Birds of a Feather Flock Together: A Close Look at Cooperation Emergence via Multi-Agent RL

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Abstract

How cooperation emerges is a long-standing and interdisciplinary problem. Game-theoretical studies on social dilemmas reveal that altruistic incentives are critical to the emergence of cooperation but their analyses are limited to stateless games. For more realistic scenarios, multi-agent reinforcement learning has been used to study sequential social dilemmas (SSDs). Recent works show that learning to incentivize other agents can promote cooperation in SSDs. However, we find that, with these incentivizing mechanisms, the team cooperation level does not converge and regularly oscillates between cooperation and defection during learning. We show that a second-order social dilemma resulting from the incentive mechanisms is the main reason for such fragile cooperation. We formally analyze the dynamics of second-order social dilemmas and find that a typical tendency of humans, called homophily, provides a promising solution. We propose a novel learning framework to encourage homophilic incentives and show that it achieves stable cooperation in both SSDs of public goods and tragedy of the commons.

1 Introduction

Charles Darwin and his grand theory of evolution form the basics of the modern conception of the origin of species [1, 2]. One core idea of evolution theory states that individual fitness is key to surviving over the long term. However, this idea of survival of the fittest seems to run counter to cooperative or altruistic behaviors of some social species [3]. Historically, the problem of how cooperation emerges among self-interested agents has long perplexed scientists from various fields, such as evolutionary biology, animal behavioristics [4], and neuroscience [5], and is listed as one of the 125 most compelling science questions for the 21st century [6, 7].

Evolutionary game theory (EGT) provides a mathematical tool for studying the emergence of cooperation [8–11], which quantifies cooperation and predicts behavioral outcomes under different circumstances. Game theory has helped reveal that cooperation emergence is highly related to altruistic incentives [12–14] – individuals will pay costs to punish or reward others, even though there is no immediate gain by these actions for themselves [15–19]. Despite this progress, EGT studies cooperation emergence and altruistic incentives by modelling the evolutionary dynamics of several fixed policies on stateless games like iterated social dilemmas [20–22]. For comparison, real-world social dilemmas are temporally extended, where cooperation, defection, punishing, and rewarding are policies that should be learned.

Deep multi-agent reinforcement learning (MARL) shows promise to fill the gap to study how cooperation emerges on more realistic sequential social dilemmas [23]. Recently, Yang et al. [24]
and Lupu and Precup [25] show that the presence of incentive actions can encourage cooperative behaviors in public goods dilemmas and tragedy of the commons dilemmas, respectively. In these learning frameworks, each agent learns a behavior policy for selecting physical actions to execute in the environment and an incentive policy for rewarding or punishing others. However, these methods do not effectively scale up and limit in very small settings with two or three agents. With further investigation, we also observe that these methods do not converge to stable cooperation, where the population cooperation level regularly oscillates between cooperation and complete defection.

In this paper, we first analyze the underlying reasons behind the phenomenon of unstable cooperation. We find that, although incentive actions make cooperation more likely to emerge, they also introduce a second-order social dilemma into the system – If someone else would spend energy on punishing or rewarding others, why should I bother to do these [26]? The consequence is that more and more second-order free-riders would exploit those agents who make an effort to incentivize others, resulting in a degraded incentivizing mechanism and thus collapsed cooperation.

To solve this problem, we first illustrate the dynamics of and formally analyze the impetus for the second-order social dilemma on a fully-featured case study. Based on these analyses, we propose a novel learning mechanism by encouraging agents with similar environmental behaviors to have similar incentivizing behaviors. Our method is inspired by a concept called homophily, a particularly common tendency for human individuals to associate or bind with similar others, as in the proverb birds of a feather flock together.

It is worth noting that multi-person social dilemmas are classified into two broad categories: public goods and the tragedy of the commons [27–30]. We evaluate our method on both of these sequential social dilemmas and show that the agent population learns stable cooperative behaviors with great efficiency and stability. Visualization of the evolution process of cooperation shows that homophily effectively enables stable cooperation by preventing agents that conduct altruistic incentives from being exploited by second-order free-riders.

2 Preliminary and Related Works

Social Dilemmas (SDs) are among the most important settings used to study the emergence of cooperation. In a social dilemma, there exists a tension between the individual and collective rationality, in which individually reasonable behavior results in a situation where everyone suffers in the long run. Although studies on SDs have contributed significantly to the research of cooperation emergence for decades [31–33], they focus on stateless games and fixed policies. To be more realistic as in real-world situations, in this paper, we consider Sequential Social Dilemmas (SSDs, [23,34]).

An SSD can be modelled as a partially-observable general-sum Markov game [35] \( \mathcal{M} = (I, S, \{A_i\}, \mathcal{P}, \mathcal{O}, \{\mathcal{O}_i\}, \{\mathcal{R}_i\}, n, \gamma) \), where \( I \) is a finite set of \( n \) agents and \( \gamma \) is a discount factor. At each time step, agent \( i \) draws a partial observation \( o_i \in \mathcal{O}_i \) of the state \( s \in S \) according to the observation function \( O(s, i) \). Based on the observation, agent \( i \) selects an action \( a_i \in A_i \), which together form a joint action \( a \), leading to a next state \( s' \) according to the stochastic transition function \( \bar{P}(s'|s, a) \) and individual rewards \( r_i = R_i(s', a) \) for each agent. In SSDs, instead of taking atomic cooperation or defection actions, agents must learn cooperation or defection strategies consisting of potentially long sequences of environmental actions. The goal of each agent is to maximize the local expected return:

\[
Q_i(s, a) = \mathbb{E}_{s_0, a_0} \sum_{t=0}^{\infty} \gamma^t R_i(s_t, a_t) | s_0 = s, a_0 = a.
\]

Altruistic incentive, including altruistically rewarding and punishing others, is known as one of the solutions for social dilemmas [28]. However, it introduces the problem of second-order social dilemma (2nd-SD), which arises from each individual’s inclination to free ride on a mechanism that is designed to solve the first-order social dilemma. To solve 2nd-SDs, previous works either introduce extra punishing mechanisms [12,36] or change the game settings to enable the amount of public goods to grow exponentially with the number of contributors [37]. These works analyze the dynamics of predefined and fixed mechanisms and focus on stateless games. However, solving 2nd-SDs in sequential settings presents unique challenges—extra mechanisms should be learned with the risk of introducing a higher-order social dilemma—and remains largely untouched in the literature.

We propose to solve 2nd-SDs in general cases using the tendency of homophily. Homophily [38] states that similar individuals tend to associate with each other. Although the concept of homophily
has been well studied in network science [39], the relationship between homophily and cooperation emergence among self-interested agents is still unclear.

Recent works study some other mechanisms which may encourage cooperation in SSDs. Hughes et al. [40] study the effects of inequality aversion, which bypasses the problem of second-order social dilemmas because the punishment does not incur costs to any agents other than the punished ones. Jaques et al. [41] find that encouraging mutual influence among agents can promote collective behaviors. We empirically compare with these methods in Sec. 5.2.

In the following sections, we will first provide a case study to show the influence of social dilemmas, second-order social dilemmas, and how homophily can solve 2nd-SDs. Based on these analyses, we introduce how to encourage homophily in temporally extended cases in Sec. 4.

3 Case Study: Fragile Cooperation

In this section, we provide a detailed case study to explain first- and second-order social dilemmas, and demonstrate that homophily can promote cooperation by alleviating the second-order social dilemma. For clarity, in this section, we use one-step games to illustrate our ideas, which will inspire our extension to sequential decision-making settings in Sec. 4.

We adopt a classic problem setting [42–45]. A population of $n$ agents has an opportunity to create a public good, from which all can benefit, regardless of whether they have contributed to the good. Specifically, there are three strategies (atomic actions). Contributors ($C$) pay a cost $c$ to increase the size of public good by $b$. Defectors ($D$) do not contribute. The public good is uniformly distributed among cooperators and defectors. Agents can also choose to neither contribute to nor benefit from the public good, but receive a fixed reward $\sigma$, as Nonparticipants ($N$). For clarity, we conduct analyses using an illustrative example with $n = 10$, $b = 3$, $c = 1$, $\sigma = 1$. We provide a sensitivity analysis regarding parameters at the end of this section to consolidate that our conclusion generally holds.

Figure 1: First-order social dilemmas.

A: Cooperation is fragile in first-order social dilemmas. We first showcase the influence of 1st-SDs. The Schelling diagram [46, 47] (Fig. 1(a)) proves the existence of social dilemmas in this case. To visualize the learning dynamics of MARL algorithms under 1st-SDs, we learn independent policies for agents using REINFORCE [48]. In Fig. 1(b), we plot the change of the proportion of cooperative agents in the population under 3 random seeds. We observe that the cooperation level oscillates during learning. For explanation, we visualize the dynamics of population constituent in a ternary plot (Fig. 1(c)). Each point $X$ inside the equilateral triangle represents a distribution of population members ($p_C, p_D, p_N$), where $p_C + p_D + p_N = 1$, $p_C, p_D, p_N$ are represented by the distances from point $X$ to the edges $ND, CN$, and $CD$, respectively. Trajectories in Fig. 1(c) correspond to the curves with the same color in Fig. 1(b). We can observe that all the trajectories rotate counterclockwise in the vicinity of vertex $N$ regardless of the starting position.

Formally, we calculate the closed-from gradients of agents’ true value functions and visualize the gradient field in Fig. 1(d). It can be observed that cooperation is not a stable solution, which can be easily taken over by defectors, and then by nonparticipants. This phenomenon is the results of first-order social dilemmas, where cooperation is exploited by defection, eventually leading the system to a very ineffective state. We refer readers to Appendix E for the detailed proof.

B: Unexploitable altruistic incentives make cooperation possible. To introduce altruistic incentives into the system, we add Punishers ($P$) as the fourth type of strategy (atomic action). The same as contributors, a punisher contributes to and benefits from the public good, and importantly, it also pays a cost $k$ to incur a punishment $p$ on defectors. This punishment is altruistic because it reduces its local immediate reward but benefits the team in the long run.
To show the effect of altruistic incentives, we need to guarantee that no agent can exploit altruistic incentives by being a pure contributor that does not spend energy to punish defectors. Therefore, we first consider the setting where punishers also pay a cost \(\alpha k\) to incur a punishment \(\alpha p\) on the pure contributors for not punishing defectors [12]. We denote this punishing type by \(PA\), which represents a kind of \textit{unexploitable altruistic incentives}.

For simplicity, we illustrate our analyses with \(p = 2, k = 0.35, \alpha = 1\) (sensitivity analysis is deferred to the end of this section). Each horizontal plane in Fig. 2(a) shows the Schelling diagram under the corresponding number of first-order defectors, which proves that 2nd-SDs do not exist in this case. We visualize the dynamics of independent REINFORCE learners under this situation. In Fig. 2(b), we present three trajectories showing the change of the population during three runs. In this quaternary plot, each point \(X\) represents a distribution of the population \((p_C, p_D, p_N, p_P)\). Here, \(p_C + p_D + p_N + p_P = 1\) and \(p_C, p_D, p_N, p_P\) are represented by the distances from \(X\) to faces \(DNP, CNP, CDP, CDN\), respectively. We see that although two trajectories are trapped in the \(C-D-N\) plane and similar to those in Fig. 1(c), one of the three trajectories finds the stable cooperation solution \(PA\).

Formally, we calculate and plot the closed-form gradients in Fig. 3(a), where the green (blue) region indicates that a population initialized there would converge to cooperative (non-cooperative) solution. This figure proves that introducing unexploitable altruistic incentives creates a “safe region” near \(PA\), and the populations initialized there converge to cooperative solutions.

\[\begin{align*}
\text{(a) Schelling diagram} & \quad \text{(b) Trajectory in the policy space} \\
& \quad \text{(c) Schelling diagram} \\
& \quad \text{(d) Gradient field} \\
\end{align*}\]

\[\begin{align*}
\text{C: Exploitable altruistic incentives suffer from 2nd-SDs, which again lead to fragile cooperation.} & \\
\text{Now we restrict the punishments incurred by punishers, and they can only pay a cost } k \text{ to incur a punishment } p \text{ on defectors. Now the punishers can be exploited by pure cooperators who do not pay for but benefit from punishments. We call this type of punishers the \textit{exploitable punishers}. On each horizontal plane in Fig. 2(c), we show the Schelling diagram with different numbers of first-order defectors, which reveals the existence of second-order social dilemmas.}
\end{align*}\]

Formally, assume that the probability of agent \(i\) taking three actions are \(\theta_{i,C}, \theta_{i,D}, \theta_{i,P}\), respectively. It can be derived (Appendix E) that the gradient of agent \(i\)’s value function w.r.t. the probability of second-order cooperative action \(\theta_{i,P}\) minus the the gradient w.r.t the probability of second-order defective action \(\theta_{i,D}\) is \(-k \sum_{j \neq i} \theta_{j,D}\), where \(k > 0\) is the punishment cost. The gradient is negative for \(\forall \theta_{i,D}\), which indicates that second-order cooperators would be taken over by second-order defectors. This is the second-order social dilemma. The result is that only strategies \(C, D, N\) exist, after which the system degrades due to the 1st-SD as discussed before. We plot the closed-form gradients in Fig. 2(d), from which we observe that the “safe region” disappears, and, for any initialization, the population ends with non-cooperation.

\[\begin{align*}
\text{Takeaways} & \quad \text{We conclude that only unexploitable incentives can make cooperation a stable solution. It becomes particularly problematic in temporally extended cases, where the incentivizing policies need to be learned. It is typical that some agents would learn altruistic incentives earlier than others. However, as analysed before, these altruistic agents will be exploited by other agents, leading to degraded altruistic behaviors. Further, with collapsed altruistic incentivizing mechanisms, the population falls back to a 1st-SD, making cooperation much less likely to emerge.}
\end{align*}\]
D: Homophily solves second-order social dilemmas. To show the effect of homophily, based on the settings in part C, we further encourage agents with similar acting behaviors to have similar incentivizing behaviors. Since only contributors and punishers have the same acting behavior of contributing to the public good, we encourage their incentives to be the same by converting the minority of P and C to the majority with a probability of 0.2.

Again, we calculate the closed-form gradients after adding this inclination. We find that the “safe region” reappears (Fig. 3(b)). The gradient w.r.t. \( \theta_i,P \) minus the gradient w.r.t \( \theta_i,C \) is
\[
-k \sum_{j \neq i} \theta_{j,D} + 2\lambda \text{sign}(\sum_{j \neq i}(\theta_{j,P} - \theta_{j,C})) \min(\theta_i,C, \theta_j,P),
\]
which is positive when close to point P. Interestingly, the “safe region” is larger than that in Fig. 3(a), which exists due to unexploitable altruistic incentives. In this way, we conclude that homophily helps solve second-order social dilemmas.

Sensitivity analyses of the key parameters used in this section. We use one-at-a-time method and show the result with a Tornado Diagram in Fig. 4. When homophily is not introduced, with a 20% perturbation of default parameters, 2nd-SDs persist and the “cooperative volume” (green region in Fig. 2(d)) is always 0 (Fig. 4(left)). In contrast, when homophily is introduced, the cooperative volume (green region in Fig. 3(b)) fluctuates within a reasonable range and is always larger than 0.1 (Fig. 4(right)), which allows cooperation emergence. These results consolidate the robustness of our observations and method across a wide range of conditions.

By this case study, we show that homophilic incentives encourage cooperation emergence. However, this study focuses on one-step games and predefines the mechanism of punishers. The question is how to encourage homophily in realistic settings without depending on any predefined mechanisms.

4 Methods

As discussed in the previous section, second-order social dilemmas disturb the learning process of incentivizing actions – agents who learn altruistic punishing or rewarding earlier tend to be exploited by other agents. Consequently, the altruistic incentivizing behaviors are typically taken over and the population would fall back to first-order social dilemmas, resulting in a hopeless loop.

In this section, we discuss how to introduce homophily into sequential social dilemmas so that the loop can be broken and cooperation is possible to emerge and stabilize. We propose to encourage homophily by encouraging agents with similar acting (environmental) behaviors to have similar incentivizing behaviors. We now describe our learning framework shown in Fig. 5.

4.1 Incentivizing and environmental behavior learning

To enable incentivizing behaviors, we add incentivizing actions to the action space. We use \( a_{i \rightarrow j} \) to denote the incentivizing action from \( i \) to \( j \). The action \( a_{i \rightarrow j} \) induces an inter-agent reward \( \eta' r_{i \rightarrow j} \) to agent \( j \). Here, \( \eta' > 0 \) is a scaling factor. In this paper, we consider three types of incentivizing actions with a positive, negative, and zero \( r_{i \rightarrow j} \), respectively. Since we consider altruistic incentives, the action \( a_{i \rightarrow j} \) itself costs \( \eta'' |r_{i \rightarrow j}| \), where \( \eta'' > 0 \) is also a scaling factor.

Each agent learns two Q functions, for selecting environmental actions and incentivizing actions, respectively. At each step, agents first simultaneously select environmental actions \( a_i \) according to \( Q^i_{\text{env}}(\tau, a_i) \), which is based on local action-observation history and is parameterized by \( \theta_i \). Then, conditioned on environmental actions of other agents, \( a_i \), each agent \( i \) decides its incentivizing actions \( a_{i \rightarrow -i} \) according to \( Q^i_{\text{inc}}(\tau_i, a_{-i}, a_{i \rightarrow -i}) \) parameterized by \( \phi_i \).
One question is what rewards should be considered when training \( Q_{\phi_i}^{i,\text{inc}} \). Intuitively, incentivizing actions are expected to positively influence the return given by the environment. Therefore, we include environment rewards \( r_i \). We also consider the costs of incentivizing actions to prevent agents from excessively giving incentives. Moreover, we ignore the rewards received from other agents, which can effectively prevent agents from learning trivial and detrimental policies, such as keeping exchanging positive incentives regardless of the observations.

Another question of learning \( Q_{\phi_i}^{i,\text{inc}} \) is that it requires \( 3^n - 1 \) outputs using a conventional deep Q-network and most output heads would remain unchanged for long stretches of time. To solve this problem, agent \( i \) can learn \( n - 1 \) incentivizing Q functions \( Q_{\phi_i}^{i,\text{inc}} \), each of which corresponds to one agent \( j \neq i \). However, this alternative arises a new question because the environment rewards are considered when training \( Q_{\phi_i}^{i,\text{inc}} \) but they do not present an explicit decomposition over agents. To solve this problem, we propose to estimate \( Q_{\phi_i}^{i,\text{inc}} \) as a summation:

\[
Q_{\phi_i}^{i,\text{inc}}((\tau_i, a_i), a_{i \rightarrow i}) = \sum_{j \neq i} Q_{\phi_i}^{i,\text{inc}}((\tau_i, a_j), a_{i \rightarrow j}).
\]

Here, parameters of \( Q_{\phi_i}^{i,\text{inc}} \) are shared to accelerate training. This formulation is similar to VDN \([49]\). The difference is that we sum incentivizing Q’s of a single agent, rather than Q’s of different agents.

With these formulations, we train each agent’s incentivizing Q by minimizing the following TD loss:

\[
\mathcal{L}_i^{\text{inc}}(\phi_i) = \mathbb{E}_D \left[ (r_i - \gamma \sum_{j \neq i} r_{j \rightarrow j} + \gamma^{\text{inc}} \max_{a_i' \rightarrow i} Q_{\phi_i}^{i,\text{inc}}((\tau_i, a_i'), a_{i \rightarrow i}) - Q_{\phi_i}^{i,\text{inc}}((\tau_i, a_i), a_{i \rightarrow i}))^2 \right],
\]

where \( \gamma^{\text{inc}} \) is the discount factor, \( \phi_i^{-} \) is parameters of a target network that are periodically copied from \( \phi_i \), and the expectation is estimated by uniform samples from a replay buffer \( D \).

Environmental Q function is trained with rewards from the environment and the incentives received from other agents, and we minimize the following TD loss for learning \( Q_{\phi_i}^{i,\text{env}} \):

\[
\mathcal{L}_i^{\text{env}}(\theta_i) = \mathbb{E}_D \left[ (y_i^{\text{env}} - Q_{\theta_i}^{i,\text{env}}(\tau_i, a_i))^2 \right].
\]

4.2 Homophily

Directly learning incentivizing policies can be difficult due to second-order social dilemmas as we discussed in Sec.3. To solve this problem and inspired by the stateless case in Sec.3 Part D, we encourage agents to be homophilic, i.e., agents with similar environmental behaviors should have similar incentive behaviors, which can be expressed as a loss to be minimized:

\[
\mathcal{L}_i^{\text{homo}}(\phi_i) = \mathbb{E}_D \left[ -\sum_{j \neq i} S_{\text{env}}(i, j) S_{\text{inc}}(i, j; \phi_i) \right],
\]

where \( S_{\text{env}} \) is 1 or 0, indicting the environmental behaviors are similar or not. \( S_{\text{inc}} \) measures the similarity between incentivizing behaviors of two agents.

The first question is how to define \( S_{\text{inc}}(i, j; \phi_i) \). The idea is to measure the similarity between two agents’ incentive behaviors by comparing their incentive actions to each of other agents. For each agent i, we measure its similarity to agent j as:

\[
S_{\text{inc}}(i, j; \phi_i) = -\sum_{k \neq i, j} \mathcal{C} \mathcal{E} \left[ P_{a_j \rightarrow k} \| \sigma(Q_{\phi_i}^{i,\text{inc}}((\tau_i, a_k))) \right],
\]

where \( \sigma(\cdot) \) is the softmax function, \( P_{a_j \rightarrow k} \) is a categorical distribution over agent j’s incentive actions, with a probability of 1 for the action that agent j takes for agent k (\( a_{j \rightarrow k} \)). The cross entropy \( \mathcal{C} \mathcal{E} [\|\|] \) measures the distance between these two distributions.
We test our method on sequential social dilemmas. There are two broad categories of multi-person social dilemmas [28]: Public goods dilemmas and Tragedy of commons dilemmas. In Public goods dilemmas, individuals pay an immediate and personal cost in order to generate a benefit that is shared by all participants. In Tragedy of commons dilemmas, individuals are tempted by an immediate and personal benefit, which induces a cost shared by all in the long run, such as depleting the public resource. In this paper, we consider sequential versions of these two dilemmas, Cleanup and Harvest [23]. The detailed settings are described in Appendix C.1.

In our framework, each agent has an environmental and an incentivizing Q function. The Q network architecture is the same for all agents but they do not share parameters. We set different discount factors for the two Q functions: $\gamma^\text{env} = 0.95$ and $\gamma^\text{inc} = 0.995$. To prevent the influence of incentives from being so strong that they interfere with environmental behavior learning, we set the incentive effect factor $\eta^e$ to 1.0 in all our experiments. Moreover, we find that a value of 0.1 for the incentive cost factor $\eta^c$ prevents the costs from being so large that no one wants to incentivize others, and from being so small that incentives proliferate. For other details, we refer readers to Appendix C.

### 4.3 Discussion

Is homophily the only possible solution for 2nd-SDs? No, it is not, but homophily has several advantages over other possible solutions. There are three types of solutions for (1st-) SDs [28]. (1) Structural solutions modify the game settings [50] and thus violate the assumption of the study of cooperation emergence. (2) Strategic solutions, such as tit-for-tat [51] and partner selection [33], typically require identifying cooperative and defective behaviors. Such approaches face major challenges in temporally extended cases – the co-learning of cooperation/defection detection and incentivizing mechanism is fragile and suffers from extremely postponed learning signals from each other. (3) Conventional motivational solutions like altruism may introduce higher-order SDs as shown in Sec. 5. The advantage of homophily is that it avoids higher-order SDs (e.g., 3rd-SDs) while not requiring identifying cooperation/defection.

### 5 Experiments

Our experiments aim to answer the following questions: (1) Can homophily promote the emergence of cooperation? (Sec. 5.2) (2) What is the contribution of each component in the proposed learning framework? (Sec. 5.3) (3) How does cooperation emerge and evolve under homophilic incentives? (Sec. 5.4) (4) How does homophily affect incentive behaviors? (Sec. 5.5)

#### 5.1 Experimental Setup

We test our method on sequential social dilemmas. There are two broad categories of multi-person social dilemmas [28]: Public goods dilemmas and Tragedy of commons dilemmas. In Public goods dilemmas, individuals pay an immediate and personal cost in order to generate a benefit that is shared by all participants. In Tragedy of commons dilemmas, individuals are tempted by an immediate and personal benefit, which induces a cost shared by all in the long run, such as depleting the public resource. In this paper, we consider sequential versions of these two dilemmas, Cleanup and Harvest [23]. The detailed settings are described in Appendix C.1.

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5.2 Performance

To test whether homophilic learning can promote the emergence of cooperation, we test our method on CleanUp and Harvest with different numbers of agents and compare against various baselines: LIO [24], Inequity Aversion [40], Social Influence [41], and Selfish Actor-Critic. The details of baselines can be found in Appendix D.

We test all methods with 5 random seeds and show the median value as well as 95% confidence intervals in Fig. 6. It can be observed that our method helps agents learn cooperation with efficiency and stability. In comparison, baseline algorithms either cannot learn any cooperation strategies or the cooperation level oscillates. Inequity aversion oscillates on CleanUp (n=5), which can be proved by its large confidence intervals, and cannot learn to cooperate on Harvest (n=10). Social influence proves that cooperation can be achieved by encouraging agents to influence each other, but it requires many samples (typically 100M as reported in [41]) to learn cooperative strategies. In contrast, our method needs around 5M samples to learn stable cooperative strategies. LIO can learn cooperation within 2M timesteps on CleanUp (n=3), but is less effective in dilemmas with more agents.

5.3 Ablation Study

There are three contributions that characterize our method. (1) First and the most important, the homophily learning objective. (2) Discrete incentive actions and factored incentive Q-functions for each agent. (3) Excluding received incentives when training incentive Q-functions. In this section, we design the following ablations to test the contribution of each of these components.

(1) Without homophily (w/o homophily). We exclude the homophily loss $L_{\text{homo}}$ from our learning objective. We can see that the team performance drops significantly, especially in tasks with more agents. Moreover, without homophily loss, our method performs worse than all baselines on CleanUp (n=5) and (n=10). These observations suggest that our method works mainly because of the homophily loss. (2) Continuous incentivizing actions. Ablation Cont. inc. actions shows the influence of discrete actions. We learn a continuous incentivizing rewarding function for w/o homophily. We can observe further performance decrease on CleanUp (n=3) and Harvest (n=10). We hypothesize that this is because the search space for incentivizing policies grows, making the strategy more difficult to learn. (3) Train incentivizing Q’s with received incentives. We ignore incentives received by agents when training incentivizing strategies. For comparison, ablation w/ inc. shows what would happen if they are included. We can observe that w/ inc. significantly underperforms the original method on all environments. The reason is that agents learn to give each other positive incentives excessively regardless of observations. Since received incentives are also considered in Q-learning for acting behaviors, excessive incentives would overwhelm environmental rewards and significantly hurt learning performance.

5.4 Evolution of Cooperation

To clearly show the evolution of emergent cooperation, the problem of second-order social dilemmas, and how homophily alleviates this problem, according to different team returns, we select four stages during learning and analyze their corresponding behaviors (Fig. 7).

Phase 1: Exploring incentives. This stage starts at the beginning of the training and extends until $T \approx 2.0M$. During this stage, agents are learning basic dynamics of the environment. For example, as shown in the first row of Fig. 7 agents have not learned to eat apples to get rewarded. Meanwhile, during exploration, agents occasionally give incentives to agents who cleaned wastes ($r_1 + 3$), which enables learning incentivizing behaviors in the following stages.

Phase 2: Second-order social dilemmas. This stage starts at the rising point of the learning curve ($T \approx 2.0M$) and ends at $T \approx 3.3M$. Some agents (the pink agent in the second row of Fig. 7) learn to give positive rewards to cleaning agents, which indicates the emergence of cooperation. However, other agents (e.g., orange and blue) typically do not give positive incentives but can enjoy the benefits of others’ incentive behaviors. We can observe an oscillation of team return during this stage. This is the effect of second-order social dilemmas. If there are no additional restrictions (such as homophily) to deal with this problem, the team will fall back to the state where no one wants to perform incentives, resulting in the collapse of cooperation.
Phase 3: Homophily solves second-order social dilemmas. After some oscillations of cooperation, the homophily loss gradually encourages agents with similar environmental behaviors to have similar incentivizing behaviors. As shown in the third row of Fig. 7, although there are still some noisy incentives at this stage, agents who are close to the apple-spawning region simultaneously reward cleaning agents and punish those who are next to the wastes but do not clean them. These incentivizing behaviors indicate that the population has gotten over the second-order social dilemma with the help of homophily. Correspondingly, the team return increases in this stage (from 3.3M to 3.9M).

Phase 4: Stabilized cooperation. This stage starts at $T \approx 3.9M$. Taking advantage of the effect of homophily, during this stage, there are no second-order free-riders and all incentive rewards are given by agents harvesting apples to agents in the region of wastes. Moreover, screenshots show that agents learn an efficient division of labor – three agents eat apples and get environmental rewards while two agents clean the wastes and get rewards from harvesting agents. These incentivizing and environmental behaviors are a stable solution only when homophily learning objective is included.

Based on the illustrations of the evolution of cooperation, we conclude that homophily prevents altruistic incentivizing behaviors from being exploited by second-order free riders, and thus solves the problem of 2nd-SDs and leads to stable cooperation. For detailed agent behaviors at different stages, we refer readers to our online videos.

5.5 Homophilic Incentives

In previous sections, we show that homophilic incentives can promote cooperation, but how homophily affects incentivizing behaviors remains largely unclear. To make up for this, we compare our method with the ablation w/o homophily on Cleanup ($n=3$) by plotting their collective return and altruistic incentive (the average incentive that each Cleaner receives at each time step) in Fig. 8.

We can observe a close connection between incentives and cooperation. Intuitively, the more positive incentives cleaners receive, the more apples are expected to spawn and be collected. However, without homophily, the received incentives oscillate.

![Figure 7: Evolution of cooperation in Cleanup. Left: Sum of environmental rewards received by all agents. Middle: Environmental and incentivizing behaviors at four different stages of learning. Right: Corresponding descriptions.](image)

![Figure 8: Homophily eliminates incentive oscillations.](image)

https://sites.google.com/view/homophily/
dramatically, which is caused by second-order social dilemmas and is in line with the discussions before. In comparison, our method keeps incentivizing cleaners and thus learn cooperation with stability.

6 Closing Remarks

In this paper, we study the problem of cooperation emergence. We show that altruistic incentives make cooperation possible but cannot stabilize due to second-order social dilemmas. We then formally and empirically show that homophily, a common tendency typical of humans, may solve this problem. Combined with deep MARL, we propose an implementation of homophilic learning for sequential social dilemmas. We expect that our work can encourage future works on studying the exciting topics of cooperation emergence, evolution, and stability.

References

[1] Bentley Glass, Owsei Temkin, and William L Straus. Forerunners of darwin, 1745-1859. 1968.
[2] Jerry A Coyne. Why evolution is true. Oxford University Press, 2010.
[3] JU Jarvis. Eusociality in a mammal: cooperative breeding in naked mole-rat colonies. Science, 212(4494):571–573, 1981.
[4] Craig Packer, Dennis A Gilbert, AE Pusey, and SJ O’Brieni. A molecular genetic analysis of kinship and cooperation in african lions. Nature, 351(6327):562–565, 1991.
[5] James K Rilling, David A Gutman, Thorsten R Zeh, Giuseppe Pagnoni, Gregory S Berns, and Clinton D Kilts. A neural basis for social cooperation. Neuron, 35(2):395–405, 2002.
[6] Donald Kennedy. 125. Science, 309(5731):19–20, 2005.
[7] Elizabeth Pennisi. How did cooperative behavior evolve? Science, 309(5731):93–93, 2005.
[8] Martin Nowak and Karl Sigmund. Chaos and the evolution of cooperation. Proceedings of the National Academy of Sciences, 90(11):5091–5094, 1993.
[9] Damien Challet and Y-C Zhang. Emergence of cooperation and organization in an evolutionary game. Physica A: Statistical Mechanics and its Applications, 246(3-4):407–418, 1997.
[10] Martin A Nowak, Akira Sasaki, Christine Taylor, and Drew Fudenberg. Emergence of cooperation and evolutionary stability in finite populations. Nature, 428(6983):646–650, 2004.
[11] Christian Hilbe, Štěpán Šimsa, Krishnendu Chatterjee, and Martin A Nowak. Evolution of cooperation in stochastic games. Nature, 559(7713):246–249, 2018.
[12] James H Fowler. Altruistic punishment and the origin of cooperation. Proceedings of the National Academy of Sciences, 102(19):7047–7049, 2005.
[13] Erol Akçay and Joan Roughgarden. The evolution of payoff matrices: providing incentives to cooperate. Proceedings of the Royal Society B: Biological Sciences, 278(1715):2198–2206, 2011.
[14] Yuk-fai Fong and Jay Surti. The optimal degree of cooperation in the repeated prisoners’ dilemma with side payments. Games and Economic Behavior, 67(1):277–291, 2009.
[15] Elinor Ostrom, James Walker, and Roy Gardner. Covenants with and without a sword: Self-governance is possible. American political science Review, 86(2):404–417, 1992.
[16] Werner Güth. An evolutionary approach to explaining cooperative behavior by reciprocal incentives. International Journal of Game Theory, 24(4):323–344, 1995.
[17] Ernst Fehr and Simon Gächter. Altruistic punishment in humans. Nature, 415(6868):137–140, 2002.
[18] Robert Boyd, Herbert Gintis, Samuel Bowles, and Peter J Richerson. The evolution of altruistic punishment. *Proceedings of the National Academy of Sciences*, 100(6):3531–3535, 2003.

[19] Thomas Mussweiler and Axel Ockenfels. Similarity increases altruistic punishment in humans. *Proceedings of the National Academy of Sciences*, 110(48):19318–19323, 2013.

[20] Robert Boyd. Mistakes allow evolutionary stability in the repeated prisoner’s dilemma game. *Journal of theoretical Biology*, 136(1):47–56, 1989.

[21] David G Rand and Martin A Nowak. The evolution of antisocial punishment in optional public goods games. *Nature communications*, 2(1):1–7, 2011.

[22] Alexander J Stewart, Todd L Parsons, and Joshua B Plotkin. Evolutionary consequences of behavioral diversity. *Proceedings of the National Academy of Sciences*, 113(45):E7003–E7009, 2016.

[23] Joel Z Leibo, Vinicius Zambaldi, Marc Lanctot, Janusz Marecki, and Thore Graepel. Multi-agent reinforcement learning in sequential social dilemmas. In *Proceedings of the 16th Conference on Autonomous Agents and MultiAgent Systems*, pages 464–473. International Foundation for Autonomous Agents and Multiagent Systems, 2017.

[24] Jiachen Yang, Ang Li, Mehrdad Farajtabar, Peter Sunehag, Edward Hughes, and Hongyuan Zha. Learning to incentivize other learning agents. *arXiv preprint arXiv:2006.06051*, 2020.

[25] Andrei Lupu and Doina Precup. Gifting in multi-agent reinforcement learning. In *Proceedings of the 19th International Conference on Autonomous Agents and MultiAgent Systems*, pages 789–797, 2020.

[26] Anna Dreber, David G Rand, Drew Fudenberg, and Martin A Nowak. Winners don’t punish. *Nature*, 452(7185):348–351, 2008.

[27] G HARDIN. Tragedy of the commons. new series, vol. 162, no. 3859, 1968.

[28] Peter Kollock. Social dilemmas: The anatomy of cooperation. *Annual Review of Sociology*, 24:183–214, 1998.

[29] John O Ledyard. Public goods: A survey of experimental research. 1994.

[30] Garrett Hardin. The tragedy of the commons. *Journal of Natural Resources Policy Research*, 1(3):243–253, 2009.

[31] R Axelrod and W. D. Hamilton. The evolution of cooperation. *Science*, 1(1):1390–1396, 1987.

[32] Alexander Peysakhovich and Adam Lerer. Consequentialist conditional cooperation in social dilemmas with imperfect information. *arXiv preprint arXiv:1710.06975*, 2017.

[33] Nicolas Anastassacos, Stephen Hailes, and Mirco Musolesi. Partner selection for the emergence of cooperation in multi-agent systems using reinforcement learning. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 34, pages 7047–7054, 2020.

[34] Mariana Blanco, Dirk Engelmann, Alexander K Koch, and Hans-Theo Normann. Preferences and beliefs in a sequential social dilemma: a within-subjects analysis. *Games and Economic Behavior*, 87:122–135, 2014.

[35] Michael L. Littman. *Markov games as a framework for multi-agent reinforcement learning*. Morgan Kaufman Publishers, Inc., 1994.

[36] Garrison W Greenwood. Altruistic punishment can help resolve tragedy of the commons social dilemmas. In *2016 IEEE Conference on Computational Intelligence and Games (CIG)*, pages 1–7. IEEE, 2016.

[37] Hang Ye, Shu Chen, Jun Luo, Fei Tan, Yongmin Jia, and Yefeng Chen. Increasing returns to scale: The solution to the second-order social dilemma. *Scientific reports*, 6(1):1–10, 2016.
[38] Miller McPherson, Lynn Smith-Lovin, and James M Cook. Birds of a feather: Homophily in social networks. *Annual review of sociology*, 27(1):415–444, 2001.

[39] Gueorgi Kossinets and Duncan J Watts. Origins of homophily in an evolving social network. *American journal of sociology*, 115(2):405–450, 2009.

[40] Edward Hughes, Joel Z Leibo, Matthew Phillips, Karl Tuyls, Edgar Dueñez-Guzman, Antonio García Castañeda, Iain Dunning, Tina Zhu, Kevin McKee, Raphael Koster, et al. Inequity aversion improves cooperation in intertemporal social dilemmas. In *Advances in Neural Information Processing Systems*, pages 3330–3340, 2018.

[41] Natasha Jaques, Angeliki Lazaridou, Edward Hughes, Caglar Gulcehre, Pedro Ortega, Dj Strouse, Joel Z Leibo, and Nando De Freitas. Social influence as intrinsic motivation for multi-agent deep reinforcement learning. In *International Conference on Machine Learning*, pages 3040–3049, 2019.

[42] Christoph Hauert, Arne Traulsen, Hannelore Brandt, Martin A Nowak, and Karl Sigmund. Via freedom to coercion: The emergence of costly punishment. *Science*, 316(5833):1905–1907, 2007.

[43] Hauert, Christoph, Monte, Silvia, De, Hofbauer, Josef, Sigmund, and Karl. volunteering as red queen mechanism for cooperation in public goods games. *Science*, 2002.

[44] Dirk Semmann, Hans Juergen Krambeck, and Manfred Milinski. volunteering leads to rock-paper-scissors dynamics in a public goods game. *Nature*, 425(6956):390, 2003.

[45] Christoph Hauert, Silvia De Monte, Josef Hofbauer, and Karl Sigmund. Replicator dynamics for optional public good games. *Journal of Theoretical Biology*, 218(2):187–194, 2002.

[46] Thomas C Schelling. Hockey helmets, concealed weapons, and daylight saving: A study of binary choices with externalities. *Journal of Conflict resolution*, 17(3):381–428, 1973.

[47] Julien Perolat, Joel Z Leibo, Vinicius Zambaldi, Charles Beattie, Karl Tuyls, and Thore Graepel. A multi-agent reinforcement learning model of common-pool resource appropriation. *arXiv preprint arXiv:1707.06600*, 2017.

[48] Ronald J Williams. Simple statistical gradient-following algorithms for connectionist reinforcement learning. *Machine learning*, 8(3-4):229–256, 1992.

[49] Peter Sunehag, Guy Lever, Audrunas Gruslys, Wojciech Marian Czarnecki, Vinicius Zambaldi, Max Jaderberg, Marc Lanctot, Nicolas Sonnerat, Joel Z Leibo, Karl Tuyls, et al. Value-decomposition networks for cooperative multi-agent learning based on team reward. In *Proceedings of the 17th International Conference on Autonomous Agents and MultiAgent Systems*, pages 2085–2087. International Foundation for Autonomous Agents and Multiagent Systems, 2018.

[50] Amnon Rapoport, Gary Bornstein, and Ido Erev. Intergroup competition for public goods: Effects of unequal resources and relative group size. *Journal of Personality and Social Psychology*, 56(5):748–756, 1989.

[51] Robert Axelrod and William D. Hamilton. *The Evolution of Cooperation*. 1984.

[52] Mikayel Samvelyan, Tabish Rashid, Christian Schroeder de Witt, Gregory Farquhar, Nantas Nardelli, Tim G. J. Rudner, Chia-Man Hung, Philip H. S. Torr, Jakob Foerster, and Shimon Whiteson. The StarCraft Multi-Agent Challenge. *CoRR*, abs/1902.04043, 2019.

[53] Eugene Vinitsky, Natasha Jaques, Joel Leibo, Antonio Castaneda, and Edward Hughes. An open source implementation of sequential social dilemma games. *https://github.com/eugenevinitsky/sequential_social_dilemma_games*, 2019. GitHub repository.

[54] Dan Pelleg, Andrew W Moore, et al. X-means: Extending k-means with efficient estimation of the number of clusters. In *International Conference of Machine Learning*, volume 1, pages 727–734, 2000.
Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper’s contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] Please refer to Appendix F.
   (c) Did you discuss any potential negative societal impacts of your work? [N/A] Our approach do not have potential negative societal impacts.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]

2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [N/A] Our theoretical results do not rely on additional assumptions.
   (b) Did you include complete proofs of all theoretical results? [Yes] Please refer to Appendix E.

3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] We include them in the supplemental material.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] Please refer to Appendix C.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] We include them in all our figures. (Fig. 6)
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] Please refer to Appendix C.

4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes] Our method is built on the open-sourced codebase PyMARL [52] and Sequential Social Dilemma Games (SSDG) [53]. See Appendix C.
   (b) Did you mention the license of the assets? [Yes] We mention that the open-sourced repository PyMARL is licensed under Apache License v2.0 and Sequential Social Dilemma Games (SSDG) is licensed under MIT License in the supplemental material.
   (c) Did you include any new assets either in the supplemental material or as a URL? [Yes] We include our codebase for the homophily framework in the supplemental material.
   (d) Did you discuss whether and how consent was obtained from people whose data you’re using/curating? [N/A] The codebases we use are open-sourced.
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A] Our data does not include such content.
5. If you used crowdsourcing or conducted research with human subjects...

   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]

   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]

   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]
A Details of case study

A.1 Problem settings

From the perspective of multi-agent reinforcement learning, we provide a detailed case study to explain both first- and second-order social dilemmas, and demonstrate that homophily can promote cooperation by alleviating second-order social dilemmas. The case study is based on the classic problem setting from \[12\] for its modeling of the public goods dilemma.

A population of \( n \) agents has an opportunity to create a public good that will be equally distributed to all participants. There are several possible strategies in this population. Contributors (\( C \)) pay a cost \( c \) to increase the size of public goods by \( b \). Defectors (\( D \)) do not contribute but benefit from the public goods. Agents can also choose to neither contribute to nor benefit from the public goods, which is the same as contributors, and importantly, it also pays a cost \( k \) to incur a punishment \( p \) on defectors. To guarantee that no agent can exploit altruistic incentives by being a pure contributor on defectors. Therefore, in this part, we consider Contributors (\( C \)), Defectors (\( D \)), and Nonparticipants (\( N \)). Assume that the proportion of each strategy is \( p_C, p_D, \) and \( p_N \), respectively, and \( p_C + p_D + p_N = 1 \). Then the rewards at each step are

\[
 r = \begin{cases} 
 b_{PC} \frac{1}{1-p_N} - c, & \text{Contributors (} C \text{)} \\
 b_{PC} \frac{1}{1-p_N}, & \text{Defectors (} D \text{)} \\
 \sigma, & \text{Nonparticipants (} N \text{)} 
\end{cases}

(7)

From Eq. 7 we can see that the rewards of defectors are always higher than those of contributors, which leads to first-order social dilemmas (1st-SDs or SDs).

In Sec. 3 Part A, to showcase the influence of first-order social dilemmas, we consider Contributors (\( C \)), Defectors (\( D \)), and Nonparticipants (\( N \)). Assume that the proportion of each strategy is \( p_C, p_D, p_N \), and \( p_{PA} \), respectively, and \( p_C + p_D + p_N + p_{PA} = 1 \). Then the rewards at each step are

\[
 r = \begin{cases} 
 \frac{b_{PC} + p_{PA}}{1-p_N} - c - \alpha p_{PA}, & \text{Contributors (} C \text{)} \\
 \frac{b_{PC} + p_{PA}}{1-p_N} - p_{PA}, & \text{Defectors (} D \text{)} \\
 \sigma, & \text{Nonparticipants (} N \text{)} \\
 \frac{b_{PC} + p_{PA}}{1-p_N} - c - k p_D - \alpha k p_C, & \text{Unexploitable Punishers (} PA \text{)} 
\end{cases}

(8)

In Sec. 3 Part B, to show the effect of unexploitable altruistic incentives, we consider Contributors (\( C \)), Nonparticipants (\( N \)), and Exploitable Punishers (\( PA \)). Assume that the proportion of each strategy is \( p_C, p_D, p_N \), and \( p_p \), respectively, and \( p_C + p_D + p_N + p_p = 1 \). Then the rewards each step are

\[
 r = \begin{cases} 
 \frac{b_{PC} + p_{PP}}{1-p_N} - c, & \text{Contributors (} C \text{)} \\
 \frac{b_{PC} + p_{PP}}{1-p_N} - p_{PP}, & \text{Defectors (} D \text{)} \\
 \sigma, & \text{Nonparticipants (} N \text{)} \\
 \frac{b_{PC} + p_{PP}}{1-p_N} - c - k p_D, & \text{Exploitable Punishers (} P \text{)} 
\end{cases}

(9)

From Eq. 9 we can find that the rewards of pure contributors are always higher than those of exploitable punishers, which leads to the second-order social dilemmas (2nd-SDs).

In Sec. 3 Part D, to show the effect of homophily, based on the settings of Eq. 9 which suffer from 2nd-SDs, we further encourage agents with similar acting behaviors to have similar incentivizing behaviors. In the considered setting, only contributors and punishers have the same acting behavior.
of contributing to the public goods. Therefore, we encourage their incentivizing behaviors to be the same by converting the minority of punishers and contributors to the majority of them with probability 0.2. (For example, if 30% of the agents are punishers and 20% of them are contributors, then contributors become punishers with probability 0.2.)

In all our simulations, we set \( n = 10, b = 3, c = 1, \sigma = 1, p = 2, k = 0.35, \) and \( \alpha = 1. \) A sensitivity analysis is provided in Sec. 3 of the main text to demonstrate that our observation and conclusion are solid for a large range of parameters. Agents use REINFORCE policy gradients [48] to learn independent local policies for selecting strategies (atomic actions).

### A.2 Visualization and Coordinate transformation

In order to demonstrate the evolution of population, we employ two visualization methods, the ternary plot (for \( p_C, p_D, p_N \) in Sec. 3 Part A) and quaternary plot (for \( p_C, p_D, p_N, p_P \) in Sec. 3 Part B and \( p_C, p_D, p_N, p_P \) in Sec. 3 Part C, D).

**Ternary plot**, an equilateral triangle periphery with several trajectories inside, reveals the dynamics of population constituents (three different strategies), as shown in Fig. 1(c) in the paper. Each point \( X \) inside the equilateral triangle represents a distribution of the population (of three strategies), as shown in Fig. 1(c) in the paper. Each point \( X \) has coordinates before trajectories can be plotted. We now describe the details of coordinate transformation.

However, ternary plot can only visualize the evolutionary trajectories of three strategies. When the fourth strategy is introduced, we resort to the **quaternary plot** in 3-dimensional space. For any interior point \( X \) of a regular tetrahedron \( CDNP \) (Fig. 9), the sum of distances from point \( X \) to four faces \( NCD, PCN, DPN, \) and \( PCD \) is a constant. Therefore, we can still use an interior point \( X \) to represent a population distribution and represent \( p_C, p_D, p_N, p_P \) by the distances from \( X \) to different faces.

Point-to-face distances have to be transformed into rectangular coordinates before trajectories can be plotted. We now describe the details of coordinate transformation.

We first plot a regular tetrahedron in the three-dimensional rectangular coordinate system, with four vertices \( P(0,0,1), N(\sqrt{2},0,0), C(-\sqrt{2},0,0), D(-\sqrt{2},0,0) \) as in Fig. 9. To simplify notations, we denote the distance from an interior point \( X \) to faces \( DNP, CNP, CDP, \) and \( CDN \) by \( p_C, p_D, p_N, \) and \( p_P, \) respectively.

It can be calculated that the equation for plane \( PNC \) is

\[
\sqrt{2}x + \sqrt{6}y + z = 1
\]

and the equation for plane \( PND \) is

\[
\sqrt{2}x - \sqrt{6}y + z = 1.
\]

Next, using formula in analytical geometry for calculating the distance from a point to a given plane, we can derive

\[
\begin{align*}
p_D &= \frac{1}{3}\sqrt{2}x + \sqrt{6}y + z - 1, \\
p_C &= \frac{1}{3}\sqrt{2}x - \sqrt{6}y + z - 1, \\
p_P &= z.
\end{align*}
\]

Finally, we solve the above system of equations and get

\[
\begin{align*}
x &= \frac{\sqrt{2}}{12}(2 - 3p_D - 3p_C - 2p_P), \\
y &= \frac{\sqrt{6}}{12}(p_D - p_C), \\
z &= p_P.
\end{align*}
\]
The more homophilic a population is, the more possible cooperation would emerge. The cooperation proportion and gradient field in the population policy space under different degrees of homophily are shown. The increasing volume of the “safe region” and the cooperation proportion increases with the degree of homophily.

With Eq. [11] we can calculate the corresponding coordinate in the three-dimensional rectangular coordinate system of any population distribution. Connecting all points into a curve gives the 3D quaternary plot.

B More results and analyses

B.1 Case study: Limit cycle

In Fig. 10, we present a limit cycle in the population policy space. A limit cycle is a closed trajectory, and any population initialized on the cycle would keep looping over it and never converge to a stable solution. It is worth noting that although homophilic incentives make cooperation possible (Fig. 3(b) in the main text), they cannot eliminate limit cycles in the non-cooperative (blue) region.

B.2 Case study: Degree of homophily

In Sec. 3 Part D, we encourage agents with similar acting behaviors to have similar incentivizing behaviors by converting the minority of punishers and contributors to the majority of them with probability $\lambda$ ($\lambda=0.2$ in the paper). We call $\lambda$ the degree of homophily.

To further show the influence of $\lambda$, in Fig. 11 we plot how the cooperation proportion changes with respect to the degree of homophily. Cooperation proportion is the ratio of the volume of the cooperative (green) region to the volume of the regular tetrahedron. We observe that the cooperation proportion increases with the degree of homophily, and gradually converges to a constant value 0.4. We further present the gradient field under several degrees of homophily. As expected, the volume of the “safe region” increases with the degree of homophily.
These results demonstrate that the more homophilic a population is, the more possible cooperation would emerge.

C Details of experiments

Our method is built on the open-sourced codebase PyMARL [52] and Sequential Social Dilemma Games (SSDG) [53]. We now discuss the specific environmental settings and implementation details.

C.1 Sequential Social Dilemmas

In Cleanup game (Fig. 12(a)), the apple regrowth rate decreases linearly with the density of waste and would reduce to zero as the amount of waste exceeds a saturation threshold. At the start of each episode, the environment resets with waste just beyond the saturation threshold. To enable apple reproduction, agents can fire a cleaning beam to clear waste within the beam range, but this action induces no immediate reward. Additionally, waste is produced with a certain probability during the episode, so agents need to keep cleaning waste to maintain the provision of apples. We have a dilemma in this game. There is a distance between the waste field and the apple field. It is personally more rewarding to stay in the apple field to wait for the spawned apples, but some agents have to sacrifice, leave the apple field, and contribute to the public goods by cleaning waste.

In Harvest game (Fig. 12(b)), the apple reproduction rate grows with the density of uncollected apples around it. If all apples in a local area are harvested then no apple will re-spawn until the next episode. There is a dilemma in the game. For individual short-term interests, agents tend to harvest as rapidly as possible, which will deplete local resources and harm long-term collective interests. However, agents who abstain from personal benefits for the good of the group are easily exploited by defecting and over-harvesting agents.

C.2 Environments

To focus on the problem of social dilemmas, for all experiments, including baselines and ablations, we remove agent rotation actions in SSDG and set the orientation of all agents to face “up”, like in previous works studying social dilemmas [24]. For our method, we disable the “fining” action and use incentive actions as the way to incentivize other agents. In both Cleanup and Harvest game, eating an apple will provide a local reward of +1, and there are no other environmental rewards.

In Cleanup, agents are equipped with a cleaning beam, which allows them to remove waste. We test our method on three Cleanup maps with different numbers of agents. In Table 1 we show the details of each map.

| Parameter          | n=3   | n=5   | n=10  |
|--------------------|-------|-------|-------|
| Map Size           | 10×10 | 25×18 | 48×18 |
| View Size          | 7     | 15    | 15    |
| Max Steps          | 50    | 100   | 100   |
| Apple Respawn Probability | 0.3  | 0.05  | 0.05  |
| Depletion Threshold | 0.4   | 0.99  | 0.99  |
| Restoration Threshold | 0.0  | 0.0   | 0.0   |
| Waste Spawn Probability | 0.5  | 0.05  | 0.05  |

In Harvest, the apple spawning rate at each point is related to the current number of apples within an ℓ1-distance of 2, and the spawn probability is 0, 0.05, 0.08, and 0.1 when there are 0, 1, 2, and ≥3 apples within the distance, respectively.
C.3 Implementation

Network architecture There are two main components in our methods: environmental Q-functions and incentivizing Q-functions. In the study of social dilemmas, agents learn independently, so we do not share parameters among different agents, except for the RGB preprocessing network, which has the following architecture: 1 convolutional layer (6 filters, $3 \times 3$ kernel with stride 1), 1 flatten layer, and 1 dense layer (32 neurons) with LeakyReLU activation. The environmental Q-functions and incentivizing Q-functions take the output of the RGB preprocessing network as input.

The environmental Q-function consists of three layers: a fully-connected layer with LeakyReLU as activation, followed by a 64 bit GRU, and followed by another fully-connected layer that outputs an estimated utility for each action. The incentivizing Q-function has the same architecture as the acting Q-function, except that the last layer additionally takes the target agent’s environmental action as input.

Optimization For all experiments, we set the loss scaling factor $\lambda_{\text{inc}} = 1$, $\lambda_{\text{homo}} = 0.01$, discount factor $\gamma_{\text{env}} = 0.95$, $\gamma_{\text{inc}} = 0.995$, incentive effect factor $\eta^e = 1.0$, and incentive cost factor $\eta^c = 0.1$. The optimization is conducted using Adam with a learning rate of 0.0001. For exploration, we use $\epsilon$-greedy with $\epsilon$ annealed linearly from 1.0 to 0.05 over 50K time steps and kept constant for the rest of the training. We run one environment each time to collect samples. Batches of 16 episodes are sampled from the replay buffer (whose size is 5000), and the whole framework is trained end-to-end on fully unrolled episodes.

Experiments are carried out on NVIDIA GTX 2080 Ti GPU. For a 10-agent environment (like Cleanup $(n=10)$), our method requires approximately 60G of RAM and 0.9G of video memory, and takes about 115 hours to finish 5M timesteps of training.

C.4 Similarity of environmental behaviors

In Sec. 4.2 of the paper, we discuss how to encourage homophily in temporally extended cases. A challenge is to measure the similarity of environmental behaviors. In this paper, we use the X-means [54] implementation provided by PyClustering [55] to identify similar behaviors. The behavioral features include the changes made to common information like the amount of harvesting, the amount of cleanup, etc., in the last 10 timesteps. When clustering, the minimum and maximum number of clusters are set to 2 and 4, respectively.

D Details of baselines and ablations

We compare our method against various baselines and ablations. For LIO [24], Inequity Aversion [40], and Social Influence [41], we use the codes provided by the authors and the hyper-parameters that have been fine-tuned on the Sequential Social Dilemma Games (SSDG) [53]. For Selfish Actor-Critic, we use the default implementation in SSDG.

The ablation Cont. inc. actions, which learns continuous incentives, uses the same implementation and hyperparameter settings as LIO, but with the only difference that the incentive cost is changed from the default value of LIO to 0.1, which is the same as in our method. Ablation w/o homophily and w/ inc use the identical network structure and hyper-parameter settings as our method. The differences are that w/o homophily does not use the homophily loss by setting homophily loss scaling factor $\lambda_{\text{homo}}$ to 0, and w/ inc additionally uses received incentives to train incentive Q-functions. For all the experiments, we keep the game settings to be the same for fair comparisons.

E Formal Analysis

In this section, we formally calculate the closed-form gradients in the policy space for the case study problem, which are visualized as ternary plots or quaternary plots in Sec. 3 of the paper.

E.1 Notations

Suppose a team of $n$ agents joins the public goods game introduced in Sec. 3, where the reward functions can be found in Appendix A. The action set $A$ is identical for all agents and depends on the
We first define two frequently used equations. Let \( \pi \sum \) where \( \pi \sum \) and use the notation \( d_\mathcal{I} = (d_1, \cdots, d_{i-1}, d_{i+1}, \cdots, d_n) \), where \( d_k \equiv \mathbb{I}(a_k = N) \in \{0, 1\} \) is the indicator variable, i.e., \( d_k = 1 \) if \( a_k = N \) and otherwise \( d_k = 0 \). We have

\[
E_{-i} = \sum_{d_i \in (0,1)^{n-1}} \frac{1}{n - \sum_{k \neq i} d_k} \prod_{k \neq i} (1 - \theta_{k,N}^{\mathcal{I}})^{1-d_k} \theta_{k,N}^{d_k}.
\]

Note that \( \frac{\partial}{\partial \theta_{i,N}} E_{-i} = 0 \). Similarly, we define

\[
E_{-ij} = \mathbb{E}_\pi \left[ \frac{1}{n - \sum_{k \neq \{i,j\}} d_k} \prod_{k \neq \{i,j\}} (1 - \theta_{k,N}^{\mathcal{I}})^{1-d_k} \theta_{k,N}^{d_k} \right]
\]

and use the notation \( d_{-ij} = (d_1, \cdots, d_{i-1}, d_{i+1}, \cdots, d_{j-1}, d_{j+1}, \cdots, d_n) \), where \( d_k \equiv \mathbb{I}(a_k = N) \in \{0, 1\} \). We have

\[
E_{-ij} = \sum_{d_{-ij} \in (0,1)^{n-2}} \frac{1}{n - \sum_{k \neq \{i,j\}} d_k} \prod_{k \neq \{i,j\}} (1 - \theta_{k,N}^{\mathcal{I}})^{1-d_k} \theta_{k,N}^{d_k}.
\]

Note that \( \frac{\partial}{\partial \theta_{i,N}} E_{-ij} = 0 \).

### E.2 Sec. 3 Part A

To showcase the influence of first-order social dilemmas, in Sec. 3 Part A we consider three atomic actions, \( C, D, N \). Assume that agent \( i \) chooses actions from \( \mathcal{A} = \{C, D, N\} \) with probabilities \( \theta_i,C, \theta_i,D, \theta_i,N \). The reward function is defined in Eq.\[7\] in Appendix A.1. We can calculate the value function of agent \( i \):

\[
V_i^\pi = \mathbb{E}_\pi \left[ r_i(a_1, \cdots, a_n) \right]
\]

\[
= \mathbb{E}_\pi \left[ \mathbb{I}(a_i = C) \left( \frac{b}{n - \sum_{j \neq i} \mathbb{I}(a_j = N)} \left( \sum_{j \neq i} \mathbb{I}(a_j = C) + 1 \right) - c \right) 
+ \mathbb{I}(a_i = D) \frac{b}{n - \sum_{j \neq i} \mathbb{I}(a_j = N)} \left( \sum_{j \neq i} \mathbb{I}(a_j = C) \right) 
+ \mathbb{I}(a_i = N) \sigma \right]
\]

\[
= \theta_{i,C} \left( b \left( \sum_{j \neq i} \theta_{j,C} E_{-ij} + E_{-i} \right) - c \right) + \theta_{i,D} b \sum_{j \neq i} \theta_{j,C} E_{-ij} + \theta_{i,N} \sigma.
\]
where \( E_{-i} \) and \( E_{-ij} \) are defined as in Eq. 12 and Eq. 13, respectively. Then we can calculate the derivatives of the value function w.r.t each parameter:

\[
\frac{\partial V^\pi_i}{\partial \theta_{i,C}} = b \left( \sum_{j \neq i} \theta_{j,C} E_{-ij} + E_{-i} \right) - c, \tag{14}
\]

\[
\frac{\partial V^\pi_i}{\partial \theta_{i,D}} = b \sum_{j \neq i} \theta_{j,C} E_{-ij}, \tag{15}
\]

\[
\frac{\partial V^\pi_i}{\partial \theta_{i,N}} = \sigma. \tag{16}
\]

The above equations are used to plot Fig. 1(d) of the paper.

### E.3 Sec. 3 Part B

To introduce altruistic incentives into the system, we add the fourth type of atomic action, \( PA \). We consider unexploitable punishments here, and exploitable punishments in the next subsection. Agent \( i \) chooses actions from \( A = \{C, D, N, PA\} \) with probabilities \( \theta_{i,C}, \theta_{i,D}, \theta_{i,N}, \theta_{i,PA} \). The reward function in this case is defined in Eq. 8 in Appendix A.1. We can calculate the value function of agent \( i \),

\[
V^\pi_i = \mathbb{E}_\pi \left[ r_i(a_1, \cdots, a_n) \right] = \mathbb{E}_\pi \left[ I(a_i = C) \left( b - \frac{1}{n} \sum_{j \neq i} I(a_j = N) \left( \sum_{j \neq i} I(a_j = C, PA) + 1 \right) \right) - c \\
- \alpha p \frac{1}{n} \sum_{j \neq i} I(a_j = PA) \\
+ I(a_i = D) \left( b - \frac{1}{n} \sum_{j \neq i} I(a_j = N) \left( \sum_{j \neq i} I(a_j = C, PA) \right) - p \frac{1}{n} \sum_{j \neq i} I(a_j = PA) \right) \\
+ I(a_i = N) \sigma \\
+ I(a_i = PA) \left( b - \frac{1}{n} \sum_{j \neq i} I(a_j = N) \left( \sum_{j \neq i} I(a_j = C, PA) + 1 \right) \right) - c \\
- \alpha k \frac{1}{n} \sum_{j \neq i} I(a_j = C) - k \frac{1}{n} \sum_{j \neq i} I(a_j = D) \right] \\
= \theta_{i,C} \left( b \left( \sum_{j \neq i} (\theta_{j,C} + \theta_{j,PA}) E_{-ij} + E_{-i} \right) - c - \alpha p \frac{1}{n} \sum_{j \neq i} \theta_{j,PA} \right) \\
+ \theta_{i,D} \left( b \sum_{j \neq i} (\theta_{j,C} + \theta_{j,PA}) E_{-ij} - p \frac{1}{n} \sum_{j \neq i} \theta_{j,PA} \right) \\
+ \theta_{i,N} \sigma \\
+ \theta_{j,PA} \left( b \left( \sum_{j \neq i} (\theta_{j,C} + \theta_{j,PA}) E_{-ij} + E_{-i} \right) - c - \alpha k \frac{1}{n} \sum_{j \neq i} \theta_{j,C} - k \frac{1}{n} \sum_{j \neq i} \theta_{j,D} \right),
\]
The above equations are used to plot Fig. 3(a) of the paper.

E.4 Sec. 3 Part C

Now we consider exploitable punishments. Agent $i$ chooses actions from $A = \{C, D, N, P\}$ with probabilities $\theta_i, C, \theta_i, D, \theta_i, N, \theta_i, P$. The reward function is defined in Eq. 9 in Appendix A.1. We can calculate the value function of agent $i$:

\[
V_i = \mathbb{E}_\pi \left[ r_i(a_1, \cdots, a_n) \right] = \mathbb{E}_\pi \left[ \mathbb{I}(a_i = C) \left( \frac{1}{n - \sum_{j \neq i} \mathbb{I}(a_j = N)} \left( \sum_{j \neq i} \mathbb{I}(a_j = C, P) + 1 \right) - c \right) + \mathbb{I}(a_i = D) \left( \frac{1}{n - \sum_{j \neq i} \mathbb{I}(a_j = N)} \left( \sum_{j \neq i} \mathbb{I}(a_j = C, P) \right) - p \frac{1}{n} \sum_{j \neq i} \mathbb{I}(a_j = P) \right) + \mathbb{I}(a_i = N) \sigma \right.
\]

\[
+ \mathbb{I}(a_i = P) \left( \frac{1}{n - \sum_{j \neq i} \mathbb{I}(a_j = N)} \left( \sum_{j \neq i} \mathbb{I}(a_j = C, P) + 1 \right) - c \right) - k \frac{1}{n} \sum_{j \neq i} \mathbb{I}(a_j = D) \right]
\]

\[
= \theta_i, C \left( b \left( \sum_{j \neq i} (\theta_j, C + \theta_j, P)E_{-ij} + E_{-i} \right) - c \right) + \theta_i, D \left( b \sum_{j \neq i} (\theta_j, C + \theta_j, P)E_{-ij} - p \frac{1}{n} \sum_{j \neq i} \theta_j, P \right) + \theta_i, N \sigma
\]

\[
+ \theta_j, P \left( b \left( \sum_{j \neq i} (\theta_j, C + \theta_j, P)E_{-ij} + E_{-i} \right) - c - k \frac{1}{n} \sum_{j \neq i} \theta_j, D \right)
\]

where $\mathbb{I}(a_j = C, P)$ equals one if and only if $a_j = C$ or $a_j = P$, and $E_{-i}$ and $E_{-ij}$ are defined in Eq. 12 and Eq. 13 respectively. Then we can calculate the derivatives of the value function w.r.t each parameter,
The above equations are used to plot Fig. 2(d) of the paper. It is worth noting that

\[
\frac{\partial V_i}{\partial \theta_{i,C}} = b \left( \sum_{j \neq i} (\theta_{j,C} + \theta_{j,P}) E_{ij} + E_{-i} \right) - c, \quad (21)
\]

\[
\frac{\partial V_i}{\partial \theta_{i,D}} = b \left( \sum_{j \neq i} (\theta_{j,C} + \theta_{j,P}) E_{ij} - p \frac{1}{n} \sum_{j \neq i} \theta_{j,P} \right), \quad (22)
\]

\[
\frac{\partial V_i}{\partial \theta_{i,N}} = \sigma, \quad (23)
\]

\[
\frac{\partial V_i}{\partial \theta_{i,P}} = b \left( \sum_{j \neq i} (\theta_{j,C} + \theta_{j,P}) E_{ij} + E_{-i} \right) - c - k_1 \frac{1}{n} \sum_{j \neq i} \theta_{j,D}. \quad (24)
\]

The gradient is non-positive for any \( \theta_{i,D} \), which indicates that second-order cooperators would be taken over by second-order defectors.

**E.5 Sec. 3 Part D**

Based on the settings specified in Appendix E.4, we consider homophily here. Agent \( i \) chooses actions from \( A = \{C, D, N, P\} \) with probabilities \( \theta_{i,C}, \theta_{i,D}, \theta_{i,N}, \theta_{i,P} \). The reward function is defined in Eq. 9. We can calculate the value function of agent \( i \):

\[
V_i = \mathbb{E}_\pi \left[ r_i(a_1, \cdots, a_n) \right]
\]

\[
= \mathbb{E}_\pi \left[ \mathbb{I}(a_i = C) \left( b \frac{1}{n} \sum_{j \neq i} \mathbb{1}(a_j = N) \left( \sum_{j \neq i} \mathbb{1}(a_j = C, P) + 1 \right) - c \right) \right.
\]

\[
+ \mathbb{I}(a_i = D) \left( b \frac{1}{n} \sum_{j \neq i} \mathbb{1}(a_j = N) \left( \sum_{j \neq i} \mathbb{1}(a_j = C, P) - p \frac{1}{n} \sum_{j \neq i} \mathbb{1}(a_j = P) \right) \right.
\]

\[
+ \mathbb{I}(a_i = N) \sigma
\]

\[
+ \mathbb{I}(a_i = P) \left( b \frac{1}{n} \sum_{j \neq i} \mathbb{1}(a_j = N) \left( \sum_{j \neq i} \mathbb{1}(a_j = C, P) + 1 \right) - c \right.
\]

\[
- k_1 \frac{1}{n} \sum_{j \neq i} \mathbb{1}(a_j = D) \left] \right)
\]

\[
= \theta_{i,C} \left( b \left( \sum_{j \neq i} (\theta_{j,C} + \theta_{j,P}) E_{ij} + E_{-i} \right) - c \right)
\]

\[
+ \theta_{i,D} \left( b \left( \sum_{j \neq i} (\theta_{j,C} + \theta_{j,P}) E_{ij} - p \frac{1}{n} \sum_{j \neq i} \theta_{j,P} \right) \right)
\]

\[
+ \theta_{i,N} \sigma
\]

\[
+ \theta_{i,P} \left( b \left( \sum_{j \neq i} (\theta_{j,C} + \theta_{j,P}) E_{ij} + E_{-i} \right) - c - k_1 \frac{1}{n} \sum_{j \neq i} \theta_{j,D} \right),
\]

23
where $I(a_j = C, P)$ equals one if and only if $a_j = C$ or $a_j = P$, and $E_{-i}$ and $E_{-ij}$ are defined in Eq. [12] and Eq. [13] respectively. Then we can calculate the derivatives of the value function w.r.t each parameter. Besides, to show the effect of homophily, we encourage agents with similar environmental behaviors to have similar incentivizing behaviors. Since only contributors and punishers have the same environmental behavior of contributing to the public goods, we encourage their incentivizing behaviors to be the same by converting the minority of $P$ and $C$ to the majority with a probability of $\lambda = 0.2$. For each agent, the converting direction depends on all the other agents. Specifically, if other agents choose action $P$ more often ($\text{sign}(\sum_{j \neq i}(\theta_{j,P} - \theta_{j,C})) > 0$), agent $i$ will increase the probability of choosing action $P$ by $\lambda \cdot \min(\theta_{i,C}, \theta_{i,P})$, and vice versa. Formally, taken homophily into consideration, the gradients of each parameter of agent $i$ are:

$$
\dot{\theta}_{i,C} = b \left( \sum_{j \neq i} (\theta_{j,C} + \theta_{j,P}) E_{-ij} + E_{-i} \right) - c + \lambda \cdot \text{sign} \left( \sum_{j \neq i} (\theta_{j,C} - \theta_{j,P}) \right) \min(\theta_{i,C}, \theta_{i,P}),
$$

$$
\dot{\theta}_{i,D} = b \sum_{j \neq i} (\theta_{j,C} + \theta_{j,P}) E_{-ij} - \frac{1}{n} \sum_{j \neq i} \theta_{j,P},
$$

$$
\dot{\theta}_{i,N} = \sigma,
$$

$$
\dot{\theta}_{i,P} = b \left( \sum_{j \neq i} (\theta_{j,C} + \theta_{j,P}) E_{-ij} + E_{-i} \right) - c - \frac{1}{n} \sum_{j \neq i} \theta_{j,D} + \lambda \cdot \text{sign} \left( \sum_{j \neq i} (\theta_{j,P} - \theta_{j,C}) \right) \min(\theta_{i,C}, \theta_{i,P}).
$$

The above equations are used to plot Fig. 3(b) of the paper. And it is worth noting that

$$
\dot{\theta}_{i,P} - \dot{\theta}_{i,C} = -k \frac{1}{n} \sum_{j \neq i} \theta_{j,D} + 2\lambda \cdot \text{sign} \left( \sum_{j \neq i} (\theta_{j,P} - \theta_{j,C}) \right) \min(\theta_{i,C}, \theta_{i,P}),
$$

which is positive when the population is close to point $P$, in which situation the population chooses action $P$ more often than $C$ and $D$ ($\text{sign}(\sum_{j \neq i}(\theta_{j,P} - \theta_{j,C})) > 0$ and $\sum_{j \neq i} \theta_{j,D}$ is small), and thus the agents will not deviate to second-order free-riding.

### E.6 Project onto the probability simplex

After we have obtained the gradients of each action of agent $i$, we can calculate the new policy as follows:

$$
\theta'_{i,X} = \theta_{i,X} + \beta \frac{\partial V_i}{\partial \theta_{i,X}}, \forall X \in A.
$$

where $\beta$ is the learning rate. Now $\pi'_i(a_i = X) = \theta'_{i,X}$. However, this new policy may not be in the valid probability space, i.e. $\sum_{X \in A} \pi'_i(a_i = X) = 1$ may not hold anymore. To address this issue, we project it onto the probability simplex [56][57] after each update. Let $\Pi_{\Delta^{|A|}} : \mathbb{R}^{|A|} \rightarrow \Delta^{|A|}$ denotes the projection to the valid space:

$$
\Pi_{\Delta^{|A|}}[x] = \arg \min_{z \in \Delta^{|A|}} \|x - z\|,\quad (34)
$$
where $\| \cdot \|$ denotes the regular Euclidean norm and $\Delta^{[A]}$ is the canonical simplex defined by

$$\Delta^{[A]} \coloneqq \left\{ z = (z_1, \cdots, z_{|A|})^T \in \mathbb{R}^{[A]} : 0 \leq z_i \leq 1, i = 1, \cdots, n, \text{ and } \sum_{i=1}^{|A|} z_i = 1 \right\}.$$  

Using this projection, the valid new policy of agent $i$ is

$$\pi_i' \leftarrow \Pi_{\Delta^{[A]}}[\pi_i'],$$  (35)

where $\pi_i' = (\theta_{i,x})_{x \in A}$ is the parameter vector of agent $i$. With enough updates and this projection rule, we can determine the location of the “safe region” in Fig. 2(d), Fig. 3(a) and Fig. 3(b) of the paper.

**F Limitations**

In this work, we study the problem of cooperation emergence in both single-stage and sequential social dilemmas. For single-stage social dilemmas, we provide formal analyses and numerical results for the effect of free-riders and homophily in Sec. 3 and Appendix E. However, in the main text, for sequential social dilemmas, we only provide empirical results in Sec. 5.

Our aim is to formally analyze the evolutionary dynamics of environmental behaviors and incentivizing behaviors on SSDs. However, the environmental policies and incentivizing policies are interdependent, and it is difficult to accurately account for the effect of incentivizing behaviors when considering environmental policy updates.

To better explain this challenge, we first give some notations. There are $n$ agents participating in the public goods game introduced in Sec. 3. The first-order cooperation contributes to the public goods and benefits from it, while the first-order defection does not contribute but benefits from the public goods. The second-order cooperation will pay a cost to punish those who choose first-order defection, while the second-order defection will not punish such defections. Each agent $i$ chooses actions according to its own policy $\pi_i$, which includes environmental policy $\pi_i^1(a_1^1)$ parameterized by $\theta_{i,1}$ and incentivizing policy $\pi_i^2(a_2^1)$ parameterized by $\theta_{i,2}$. We assume that the two policies are independent, i.e., $\pi_i(a_1^1, a_2^2) = \pi_i^1(a_1^1)\pi_i^2(a_2^2)$. Agent $i$ chooses first-order cooperation (or defection) with probability $\pi_i^1(a_1^1 = C) = \theta_{i,1}$ (or $\pi_i^1(a_1^1 = D) = 1 - \theta_{i,1}$) and chooses second-order cooperation (or defection) with probability $\pi_i^2(a_2^2 = C) = \theta_{i,2}$ (or $\pi_i^2(a_2^2 = D) = 1 - \theta_{i,2}$). We also assume different agents choose actions independently: $\pi(a_1^1, a_2^1, \cdots, a_n^1, a_n^2) = \prod_{j=1}^{n} \pi_j(a_j^1, a_j^2)$. We can calculate the value function of agent $i$,

$$V_i^n = \mathbb{E}_\pi[r_i(a_1^1, a_2^1, \cdots, a_n^1, a_n^2)]$$

$$= \mathbb{E}_\pi \left[ \sum_{j=1}^{n} \frac{b}{n} I(a_j^1 = C) - cI(a_j^1 = C) - p\frac{1}{n} I(a_j^1 = D) \sum_{j \neq i} I(a_j^2 = C) - k\frac{1}{n} I(a_j^2 = C) \sum_{j \neq i} I(a_j^2 = D) \right]$$

$$= \sum_{j=1}^{n} \frac{b}{n} \theta_{j,1} - c\theta_{j,1} - p\frac{1}{n} (1 - \theta_{i,1}) \sum_{j \neq i} \theta_{j,2} - k\frac{1}{n} (1 - \theta_{j,2}) \sum_{j \neq i} (1 - \theta_{j,1})$$

$$= \left( \frac{b}{n} - c \right) \theta_{i,1} + \sum_{j \neq i} \left( \frac{b}{n} \theta_{j,1} - p\frac{1}{n} (1 - \theta_{i,1}) \theta_{j,2} - k\frac{1}{n} (1 - \theta_{j,2}) (1 - \theta_{j,1}) \right).$$

The learning process of agent $i$’s incentivizing policy can be framed as a bi-level optimization problem,
With this derivative in hand, we can obtain the gradient of \( V_{i}^{π} \).

\[
\frac{∂V_{i}^{π}}{∂θ_{j,1}} = \frac{b}{n} - c + p \frac{1}{n} \sum_{k \neq j} θ_{k,2}.
\]  

(36)

With learning rate \( β \), the updated \( θ'_{j,1} \) becomes:

\[
θ'_{j,1} = θ_{j,1} + β \frac{∂V_{j}^{π}}{∂θ_{j,1}} = θ_{j,1} + β \left( \frac{b}{n} - c + p \frac{1}{n} \sum_{k \neq j} θ_{k,2} \right).
\]

(37)

Now the new value function for agent \( i \) is:

\[
V_{i}^{π'} = \left( \frac{b}{n} - c \right)θ_{i,1}' + \sum_{j \neq i} \left( \frac{b}{n}θ_{j,1}' - p \frac{1}{n}(1 - θ_{i,1}')θ_{j,2}' - k \frac{1}{n}θ_{i,2}(1 - θ_{j,1}') \right).
\]

(38)

To calculate updated incentivizing policies, we derive the gradient of \( V_{i}^{π'} \) w.r.t. \( θ_{i,1} \). Note that agent \( i \)’s incentivizing policy does not directly influence its own environmental behaviors, so we have:

\[
\frac{∂θ'_{j,1}}{∂θ_{i,2}} = \begin{cases} 
0, & j = i, \\
\frac{2p}{n}, & j \neq i.
\end{cases}
\]

With this derivative in hand, we can obtain the gradient of \( V_{i}^{π'} \) w.r.t. \( θ_{i,2} \):

\[
\frac{∂V_{i}^{π'}}{∂θ_{i,2}} = \sum_{j \neq i} \left( \frac{b}{n}θ_{j,1}' - p \frac{1}{n}(1 - θ_{i,1}')θ_{j,2}' - k \frac{1}{n}θ_{i,2}(1 - θ_{j,1}') \right)
\]

\[
= -k \frac{1}{n} \sum_{j \neq i}(1 - θ_{j,1}) + \frac{1}{n} \left( n - 1 \left( \frac{b}{n}(p + k) - kc \right) + pk \frac{1}{n} \left( n - 2 \sum_{j = 1}^{n} θ_{j,2} + nθ_{i,2} \right) \right).
\]

We find that the learning rate \( β \) has a decisive influence on the positivity and negativity of the above equation, and the direction of the gradient w.r.t. \( θ_{i,2} \) cannot be determined at each step. An alternative is to consider multiple gradient steps, calculate optimal \( V_{i}^{π} \) given incentivizing policies, and then derive the change direction of \( θ_{i,2} \) based on convergent \( V_{i}^{π} \). However, it is challenging to formally calculate the global optimal \( V_{i}^{π} \).

In addition, another problem arises when we consider the homophily constraint as a loss function. Using the definition of Eq. 4 and Eq. 5 in the paper, the homophily loss of agent \( i \) under the updated environmental policies is:

\[
L_{i}^{π'} = \sum_{j \neq i, k \notin (i,j)} (1 - θ_{k,1}') \left( θ_{i,1}'θ_{j,1}' + (1 - θ_{i,1}')(1 - θ_{j,1}') \right) (θ_{j,2} log θ_{i,2} + (1 - θ_{j,2}) log(1 - θ_{i,2})).
\]

(39)
With further calculation, we can find that the derivative of $L_{i}^{\pi}$ w.r.t $\theta_{i,2}$ has a nonlinear dependency on others’ policies, which makes the dynamics of the system hard to capture, not to mention obtaining the closed-form solution [58].

So far, we have presented the challenges of obtaining theoretical supports in temporally extended cases. These challenges have perplexed the researchers for a long time [59, 60, 40], and we believe that the solution for these questions is an important and promising direction for future work.