^{(i)}$ for some i . The simplest T_2 is to choose $T_2(s, a) = s$ if $s + a$ is illegal. In this case

$$T_2^{(i)}(o^{(i)}, a^{(i)}) = \mathbb{P}(s + a \text{ is legal} | o^{(i)}, a^{(i)}) \delta_{o^{(i)} + a^{(i)}} + \mathbb{P}(s + a \text{ is illegal} | o^{(i)}, a^{(i)}) \delta_{o^{(i)}}.$$

532 Clearly, $\mathbb{P}(s + a \text{ is legal} | o^{(i)}, a^{(i)})$ depends on the policies and positions of all the agents, then so
533 does the local transition kernels $T_2^{(i)}$.

534 A non-negative measure μ on \mathcal{S} is any function of the form $\mu(X) = \sum_{x \in X} f(x)$ with $f : \mathcal{S} \rightarrow \mathbb{R}_+$
535 any function. Defining the counting measure $\lambda(X) := \sum_{x \in X} 1 = \text{Card}(X)$ we have $\mu = f\lambda$ as
536 measures on \mathcal{S} , or equivalently, $\frac{d\mu}{d\lambda} = f$. We may thus translate any reward or probability distribution
537 on such a hypergrid as a measure.

A policy is a Markov kernel $\mathcal{S} \rightarrow \mathcal{A}$ such that $S \circ \pi = \text{Identity}$. More concretely, it means we have a function that associates to any state s a probability distribution on \mathcal{A} with support on elements of the form (s, a) with $a \in \mathcal{A}_s$. From the description of measures, such a policy is fully described by a function $q : \mathcal{A} \rightarrow \mathbb{R}_+$ such that

$$\forall s \in \mathcal{S}, \sum_{a \in \mathcal{A}_s} q(s, a) = 1.$$

538 The policy is then $\pi(s) = \sum_{a \in \mathcal{A}_s} q(s, a) \delta_{(s, a)}$.

A GFlowNet on this hypergrid in reward-less notations is given by $(F_{\text{init}}, \pi^*, F_{\text{out}}^*)$. Now, F_{init} is any measure on \mathcal{S} , it may be given by a pre-chosen family of categorical distribution of the finite set \mathcal{S} . For big W, D and I , since F_{init} have limited number of parameters, we may choose $F_{\text{init}} = C\delta_{s_1}$ for some s_1 , and some trainable constant C . The star-policy is similar to π except that the STOP action is absent:

$$\pi^*(s) = \sum_{a \in \mathcal{A}_s \setminus \{\text{STOP}\}} q^*(s, a), \quad Z(s) := \sum_{a' \in \mathcal{A}_s \setminus \{\text{STOP}\}} q(s, a').$$

Finally, F_{out} is measure and is thus of the form

$$F_{\text{out}}^*(X) := \sum_{x \in X} f_{\text{out}}^*(x)$$

539 for some function $f_{\text{out}}^* : \mathcal{S} \rightarrow \mathbb{R}_+$.

540 Standard notation GFlowNet is then recovered, given a reward $r : \mathcal{S} \rightarrow \mathbb{R}_+$, via:

- 541 • $R(X) = \sum_{x \in X} r(x)$;
- 542 • $F_{\text{out}}(X) = \sum_{x \in X} f_{\text{out}}(x)$ with $\forall s \in \mathcal{S}, f_{\text{out}}(s) = f_{\text{out}}^*(s) + r(s)$;
- 543 • $q(s, a) = \frac{f_{\text{out}}^*(s)}{f_{\text{out}}(s)} q^*(s, a)$ if $a \neq \text{STOP}$ and $q(s, \text{STOP}) = \frac{r(s)}{f_{\text{out}}(s)}$.

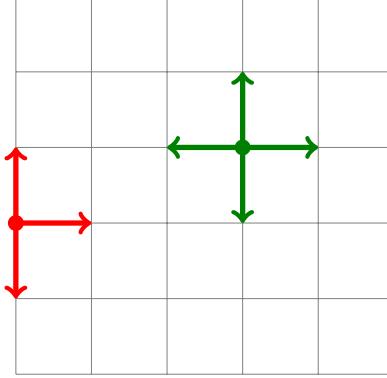


Figure 5: 2 agents on the 2D6W grid with available moves depicted.

544 **A.3 Environment structures**

545 We introduce first a hierarchy of single-agent environment structures.

- 546 547 548 • An action environment is a triplet $(\mathcal{S}, \mathcal{A}, S)$ with $\mathcal{A} \xrightarrow{S} \mathcal{S}$ a measurable map between measurable space is called of state space \mathcal{S} , action space \mathcal{A} and State map S . We denote $\mathcal{A}_s := \{a \in \mathcal{A} \mid aS = s\}$.
- 549 550 • An interactive environment is a quadruple $(\mathcal{S}, \mathcal{A}, S, T)$ where $(\mathcal{S}, \mathcal{A}, S)$ is an action environment and $T : \mathcal{A} \rightarrow \mathcal{S}$ is a quasi-Markov kernel.
- 551 552 553 • A Game environment is a quintuple $(\mathcal{S}, \mathcal{A}, S, T, R)$ where $(\mathcal{S}, \mathcal{A}, S, T)$ is an interactive environment and R is a finite non-negative non-zero measure on \mathcal{S} . We may allow the reward to be stochastic so formally, R is allowed to be random measure instead [48].

554 For multi-agent environment, we have a similar hierarchy:

- A multi-agent action environment is a tuple $(\mathcal{S}, \mathcal{A}, S, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)}, p^{(i)})_{i \in I}$ with $(\mathcal{S}, \mathcal{A}, S)$ and each $(\mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)})$ being mono-agent action environments. Furthermore, we assume $\mathcal{S} = \prod_{i \in I} \mathcal{O}^{(i)}$ and $p^{(i)} : \mathcal{S} \rightarrow \mathcal{O}^{(i)}$ are the natural projection maps. Also

$$\forall s \in \mathcal{S}, \quad \mathcal{A}_s \setminus \{\text{STOP}\} = \prod_{i \in I} \left(\mathcal{A}_{p^{(i)}(s)}^{(i)} \setminus \{\text{STOP}\} \right).$$

- 555 556 557 • A multi-agent interactive environment is a tuple $(\mathcal{S}, \mathcal{A}, S, T, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)}, p^{(i)})_{i \in I}$ where $(\mathcal{S}, \mathcal{A}, S, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)}, p^{(i)})_{i \in I}$ is a multi-agent action environment and $(\mathcal{S}, \mathcal{A}, S, T)$ is a mono-agent interactive environment.
- 558 559 560 • A multi-agent game environment is a tuple $(\mathcal{S}, \mathcal{A}, S, T, R, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)}, p^{(i)})_{i \in I}$ such that $(\mathcal{S}, \mathcal{A}, S, T, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)}, p^{(i)})_{i \in I}$ is multi-agent interactive environment and $(\mathcal{S}, \mathcal{A}, S, T, R)$ is a mono-agent game environment.

561 **A.4 GFlowNet in a Game Environment**

562 A generative flow networks may be formally defined on an action environment $(\mathcal{S}, \mathcal{A}, S)$, as a triple $(\pi^*, F_{\text{out}}^*, F_{\text{init}})$ where $\pi^* : \mathcal{S} \rightarrow \mathcal{A}$ is a Markov kernel such that $\pi^* S = \text{Id}_{\mathcal{S}}$, F_{out}^* and F_{init} are a finite non-negative measures on \mathcal{S} . Furthermore, we assume that for all $s \in \mathcal{S}$, $\pi^*(s \rightarrow \text{STOP}_s) = 0$.

565 On an interactive environment $(\mathcal{S}, \mathcal{A}, S, T)$, given a GFlowNet $(\pi^*, F_{\text{out}}^*, F_{\text{init}})$, we define the ongoing flow as $F_{\text{in}} := F_{\text{out}}^* \pi^* T + F_{\text{init}}$ and the GFlowNet induces an virtual reward $\hat{R} := F_{\text{in}} - F_{\text{out}}^*$. Note that the virtual reward is always finite as the star-outflow and the initial flow are both finite and π^* and T are Markovian.

569 **Definition 1** (Weak Flow-Matching Constraint). *The weak flow-matching constraint is defined as*

$$\hat{R} \geq 0 \tag{7}$$

570 If the GFlowNet satisfies the weak flow-matching constraint, we may define a virtual GFlowNet
 571 policy as

$$\hat{\pi} := \frac{dF_{\text{out}}^*}{dF_{\text{in}}} \pi^* \quad (8)$$

572 where δ_{STOP} is the deterministic Markov kernel sending any s to STOP_s . The virtual action and edge
 573 flows are:

$$\hat{F}_{\text{action}} := F_{\text{in}} \otimes \hat{\pi} \in \mathcal{M}^+(\mathcal{S} \times \mathcal{A}); \quad (9)$$

$$\hat{F}_{\text{edge}} := F_{\text{in}} \otimes (\hat{\pi}T) \in \mathcal{M}^+(\mathcal{S} \times \mathcal{S}). \quad (10)$$

575 In a game environment, a GFlowNet comes with an outgoing flow, a natural policy, a natural action
 576 flow and a natural edge flow

$$F_{\text{out}} := F_{\text{out}}^* + R \quad (11)$$

$$\pi := \frac{dF_{\text{out}}^*}{dF_{\text{out}}} \pi^* \quad (12)$$

$$F_{\text{edge}} := F_{\text{out}} \otimes (\pi T) \in \mathcal{M}^+(\mathcal{S} \times \mathcal{S}) \quad (13)$$

$$F_{\text{action}} := F_{\text{out}} \otimes \pi \in \mathcal{M}^+(\mathcal{S} \times \mathcal{A}). \quad (14)$$

580 By abuse of notation we also write F_{action} (resp. \hat{F}_{action}) for $F_{\text{out}}\pi$ (resp. $F_{\text{in}}\pi$). and the flow-
 581 matching property may be rewritten as follows.

582 **Definition 2** (Flow-Matching Constraint). *The flow-matching constraint on a Game environment
 583 $(\mathcal{S}, \mathcal{A}, S, T, R)$ is defined as*

$$\hat{R} = \mathbb{E}(R). \quad (15)$$

584 **Remark 1.** *In an interactive environment $(\mathcal{S}, \mathcal{A}, S, T, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)}, p^{(i)})_{i \in I}$, a GFlowNet satisfying
 585 the weak flow-matching constraint satisfies the (strong) flow-matching constraint on the Game
 586 environment $(\mathcal{S}, \mathcal{A}, S, T, \hat{R}, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)}, p^{(i)})_{i \in I}$.*

587 We may recover part of the GFlowNets $(\pi^*, F_{\text{out}}^*, F_{\text{init}})$ from any of F_{action} , \hat{F}_{action} as in general:

$$\pi^*(x \rightarrow A) = \frac{dF_{\text{action}}(\cdot \rightarrow A \setminus \text{STOP})}{dF_{\text{action}}(\cdot \rightarrow \mathcal{A} \setminus \text{STOP})} = \frac{d\hat{F}_{\text{action}}(\cdot \rightarrow A \setminus \text{STOP})}{d\hat{F}_{\text{action}}(\cdot \rightarrow \mathcal{A} \setminus \text{STOP})} \quad (16)$$

$$R = F_{\text{action}}(\cdot \rightarrow \text{STOP}) \quad \hat{R} = \hat{F}_{\text{action}}(\cdot \rightarrow \text{STOP}) \quad (17)$$

$$F_{\text{out}}^* = F_{\text{action}}(\cdot \rightarrow \mathcal{A}) - R = \hat{F}_{\text{action}}(\cdot \rightarrow \mathcal{A}) - \hat{R} \quad (18)$$

$$F_{\text{init}} = F_{\text{out}}^* T + \hat{R} \quad (19)$$

591 If the flow-matching constraint is satisfied, then

$$F_{\text{init}} = F_{\text{out}}^* T + R. \quad (20)$$

592 Before going further, the presence densities.

593 **Definition 3.** *Let $\mathbb{F} = (\pi^*, F_{\text{out}}, F_{\text{init}})$ be a GFlowNet in an interactive environment
 594 $(\mathcal{S}, \mathcal{A}, S, T, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)}, p^{(i)})_{i \in I}$.*

The initial density of \mathbb{F} is the probability distribution

$$\nu_{\mathbb{F}, \text{init}} := \frac{1}{F_{\text{init}}(\mathcal{S})} F_{\text{init}}$$

The virtual presence density of \mathbb{F} is the probability distribution $\hat{\nu}_{\mathbb{F}}$ defined by

$$\hat{\nu}_{\mathbb{F}} \propto \sum_{t=0}^{\infty} \nu_{\mathbb{F}, \text{init}} \hat{\pi}^t.$$

The anticipated presence density of \mathbb{F} is the probability distribution $\bar{\nu}_{\mathbb{F}}$ defined by

$$\bar{\nu}_{\mathbb{F}} := \frac{1}{F_{\text{in}}(\mathcal{S})} F_{\text{in}}.$$

In a game environment, the presence density of \mathbb{F} is the probability distribution $\nu_{\mathbb{F}}$ defined by

$$\nu_{\mathbb{F}} \propto \sum_{t=0}^{\infty} \nu_{\mathbb{F}, \text{init}} \pi^t.$$

595 **Lemma 1.** *Let \mathbb{F} be a GFlowNet in an interactive environment satisfying the weak flow-matching
596 constraint. If $\hat{\nu}_{\mathbb{F}} \gg \bar{\nu}_{\mathbb{F}}$, then $\hat{\nu}_{\mathbb{F}} = \bar{\nu}_{\mathbb{F}}$.*

597 *Proof.* Let $(\mathcal{S}, \mathcal{A}, S, T, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)}, p^{(i)})_{i \in I}$ be the interactive environment and let $\mathbb{F} =$
598 $(\pi^*, F_{\text{out}}, F_{\text{init}})$. To begin with, $\mathbb{F}' := (\pi^*, F_{\text{init}}(\mathcal{S})\hat{\nu}_{\mathbb{F}} - \hat{R}, F_{\text{init}})$ is a GFlowNet satisfying
599 the strong flow-matching constraint for reward \hat{R} , its edgeflow F'_{edge} may be compared to the
600 edgeflow F_{edge} of \mathbb{F} : by Proposition 2 of [15], we have $F_{\text{edge}} \geq F'_{\text{edge}}$, and the difference
601 $F_{\text{edge}} - F'_{\text{edge}}$ is a 0-flow in the sense this same article. Also, the domination hypothesis implies that
602 $F'_{\text{edge}} \gg F_{\text{edge}} \gg F_{\text{edge}}^0 := F_{\text{edge}} - F'_{\text{edge}}$. Since the edge-policy of F_{edge} is the same as that of F'_{edge}
603 we deduce that it is also the same as F_{edge}^0 . By the same Proposition 2, we have $F'_{\text{out}}\pi^t \xrightarrow{t \rightarrow +\infty} 0$,
604 therefore, $\mu\pi^t \xrightarrow{t \rightarrow +\infty} 0$ for any $\mu \ll F'_{\text{out}}$. Again by domination, $F'_{\text{edge}} \gg F_{\text{edge}}^0$ we deduce that
605 $F'_{\text{out}} \gg F_{\text{out}}^0$. Therefore, $F'_{\text{out}}\pi^t \xrightarrow{t \rightarrow +\infty} 0$. Finally, since \mathbb{F}^0 is a 0-flow, $F'_{\text{out}}\pi = F_{\text{out}}^0$, we deduce
606 that $F_{\text{out}}^0 = 0$ and thus $F_{\text{edge}} = F'_{\text{edge}}$ ie $\hat{\nu}_{\mathbb{F}} = \bar{\nu}_{\mathbb{F}}$. \square

607 **Remark 2.** *As long as the GFlowNets considered are trained using an FM-loss on a training training
608 distribution ν_{state} extracted from trajectory distributions $\hat{\nu}_{\mathbb{F}}$ or $\nu_{\mathbb{F}}$ of the GFlowNets themselves,
609 we may assume that $\hat{\nu}_{\mathbb{F}} \gg \bar{\nu}_{\mathbb{F}}$ as flows are only evaluated on a distribution dominated by $\nu_{\mathbb{F}}$. The
610 singular part with respect to $\nu_{\mathbb{F}}$ is irrelevant for training purposes as well as inference purposes.
611 Therefore, we may generally assume that $\hat{\nu} = \bar{\nu}$*

612 **Remark 3.** *The main interest of the virtual reward \hat{R} is for cases where the reward is not accessible
613 or expensive to compute. Since a GFlowNet satisfying the weak flow-matching property always
614 satisfies the strong flow-matching property for the reward \hat{R} , the sampling Theorem usually applies
615 to \hat{R} . Therefore, \hat{R} may be used as a reward during inference instead of the true reward R so that we
616 actually sample using the policy $\hat{\pi}$ instead of π .*

617 A.5 MA-GFlowNets in multi-agent environments (I): Preliminaries

618 To begin with, let us define a MA-GFlowNet on a multi-agent environment.

619 **Definition 4.** *An MA-GFlowNet on a multi-agent action environment is the data of a global GFlowNet
620 \mathbb{F} on $(\mathcal{S}, \mathcal{A}, S)$ and a collection of local GFlowNets $\mathbb{F}^{(i)}$ on $(\mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)})$ for $i \in I$.*

621 We give ourselves a multi-agent interactive environment $(\mathcal{S}, \mathcal{A}, S, T, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)}, p^{(i)})$. We wish
622 to clarify the links between local and global GFlowNet.

- 623 • A priori, there the local GFlowNets are merely defined on an action environment, they lack
624 both the local transition kernel $T^{(i)}$ and the reward $R^{(i)}$.
- 625 • Given a global GFlowNet, we wish to define local GFlowNets.
- 626 • Given a family of local GFlowNets, we wish to define a global GFlowNet.

627 For simplicity sake, for any GFlowNet \mathbb{F} defined on an interactive environment satisfying the weak
628 flow-matching constraint, we set $R = \hat{R}$ and apply remark 2 assume that $\hat{\nu}_{\mathbb{F}} = \bar{\nu}_{\mathbb{F}} = \nu_{\mathbb{F}}$.

629 **Definition 5.** *Let $(\mathcal{S}, \mathcal{A}, S, T, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)}, p^{(i)})$ be a multi-agent interactive environment and let
630 $\mathbb{F} = (\pi^*, F_{\text{out}}^*, F_{\text{init}})$ be a GFlowNet on $(\mathcal{S}, \mathcal{A})$ satisfying the weak flow-matching constraint. We
631 introduce the following:*

- 632 • the local presence probability distribution $\nu_{\mathbb{F}}^{(i)} := \nu_{\mathbb{F}} p^{(i)}$;
- 633 • the measure map $o^{(i)} \mapsto \nu_{\mathbb{F}|o^{(i)}}$ as the disintegration of $\nu_{\mathbb{F}}$ by $p^{(i)}$
- 634 • the Markov kernel $\tilde{\pi}^{(i)} : \mathcal{O}^{(i)} \rightarrow \mathcal{A}$ by $\delta_{o^{(i)}} \tilde{\pi}^{(i)} := \nu_{\mathbb{F}|o^{(i)}} \pi$;
- 635 • the Markov kernel $\pi^{(i)} : \mathcal{O}^{(i)} \rightarrow \mathcal{A}^{(i)}$ by $\pi^{(i)} = \tilde{\pi}^{(i)} p^{(i)}$;
- 636 • the Markov kernel $T^{(i)} : \mathcal{A}^{(i)} \rightarrow \mathcal{O}^{(i)}$ by $T^{(i)} = S^{(i)} \tilde{\pi}^{(i)} T p^{(i)}$;

The situation may be summarized by the following diagram:

$$\begin{array}{ccc}
 (\mathcal{S}, \nu_{\mathbb{F}}) & \begin{array}{c} \xleftarrow{\pi} \\ \xleftarrow{S} \\ \xleftarrow{T} \end{array} & (\mathcal{A}, \nu_{\mathbb{F}}\pi) \\
 \downarrow p^{(i)} & \nearrow \tilde{\pi}^{(i)} & \downarrow p(i) \\
 (\mathcal{O}^{(i)}, \nu_{\mathbb{F}}^{(i)}) & \begin{array}{c} \xleftarrow{\pi^{(i)}} \\ \xleftarrow{S^{(i)}} \\ \xleftarrow{T^{(i)}} \end{array} & (\mathcal{A}^{(i)}, \nu_{\mathbb{F}}^{(i)}\pi^{(i)}) \\
 \end{array}$$

637 Before going further, we need to check that these definitions are somewhat consistent.

Lemma 2. *The following diagrams are commutative in the category of probability spaces.*

$$\begin{array}{ccc}
 (\mathcal{S}, \nu_{\mathbb{F}}) & \begin{array}{c} \xleftarrow{\pi} \\ \xleftarrow{S} \\ \xleftarrow{T} \end{array} & (\mathcal{A}, \nu_{\mathbb{F}}\pi) \\
 \downarrow p^{(i)} & \nearrow \tilde{\pi}^{(i)} & \downarrow p(i) \\
 (\mathcal{O}^{(i)}, \nu_{\mathbb{F}}^{(i)}) & \begin{array}{c} \xleftarrow{\pi^{(i)}} \\ \xleftarrow{S^{(i)}} \\ \xleftarrow{T^{(i)}} \end{array} & (\mathcal{A}^{(i)}, \nu_{\mathbb{F}}^{(i)}\pi^{(i)}) \\
 \end{array}
 \quad
 \begin{array}{ccc}
 (\mathcal{S}, \nu_{\mathbb{F}}\pi T) & \xleftarrow{T} & (\mathcal{A}, \nu_{\mathbb{F}}\pi) \\
 \downarrow p^{(i)} & & \downarrow p(i) \\
 (\mathcal{O}^{(i)}, \nu_{\mathbb{F}}^{(i)}\pi^{(i)}T^{(i)}) & \xleftarrow{T^{(i)}} & (\mathcal{A}^{(i)}, \nu_{\mathbb{F}}^{(i)}\pi^{(i)}) \\
 \end{array}$$

638 *Proof.* For the left diagram, with the definition chosen, we only need to check that $\nu_{\mathbb{F}}^{(i)}\tilde{\pi}^{(i)} = \nu_{\mathbb{F}}\pi$.

639 For all $\varphi \in L^1(\mathcal{A}, \nu_{\mathbb{F}}\pi)$ we have

$$\begin{aligned}
 \int_{s \in \mathcal{A}} \varphi(a) d(\nu_{\mathbb{F}}\pi)(a) &= \int_{s \in \mathcal{S}} \int_{a \in \mathcal{A}} \varphi(a) d\pi(s, a) d\nu_{\mathbb{F}}(s) \\
 &= \int_{o^{(i)} \in \mathcal{O}^{(i)}} \int_{s \in (p^{(i)})^{-1}(o^{(i)})} \int_{a \in \mathcal{A}} \varphi(a) d\pi(s, a) d\nu_{\mathbb{F}|o^{(i)}}(s) d\nu_{\mathbb{F}}^{(i)}(o^{(i)}) \\
 &= \int_{o^{(i)} \in \mathcal{O}^{(i)}} \int_{a \in \mathcal{A}} \varphi(a) d\tilde{\pi}^{(i)}(a) d\nu_{\mathbb{F}}^{(i)}(o^{(i)}) \\
 &= \int_{a \in \mathcal{A}} \varphi(a) d(\nu_{\mathbb{F}}^{(i)}\tilde{\pi}^{(i)})(a).
 \end{aligned}$$

For the right diagram, we need to check that $\nu_{\mathbb{F}}\pi p^{(i)} = \nu_{\mathbb{F}}^{(i)}\pi^{(i)}$ and that $\nu_{\mathbb{F}}\pi T p^{(i)} = \nu_{\mathbb{F}}^{(i)}\pi^{(i)}T^{(i)}$. We already proved the first equality for the left diagram and for the second:

$$\nu_{\mathbb{F}}\pi p^{(i)}T^{(i)} := \nu_{\mathbb{F}} \underbrace{\pi p^{(i)}S^{(i)}\tilde{\pi}^{(i)}T^{(i)}}_{=p^{(i)}} = \underbrace{\nu_{\mathbb{F}} p^{(i)}\tilde{\pi}^{(i)}T^{(i)}}_{\nu_{\mathbb{F}}^{(i)}} = \nu_{\mathbb{F}}^{(i)}\pi^{(i)}T^{(i)}$$

640 □

641 We see that from a global GFlowNet, we may build local policies as well as local transition kernels.
 642 These policies and transitions are natural in the sense that of local the induced local agent policy and
 643 transition are exactly the one we'd have if the observations of the other agents were provided as
 644 a random external parameter. The local rewards are then stochastic depending on the state of the
 645 global GFlowNet.

646 A.6 MA-GFlowNets in multi-agent environments (II): from local to global

647 We would like to settle construction of global GFlowNet from local ones, key difficulties arise:

648 • the global distributions induce local ones but the coupling of the local distributions may be
 649 non trivial;

- the defining the star-outflow and initial flow requires to find proportionality constants

$$F_{\text{in}}(\mathcal{O}^{(i)}) \propto \nu_{\mathbb{F}}^{(i)} \quad F_{\text{init}}^{(i)} \propto \nu_{\mathbb{F}^{(i)}, \text{init}};$$

650 • The coupling of the local transition kernels $T^{(i)}$ and the global one is in general non-trivial.

651 We try to solve these issues by looking at the simplest coupling: independent local agents. Recall
652 that $\mathcal{A}_s^* = \prod_{i \in I} \mathcal{A}_s^{(i),*}$ therefore, independent coupling means that $\pi^*(s \rightarrow \cdot) = \prod_{i \in I} \pi^{(i),*}(o^{(i)} \rightarrow$
653 $\cdot)$. We may generalize this relation to a coupling of GFlowNets writing $F_{\text{action}}(\prod_{i \in I} O^{(i)} \rightarrow$
654 $\prod_{i \in I} A^{(i)}) = \prod_{i \in I} F_{\text{action}}^{(i)}(O^{(i)} \rightarrow A^{(i)})$. We are led to following the definition:

655 **Definition 6.** Let $(\mathcal{S}, \mathcal{A}, S, T, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)}, p^{(i)})$ be a multi-agent interactive environment and let
656 $\mathbb{F} = (\pi^*, F_{\text{out}}^*, F_{\text{init}})$ be a global GFlowNet on it satisfying the weak flow-matching constraint. The
657 GFlowNet \mathbb{F} is said to be

658 • star-split if for some local GFlowNets $\mathbb{F}^{(i)}$ and $\forall A^{(i)} \subset \mathcal{A}^{(i)} \setminus \text{STOP}$ we have:

$$F_{\text{action}}\left(\prod_{i \in I} A^{(i)}\right) = \prod_{i \in I} F_{\text{action}}^{(i)}(A^{(i)}). \quad (21)$$

659 • strongly star-split if for some local GFlowNets $\mathbb{F}^{(i)}$ and $\forall A^{(i)}, B^{(i)} \subset \mathcal{O}^{(i)}$ we have:

$$F_{\text{edge}}\left(\prod_{i \in I} A^{(i)} \rightarrow \prod_{i \in I} B^{(i)}\right) = \prod_{i \in I} F_{\text{edge}}^{(i)}(A^{(i)} \rightarrow B^{(i)}). \quad (22)$$

660 The local GFlowNets $\mathbb{F}^{(i)}$ are called the components of the global GFlowNet \mathbb{F} .

661 However we encounter an additional difficulty: what happens when an agent decides to stop the game
662 ? Indeed, local agents have their own STOP action, we then have at least three behaviors.

1. Unilateral Stop: if any agent decides to stop, the game stops and reward is awarded.
2. Asynchronous Unanimous Stop: if an agent decides to stop, it does not act anymore, waits
665 for the other to leave the game and then reward is awarded only when all agents stopped.
3. Synchronous Unanimous Stop: if an agent decides to stop but some other does not, then the
667 stop action is rejected and the agent plays a non-stopping action.

668 Similar variations may be considered for how the initialization of agents:

1. Asynchronous Start: the game has a free number of player, agents may enter the game while
670 other are already playing.
2. Synchronous Start: the game has a fixed number of players, and agents all start at the same
672 time.

673 These 6 possible combinaisons leads to slight variations on the formalization of MA-GFlowNets
674 from local GFlowNets.

675 A.7 Initial local-global consistencies

Let us formalize Asynchronous and Synchronous starts. In synchronous case, the agents are initially distributed according to their own initial distributions and independently. Therefore, ν_{init} is a product and

$$F_{\text{init}} \propto \nu_{\text{init}} = \prod_{i \in I} \nu_{\text{init}}^{(i)} \propto \prod_{i \in I} F_{\text{init}}^{(i)}.$$

676 Also, by strong star-splitting property, $F_{\text{in}}^* = \prod_{i \in I} F_{\text{in}}^{(i),*}$. By $F_{\text{in}} = F_{\text{init}} + F_{\text{in}}^*$ we obtain the
677 definition below.

Definition 7. A strongly star-split global GFlowNet is said to have Synchronous start if

$$F_{\text{in}} = \prod_{i \in I} F_{\text{init}}^{(i)} + \prod_{i \in I} F_{\text{in}}^{(i),*}$$

On the other hand, in the asynchronous case, an incoming agent may "bind" to agent arriving at the same time and other already there hence, the initial flow is a combination of any of the products

$$F_{\text{init}} = \sum \prod_{i \in \{\text{incoming}\}} F_{\text{init}}^{(i)} \prod_{j \in \{\text{already in}\}} F_{\text{init}}^{(j),*} = \prod_{i \in I} (F_{\text{init}}^{(i)} + F_{\text{in}}^{(i),*}) - \prod_{i \in I} F_{\text{in}}^{(i),*}.$$

Definition 8. A strongly star-split global GFlowNet is said to have *Asynchronous start* if

$$F_{\text{in}} = \prod_{i \in I} (F_{\text{init}}^{(i)} + F_{\text{in}}^{(i),*}).$$

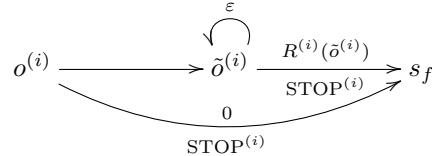
678 A.8 Terminal local-global consistencies

679 We focus on terminal behaviors 1 and 2 which we formalize as follows. Local-global consistency
680 consists in describing the formal structure linking local environments with global ones. The product
681 structure of the action space is slightly different depending on the terminal behavior. It happens that
682 we may up to formalization, we may cast Asynchronous Unanimous STOP as a particular case of
683 Unilateral STOP local-global consistency. More precisely:

684 **Definition 9** (Unilateral STOP Local-Global Consistency). *With the same notations as above, we say
685 that a multi-agent action environment has unilateral STOP if*

$$\mathcal{A}_s := \left(\prod_{i \in I} \mathcal{A}_{o^{(i)}} \right) / \sim \quad a_1 \sim a_2 \Leftrightarrow \exists i, j \in I, a_1^{(i)} = \text{STOP}^{(i)}, a_2^{(j)} = \text{STOP}^{(j)}. \quad (23)$$

Definition 10 (Asynchronous Unanimous STOP Local-Global Consistency). *With the same notations
as above, we say that a multi-agent game environment has Asynchronous Unanimous STOP if it has
Unilateral STOP and the observation space $\mathcal{O}^{(i)}$ may be decomposed into $\mathcal{O}^{(i)} = \mathcal{O}_{\text{life}}^{(i)} \cup \mathcal{O}_{\text{purgatory}}^{(i)}$
and for any observation $o^{(i)} \in \mathcal{O}_{\text{life}}^{(i)}$ we have some $\tilde{o}^{(i)} \in \mathcal{O}_{\text{purgatory}}^{(i)}$ such that :*



686 where the value on top of arrows are constrained flow values.

687 The formal definition of Unilateral STOP is straightforward as any local STOP activates the global
688 STOP so that any combination of local actions that contains at least one STOP is actually a global
689 STOP. The quotient by the equivalence relation formalizes this property. Regarding Asynchronous
690 Unanimous STOP, the chosen formalization allows to store the last observation of an agent while it is
691 put on hold until global STOP. Indeed, a standard action ($\neq \text{STOP}$) is invoked to enter purgatory,
692 the reward is supported on purgatory and as long as all the agent are not in purgatory its value is
693 zero (recall that from the viewpoint of a given agent, $R^{(i)}$ is stochastic but in fact depends on the
694 whole global state). The local STOP action is then never technically called on an "alive" observation,
695 once in purgatory the ε self-transition is called by default as long as the reward is non zero, hence
696 until all agents are in purgatory. When the reward is activated, the policy at a purgatory state $\tilde{o}^{(i)}$ is
697 then $\frac{d\varepsilon}{d(\varepsilon + R^{(i)})} \delta_{\tilde{o}^{(i)}} + \frac{dR^{(i)}}{d(\varepsilon + R^{(i)})} \delta_{\text{STOP}}$. As $\varepsilon \rightarrow 0^+$, the policy becomes equivalent to "if reward then
698 STOP, else WAIT". This behavior is exactly the informal description of Asynchronous Unanimous
699 STOP, the formalization is rather arbitrary and does not limit the applicability as it simply helps
700 deriving formulas more easily.

701 We now prove Theorem 2 and 3, which have been integrated into the following theorem:

702 **Theorem 4.** *Let $(\mathcal{S}, \mathcal{A}, S, T, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)}, p^{(i)})$ be a multi-agent interactive environment. Let $\mathbb{F}^{(i)}$
703 be non-zero GFlowNets on $(\mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)})$ for $i \in I$ satisfying the weak flow-matching constraint,
704 then there exists a transition kernel \tilde{T} and a star-split GFlowNet on $(\mathcal{S}, \mathcal{A}, S, \tilde{T}, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, S^{(i)}, p^{(i)})$
705 whose components are the $\mathbb{F}^{(i)}$.*

706 Furthermore,

707 • if the multi-agent environment is a game environment with Asynchronous Unanimous STOP
 708 and if the global GFlowNet satisfies the strong flow-matching constraint on $\prod_{i \in I} \mathcal{O}_{\text{life}}^{(i)}$ then
 709 each local GFlowNet satisfies the strong flow-matching constraint on $\mathcal{O}_{\text{life}}^{(i)}$;
 710 • if the multi-agent environment is a game environment with Asynchronous Unanimous STOP
 711 and if each local GFlowNets satisfy the strong flow-matching constraint on $\mathcal{O}_{\text{life}}^{(i)}$ then
 712 $\hat{R} = \prod_{i \in I} \hat{R}^{(i)}$.

713 *Proof.* We simply define $\mathbb{F} = (\pi^*, F_{\text{out}}^*, F_{\text{init}})$ by $\pi^*(s) := (\prod_{i \in I} \pi^{(i),*}(o^{(i)})) / \sim$ ie the projection
 714 on \mathcal{A} of the policy toward $\prod_{i \in I} \mathcal{A}^{(i)}$, then F_{out}^* as the product of the measures $F_{\text{out}}^{(i),*}$. Then we define
 715 $\tilde{T} = \prod_{i \in I} T^{(i)}$ so that $F_{\text{in}}^*(\prod_{i \in I} A^{(i)}) = \prod_{i \in I} F_{\text{in}}^{(i),*}(A^{(i)})$ and $F_{\text{init}} := \prod_{i \in I} (F_{\text{in}}^{(i),*} + F_{\text{init}}^{(i)}) -$
 716 $\prod_{i \in I} F_{\text{in}}^{(i),*}$ as the product measure of the $F_{\text{init}}^{(i)}$. By construction this GFlowNet is star-split.

Assume that \mathbb{F} satisfies the strong flow-matching constraint. It follows that for any $A^{(i)} \subset \mathcal{O}_{\text{life}}^{(i)}$ we have

$$\prod_{i \in I} F_{\text{in}}^{(i)}(A^{(i)}) = \prod_{i \in I} F_{\text{out}}^{(i)}(A^{(i)}) = \prod_{i \in I} F_{\text{out}}^{(i),*}(A^{(i)}).$$

717 Since, by assumption, all local GFlowNets satisfy the weak flow-matching constraint, all terms in
 718 the left-hand side product are bigger than those in the right-hand side product. Equality may only
 719 occur if some term is zero on both sides or if for all $i \in I$, We conclude that the strong flow-matching
 720 constraint is satisfied for all local GFlowNets on $\mathcal{O}_{\text{life}}^{(i)}$.

If the strong flow-matching constraint is satisfied on $\mathcal{O}_{\text{life}}^{(i)}$, then $\hat{R}^{(i)} = R^{(i)} = 0$ on $\mathcal{O}_{\text{life}}^{(i)}$. By
 construction, $F_{\text{out}}^{(i),*} = F_{\text{init}}^{(i),*} = 0$ on $\mathcal{O}_{\text{purgatory}}^{(i)}$. Therefore, on purgatory, we have

$$\hat{R} = F_{\text{in}} - F_{\text{out}} = F_{\text{in}}^* - F_{\text{out}}^* = \prod_{i \in I} F_{\text{in}}^{(i),*} - \prod_{i \in I} F_{\text{out}}^{(i),*} = \prod_{i \in I} F_{\text{in}}^{(i),*} = \prod_{i \in I} \hat{R}^{(i)}.$$

721 □

722 B Algorithms

723 Algorithm 3 shows the training phase of the independent flow network (IFN). In the each round of
 724 IFN, the agents first sample trajectories with policy

$$o_t^{(i)} = p_i(s_t^{(i)}) \text{ and } \pi^{(i)}(o_t^{(i)} \rightarrow a_t^{(i)}), \quad i \in I \quad (24)$$

725 with $a_t = (a_t^{(i)} : i \in I)$ and $s_{t+1} = T(s_t, a_t)$. Then we train the sampling policy by minimizing the
 726 FM loss $\mathcal{L}_{\text{FM}}^{\text{stable}}(\mathbb{F}^{(i)}, \theta)$ for $i \in I$.

Algorithm 3 Independent Flow Network Training Algorithm for MA-GFlowNets

Require: Number of agents N , A multi-agent environment $(\mathcal{S}, \mathcal{A}, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, p_i, S, T, R)$.

Require: Local GFlowNets $(\pi^{(i),*}, F_{\text{out}}^{(i),*}, F_{\text{init}}^{(i)})_{i \in I}$ parameterized by θ .

while not converged **do**

 Sample and add trajectories $(s_t)_{t \geq 0} \in \mathcal{T}$ to replay buffer with policy according to (24)

 Generate training distribution of observations $\nu_{\text{state}}^{(i)}$ for $i \in I$ from train buffer

 Apply minimization step of FM-loss $\mathcal{L}_{\text{FM}}^{\text{stable}}(F_{\text{action}}^{(i),\theta}, R^{(i)})$ for $i \in I$.

end while

727 Algorithm 4 shows the training phase of Conditioned Joint Flow Network (CJFN). In the each round
 728 of CJFN, we first sample sample trajectories with policy

$$o_t^{(i)} = p_i(s_t^{(i)}) \text{ and } \pi_{\omega}^{(i)}(o_t^{(i)} \rightarrow a_t^{(i)}), \quad i \in I \quad (25)$$

729 with $a_t = (a_t^{(i)} : i \in I)$ and $s_{t+1} = T(s_t, a_t)$. Then we train the sampling policy by minimizing the
 730 FM loss $\mathbb{E}_{\omega} \mathcal{L}_{\text{FM}}^{\text{stable}}(F_{\text{action}}^{\theta, \text{joint}}(\cdot; \omega), R)$.

Algorithm 4 Conditioned Joint Flow Network Training Algorithm for MA-GFlowNets

Require: Number of agents N , A multi-agent environment $(\mathcal{S}, \mathcal{A}, \mathcal{O}^{(i)}, \mathcal{A}^{(i)}, p_i, S, T, R)$.
Require: Simple Random distribution (Ω, \mathbb{P})
Require: Local GFlowNets $(\pi^{(i)*}, F_{\text{out}}^{(i)*}, F_{\text{init}}^{(i)})_{i \in I}$ parameterized by θ and $\omega \in \Omega$.
while not converged **do**
 Sample $\omega_1, \dots, \omega_b \sim \mathbb{P}$ and then trajectories $(s_t^\omega)_{t \geq 0} \in \mathcal{T}$ to replay buffer with policy according to (25) for $\omega \in \{\omega_1, \dots, \omega_b\}$
 Generate training distribution of states/omega $\nu_{\text{state}}^\Omega$ from the train buffer
 Apply minimization step of the FM loss $\mathbb{E}_\omega \mathcal{L}_{\text{FM}}^{\text{stable}}(\mathbb{F}^{\theta, \text{joint}}(\cdot; \omega))$ under the constraint of Weak flow-matching.
end while

731 **C Discussion: Relationship with MARL**

732 Interestingly, there are similar independent execution algorithms in the multi-agent reinforcement
733 learning scheme. Therefore, in this subsection, we discuss the relationship between flow conservation
734 networks and multi-agent RL. The value decomposition approach has been widely used in multi-agent
735 RL based on IGM conditions, such as VDN and QMIX. For a given global state s and joint action
736 a , the IGM condition asserts the consistency between joint and local greedy action selections in the
737 joint action-value $Q_{\text{tot}}(s, a)$ and individual action values $[Q_i(o_i, a_i)]_{i=1}^k$:

$$\arg \max_{a \in \mathcal{A}} Q_{\text{tot}}(s, a) = \left(\arg \max_{a_1 \in \mathcal{A}_1} Q_1(o_1, a_1), \dots, \arg \max_{a_k \in \mathcal{A}_k} Q_k(o_k, a_k) \right), \forall s \in \mathcal{S}. \quad (26)$$

738 **assumption 1.** For any complete trajectory in an MADAG $\tau = (s_0, \dots, s_f)$, we assume that
739 $Q_{\text{tot}}^\mu(s_{f-1}, a) = R(s_f)f(s_{f-1})$ with $f(s_n) = \prod_{t=0}^n \frac{1}{\mu(a|s_t)}$.

740 **Remark 1.** Although Assumption 1 is a strong assumption that does not always hold in practical
741 environments. Here we only use this assumption for discussion analysis, which does not affect the
742 performance of the proposed algorithms. A scenario where the assumption directly holds is that we
743 sample actions according to a uniform distribution in a tree structure, i.e., $\mu(a|s) = 1/|\mathcal{A}(s)|$. The
744 uniform policy is also used as an assumption in [2].

745 **Lemma 3.** Suppose Assumption 1 holds and the environment has a tree structure, based on Theorem 2
746 and IGM conditions we have:

747 1) $Q_{\text{tot}}^\mu(s, a) = F(s, a)f(s)$;
748 2) $(\arg \max_{a_i} Q_i(o_i, a_i))_{i=1}^k = (\arg \max_{a_i} F_i(o_i, a_i))_{i=1}^k$.

749 Based on Assumption1, we have Lemma 3, which shows the connection between Theorem 2 and
750 the IGM condition. This action-value function equivalence property helps us better understand the
751 multi-flow network algorithms, especially showing the rationality of Theorem 2.

752 **C.1 Proof of Lemma 3**

753 *Proof.* The proof is an extension of that of Proposition 4 in [2]. For any (s, a) satisfies $s_f = T(s, a)$,
754 we have $Q_{\text{tot}}^\mu(s, a) = R(s_f)f(s)$ and $F(s, a) = R(s_f)$. Therefore, we have $Q_{\text{tot}}^\mu(s, a) = F(s, a)f(s)$.
755 Then, for each non-final node s' , based on the action-value function in terms of the action-value at
756 the next step, we have by induction:

$$\begin{aligned} Q_{\text{tot}}^\mu(s, a) &= \hat{R}(s') + \mu(a|s') \sum_{a' \in \mathcal{A}(s')} Q_{\text{tot}}^\mu(s', a'; \hat{R}) \\ &\stackrel{(a)}{=} 0 + \mu(a|s') \sum_{a' \in \mathcal{A}(s')} F(s', a'; \hat{R})f(s'), \end{aligned} \quad (27)$$

757 where $\hat{R}(s')$ is the reward of $Q_{\text{tot}}^\mu(s, a)$ and (a) is due to that $\hat{R}(s') = 0$ if s' is not a final state. Since
758 the environment has a tree structure, we have

$$F(s, a) = \sum_{a' \in \mathcal{A}(s')} F(s', a'), \quad (28)$$

759 which yields

$$Q_{\text{tot}}^\mu(s, a) = \mu(a|s')F(s, a)f(s') = \mu(a|s')F(s, a)f(s) \frac{1}{\mu(a|s')} = F(s, a)f(s).$$

760 According to Theorem 2, we have $F(s_t, a_t) = \prod_i F_i(o_t^i, a_t^i)$, yielding

$$\begin{aligned} \arg \max_a Q_{\text{tot}}(s, a) &\stackrel{(a)}{=} \arg \max_a \log F(s, a)f(s) \\ &\stackrel{(b)}{=} \arg \max_a \sum_{i=1}^k \log F_i(o_i, a_i) \\ &\stackrel{(c)}{=} \left(\arg \max_{a_1 \in \mathcal{A}_1} F_1(o_1, a_1), \dots, \arg \max_{a_k \in \mathcal{A}_k} F_k(o_k, a_k) \right), \end{aligned} \quad (29)$$

761 where (a) is based on the fact F and $f(s)$ are positive, (b) is due to Theorem 2. Combining with the
762 IGM condition

$$\arg \max_{a \in \mathcal{A}} Q_{\text{tot}}(s, a) = \left(\arg \max_{a_1 \in \mathcal{A}_1} Q_1(o_1, a_1), \dots, \arg \max_{a_k \in \mathcal{A}_k} Q_k(o_k, a_k) \right), \forall s \in \mathcal{S}. \quad (30)$$

we can conclude that

$$\left(\arg \max_{a_i \in \mathcal{A}_i} F_i(o_i, a_i) \right)_{i=1}^k = \left(\arg \max_{a_1 \in \mathcal{A}_1} Q_1(o_1, a_1) \right)_{i=1}^k.$$

763 Then we complete the proof. \square

764 D Additional Experiments

765 D.1 Hyper-Grid Environment

766 D.1.1 Effect of Sampling Method:

767 We consider two different sampling methods of JFN; the first one is to sample trajectories using the
768 flow function F_i of each agent independently, called JFN (IS), and the other one is to combine the
769 policies π_i of all agents to obtain a joint policy π , and then performed centralized sampling, named
770 JFN (CS). As shown in Figure 6, we found that the JFN (CS) method has better performance than
771 JFN (IS) because the error of the policy π estimated by the combination method is smaller, and
772 several better samples can be obtained during the training process. However, the JFN (IS) method
can achieve decentralized sampling, which is more in line with practical applications.

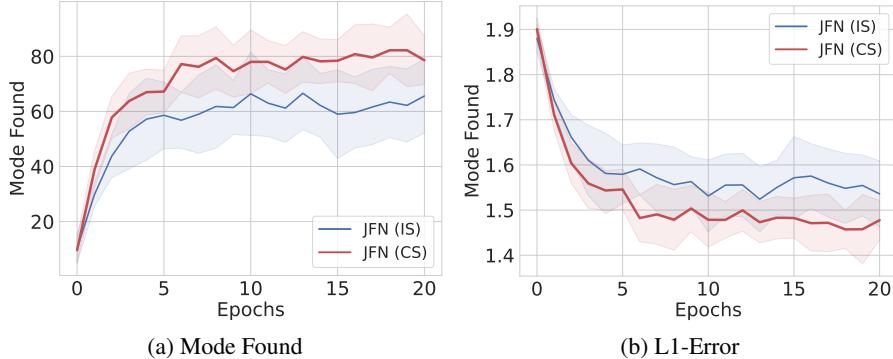


Figure 6: The performance of JFN with different methods.

773

774 **D.1.2 Effect of Different Rewards:**

775 We study the effect of different rewards in Figure 7. In particular, we set $R_0 = \{10^{-1}, 10^{-2}, 10^{-4}\}$
776 for different task challenge. A smaller value of R_0 makes the reward function distribution more
777 sparse, which makes policy optimization more difficult [2, 49, 50]. As shown in Figure 7, we found
778 that our proposed method is robust with the cases $R_0 = 10^{-1}$ and $R_0 = 10^{-2}$. When the reward
779 distribution becomes sparse, the performance of the proposed algorithm degrades slightly.

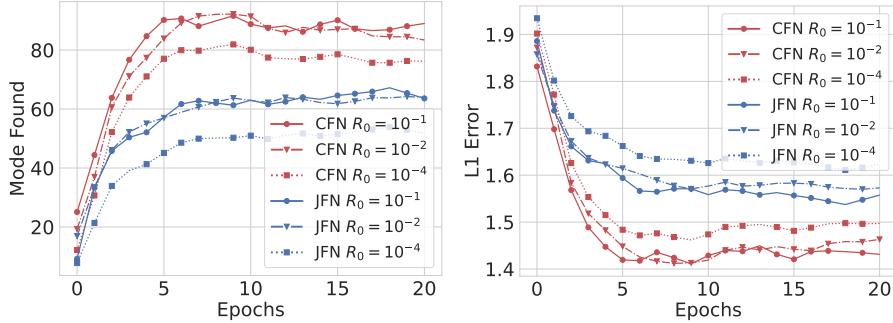


Figure 7: The effect of different reward R_0 on different algorithm.

780 **D.1.3 Flow Match Loss Function:**

781 Figure 8 shows the curve of the flow matching loss function with the number of training steps. The loss
782 of our proposed algorithm gradually decreases, ensuring the stability of the learning process. For some
783 RL algorithms based on the state-action value function estimation, the loss usually oscillates. This
784 may be because RL-based methods use experience replay buffer and the transition data distribution is
785 not stable enough. The method we propose uses an on-policy based optimization method, and the
786 data distribution changes with the current sampling policy, hence the loss function is relatively stable.
787 Then we present the experimental details on the Hyper-Grid environments. We set the same number
788 of training steps for all algorithms for a fair comparison. Moreover, we list the key hyperparameters
789 of the different algorithms in Tables 3-7.

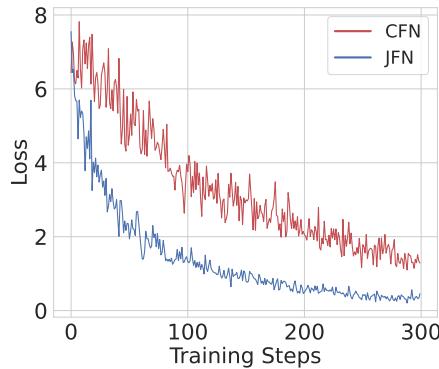


Figure 8: The flow matching loss of different algorithm.

790 In addition, as shown in Table 2, both the reinforcement learning methods and our proposed method
791 can achieve the highest reward, but the average reward of reinforcement learning is slightly better
792 for all found modes. Our algorithms do not always have higher rewards compared to RL, which is
793 reasonable since the goal of MA-GFlowNets is not to maximize rewards.

794 **D.2 StarCraft**

795 We present a visual analysis based on 3m with three identical entities attacking to win. All comparison
796 experiments adopted PyMARL framework and used default experimental parameters. Figure 9 shows

Environment	MAPPO	MASAC	MCMC	CFN	JFN
Hyper-Grid v1	2.0	1.84	1.78	2.0	2.0
Hyper-Grid v2	1.90	1.76	1.70	1.85	1.85
Hyper-Grid v3	1.84	1.66	1.62	1.82	1.82

Table 2: The best reward found using different methods.

797 the decision results of different algorithms on the 3m map. It can be found that the proposed algorithm
798 can obtain results under different reward distributions, that is, win at different costs. The costs of
799 other algorithms are often the same, which shows that the proposed algorithm is suitable for scenarios
800 with richer rewards. Figure 10 shows the performance of the different algorithms on 2s3z, which
801 shows a similar conclusion that the algorithm based on GFlowNets may be difficult to get the best
802 yield, but the goal is not to do this, but to fit the distribution better. Moreover, on StarCraft missions,
803 we did not use a clear metric to indicate the diversity of different trajectories, mainly because the
804 status of each entity includes multiple aspects, its movement range, health, opponent observation,
805 etc., which can easily result in different trajectories, but these differences do not indicate a good
806 fit for the reward distribution. As a result, it is not presented in the same way as Hyper-Grid and
807 Simple-Spread. Therefore, we used a visual method to compare the results. The maximized reward-
808 oriented algorithms such as QMIX will improve the reward by reducing the death of entities, while
the GFlowNets method can better fit the distribution on the basis of guaranteeing higher rewards.



Figure 9: The sample results of different algorithm on 3m map. **Upper:** QMIX, **Bottom:** JFN

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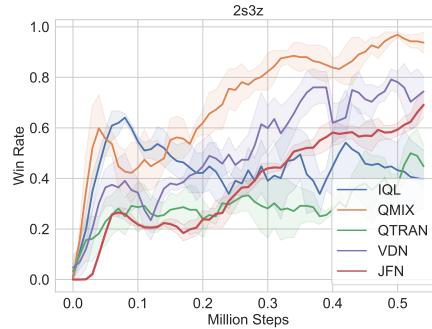


Figure 10: Average rate on 2s3z

810 D.3 Sparse-Simple-Spread Environment

811 In order to verify the performance of the CFN and JFN algorithms more extensively, we also conducted
812 experiments on Simple-Spread in the multi-agent particle environment. We compared two classic

813 Multi-agent RL algorithms, QMIX [11] and MAPPO [40], which have achieved State-of-the-Art
 814 performance in the standard simple-spread environment. Since the decision-making problems solved
 815 by GFlowNets are usually the setting of discrete state-action space, we modified Simple-Spread
 816 to meet the above conditions and named it discrete Sparse-Simple-Spread. Specifically, we set the
 817 reward function such that if the agent arrives at or near a landmark, the agent will receive the highest
 818 or second-highest reward. And this reward is given to the agent only after each trajectory ends. In
 819 addition, we fix the speed of the agent to keep the state space discrete and all agents start from the
 820 origin.

821 We adopt the average return and the number of distinguishable trajectories as performance metrics.
 822 When calculating the average return, JFN and CFN select the action with the largest flow for testing.
 823 As shown in Figure 11-Left, although the MAPPO and QMIX algorithms converge faster than the
 824 JFN, the JFN eventually achieves comparable performance. The performance of JFN is better than
 825 that of the CFN algorithm, which also shows that the method of flow decomposition can better learn
 826 the flow F_i of each agent. In each test round, we collect 16 trajectories and calculate the number of
 827 trajectories, which can be accumulated for comparison. The number of different trajectories found
 828 by JFN is 4 times that of MAPPO in Figure 11-Right, which shows that MA-GFlowNets can obtain
 829 more diverse results by sampling with the flow function. Moreover, the performance of JFN is not
 830 as good as that of the RL algorithm. This is because JFN lacks a guarantee for monotonic policy
 831 improvement [42, 43]. It pays more attention to exploration and does not fully use the learned policy,
 832 resulting in fewer high-return trajectories collected. MAPPO finds more high-return trajectories in
 833 Figure 11-Right, but it still struggles to generate more diverse results. In each sampling process, the
 834 trajectories found by MAPPO are mostly the same, while JFN does better.

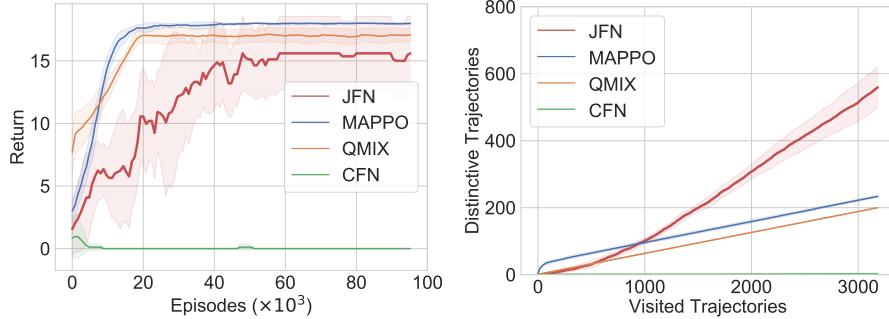


Figure 11: Average return and the number of distinctive trajectories performance of different algorithms on Sparse-Simple-Spread environments.

Table 3: Hyper-parameter of MAPPO under different environments

	Hyper-Grid-v1	Hyper-Grid-v2	Hyper-Grid-v3
Train Steps	20000	20000	20000
Agent	2	2	3
Grid Dim	2	3	3
Grid Size	[8,8]	[8,8]	[8,8]
Actor Network Hidden Layers	[256,256]	[256,256]	[256,256]
Optimizer	Adam	Adam	Adam
Learning Rate	0.0001	0.0001	0.0001
Batchsize	64	64	64
Discount Factor	0.99	0.99	0.99
PPO Entropy	1e-1	1e-1	1e-1

835 A Technical Appendices and Supplementary Material

836 Technical appendices with additional results, figures, graphs and proofs may be submitted with
 837 the paper submission before the full submission deadline (see above), or as a separate PDF in the

Table 4: Hyper-parameter of MASAC under different environments

	Hyper-Grid-v1	Hyper-Grid-v2	Hyper-Grid-v3
Train Steps	20000	20000	20000
Grid Dim	2	3	3
Grid Size	[8,8]	[8,8]	[8,8]
Actor Network Hidden Layers	[256,256]	[256,256]	[256,256]
Critic Network Hidden Layers	[256,256]	[256,256]	[256,256]
Optimizer	Adam	Adam	Adam
Learning Rate	0.0001	0.0001	0.0001
Batchsize	64	64	64
Discount Factor	0.99	0.99	0.99
SAC Alpha	0.98	0.98	0.98
Target Network Update	0.001	0.001	0.001

Table 5: Hyper-parameter of JFN under different environments

	Hyper-Grid-v1	Hyper-Grid-v2	Hyper-Grid-v3
Train Steps	20000	20000	20000
R_2	2	2	2
R_1	0.5	0.5	0.5
Grid Dim	2	3	3
Grid Size	[8,8]	[8,8]	[8,8]
Trajectories per steps	16	16	16
Flow Network Hidden Layers	[256,256]	[256,256]	[256,256]
Optimizer	Adam	Adam	Adam
Learning Rate	0.0001	0.0001	0.0001
ϵ	0.0005	0.0005	0.0005

Table 6: Hyper-parameter of CJFN under different environments

	Hyper-Grid-v1	Hyper-Grid-v2	Hyper-Grid-v3
Train Steps	20000	20000	20000
R_2	2	2	2
R_1	0.5	0.5	0.5
Grid Dim	2	3	3
Grid Size	[8,8]	[8,8]	[8,8]
Trajectories per steps	16	16	16
Flow Network Hidden Layers	[256,256]	[256,256]	[256,256]
Optimizer	Adam	Adam	Adam
Learning Rate	0.0001	0.0001	0.0001
ϵ	0.0005	0.0005	0.0005
Number of ω	4	4	4

Table 7: Hyper-parameter of CFN under different environments

	Hyper-Grid-v1	Hyper-Grid-v2	Hyper-Grid-v3
Train Steps	20000	20000	20000
Trajectories per steps	16	16	16
R_2	2	2	2
R_1	0.5	0.5	0.5
Grid Dim	2	3	3
Grid Size	[8,8]	[8,8]	[8,8]
Flow Network Hidden Layers	[256,256]	[256,256]	[256,256]
Optimizer	Adam	Adam	Adam
Learning Rate	0.0001	0.0001	0.0001
ϵ	0.0005	0.0005	0.0005

838 ZIP file below before the supplementary material deadline. There is no page limit for the technical
 839 appendices.

840 **NeurIPS Paper Checklist**

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849 • **[NA]** means either that the question is Not Applicable for that particular paper or the
850 relevant information is Not Available.
851 • Please provide a short (1–2 sentence) justification right after your answer (even for NA).

852 **The checklist answers are an integral part of your paper submission.** They are visible to the
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856 The reviewers of your paper will be asked to use the checklist as one of the factors in their evaluation.
857 While "**[Yes]**" is generally preferable to "**[No]**", it is perfectly acceptable to answer "**[No]**" provided a
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859 expensive" or "we were unable to find the license for the dataset we used"). In general, answering
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862 write a justification to elaborate. All supporting evidence can appear either in the main paper or the
863 supplemental material, provided in appendix. If you answer **[Yes]** to a question, in the justification
864 please point to the section(s) where related material for the question can be found.

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866 • **Delete this instruction block, but keep the section heading "NeurIPS Paper Checklist",**
867 • **Keep the checklist subsection headings, questions/answers and guidelines below.**
868 • **Do not modify the questions and only use the provided macros for your answers.**

869 **1. Claims**

870 Question: Do the main claims made in the abstract and introduction accurately reflect the
871 paper's contributions and scope?

872 Answer:**[Yes]**

873 Justification: Section 1 provides the MA-GFN formulation, section 2 provides theoretical
874 motivations for the Multi-agent loss, section 4 provides experimental support.

875 Guidelines:

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877 made in the paper.
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880 NA answer to this question will not be perceived well by the reviewers.
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885 **2. Limitations**

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887 Answer: **[Yes]**

888 Justification: They are discussed in section 5

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916 **3. Theory assumptions and proofs**

917 Question: For each theoretical result, does the paper provide the full set of assumptions and
918 a complete (and correct) proof?

919 Answer: **[Yes]**

920 Justification: Comprehensive justifications and proofs are provided in appendix A and C

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928 proof sketch to provide intuition.
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930 by formal proofs provided in appendix or supplemental material.
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932 **4. Experimental result reproducibility**

933 Question: Does the paper fully disclose all the information needed to reproduce the main ex-
934 perimental results of the paper to the extent that it affects the main claims and/or conclusions
935 of the paper (regardless of whether the code and data are provided or not)?

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994 • Providing as much information as possible in supplemental material (appended to the
995 paper) is recommended, but including URLs to data and code is permitted.

996 **6. Experimental setting/details**

997 Question: Does the paper specify all the training and test details (e.g., data splits, hyper-
998 parameters, how they were chosen, type of optimizer, etc.) necessary to understand the
999 results?

1000 Answer: **[Yes]**

1001 Justification: Only the Starcraft experiment requires particular Hyperparameter tuning effort
1002 due to the difference between the reward maximization objective and the GFlowNet diversity
1003 objective. Manual tuning was sufficient using standard reward temperature tuning method
1004 for similar GFlowNets training.

1005 Guidelines:

1006 • The answer NA means that the paper does not include experiments.
1007 • The experimental setting should be presented in the core of the paper to a level of detail
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1009 • The full details can be provided either with the code, in appendix, or as supplemental
1010 material.

1011 **7. Experiment statistical significance**

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1013 information about the statistical significance of the experiments?

1014 Answer: **[Yes]**

1015 Justification: Standard deviations at 2-sigma are provided on most plots.

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1040 the experiments?

1041 Answer: **[Yes]**

1042 Justification: Even though details of hardware used are not provided, all experiments were
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1058 Justification: All contributors to the work are accounted for, no non-public dataset, envi-
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