Efficient Multi-Agent Cooperation Learning through Teammate Lookahead

Anonymous authors
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Abstract

Cooperative Multi-Agent Reinforcement Learning (MARL) is a rapidly growing research field that has achieved outstanding results across a variety of challenging cooperation tasks. However, existing MARL algorithms typically overlook the concurrent updates of teammate agents. An agent always learns from the data that it cooperates with one set of (current) teammates, but then practices with another set of (updated) teammates. This phenomenon, termed as "teammate delay", leads to a discrepancy between the agent's learning objective and the actual evaluation scenario, which can degrade learning stability and efficiency. In this paper, we tackle this challenge by introducing a lookahead strategy that enables agents to learn to cooperative with predicted future teammates, allowing the explicit awareness of concurrent teammate updates. This lookahead strategy is designed to seamlessly integrate with existing gradient-based MARL methods, enhancing their performance without significant modifications to their underlying structures. The extensive experiments demonstrate the effectiveness of this approach, showing that the lookahead strategy can enhance the cooperation learning efficiency and achieve superior performance over the state-of-the-art MARL algorithms.

1 Introduction

Cooperative Multi-Agent Reinforcement Learning (MARL) techniques focus on replicating the collaborative intelligence observed in human teams Oroojlooy & Hajinezhad (2023), and advancements in recent years have showcased its remarkable potential in various application domains, including robotics Wang et al. (2022), games Berner et al. (2019), and social networks Leibo et al. (2017). Among them, multi-agent policy gradient methods stand out with the capability to handle continuous control tasks and with potential to solve intricate cooperative problems de Witt et al. (2020a); Yu et al. (2022a). Despite the ongoing progresses in this category of methods, we point out that they typically suffer from a "teammate delay" issue. Specifically, this issue occurs when an agent learns from the data that it cooperates with current teammates, but then practices with updated teammates due to the concurrent teammate updates.

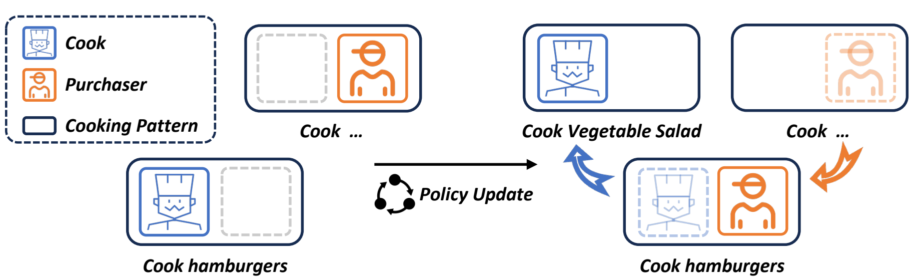


Figure 1: One simple example to show "teammate delay" issue, where *Purchaser* is expected to buy corresponding ingredients for *Cook* to cook.

For more intuitive illustration, one concrete example is shown in Figure 1. In this example, *Cook* initially wants to cook hamburgers, and *Purchaser* adjusts its policy to buy corresponding ingredients after one round of policy update. However, at this moment, *Cook* also improves its policy to cook vegetable salad. Thereby, their updated policies fail to cooperate well. This simple example reveals that updating the agents to cooperate with current teammates would lead to a training-test mismatch because the teammates update their policies as well. This gap between policy training and evaluation in each round of update can lead to severe learning inefficiency.

Although not explicitly pointing out this teammate delay issue, there exist works aiming to resolve similar problems arising from concurrent updates of teammate policies. Opponent modeling methods seek to alleviate the non-stationarity in multi-agent scenarios through explicitly modeling the teammate policies Yuan et al. (2023). They either introduce an auxiliary task of predicting teammate behaviors Hernandez-Leal et al. (2019) or learn teammate representations as extra policy conditions Papoudakis & Albrecht (2020); Cao et al. (2023). Despite their effectiveness in many problem scenarios, these methods necessitate extra teammate modeling efforts and lack theoretical analysis support. On the other hand, recent works, LOLA Foerster et al. (2018a) and COLA Willi et al. (2022), explicitly acknowledge the learning behavior of other agents and propose learning rules with opponent-learning awareness. However, these works are limited to two-player simple problems and face challenges to extend to practical cooperative scenarios. The most promising approach is one recent progress of multi-agent policy gradient method, HAPPO Kuba et al. (2021). This method proposes a sequential policy update scheme with theoretical guarantees for joint policy improvement. However, its actual implementation involves an approximation utilizing *importance sampling*, potentially influencing the actual performance due to large variance in policy gradients.

Despite all these previous efforts, how the teammate delay issue influences the cooperative policy learning and how to better mitigate its negative impact are still open questions. To answer these two questions, in this paper, we both provide a formal analysis about the impact of this issue on the policy update, which motivates us to predict future teammate policies, and propose a model-based MARL algorithm where we approximate the future teammates via conducting policy updates within the environment model. In summary, our main contributions are:

- We offer a rigorous formal analysis on policy-gradient MARL algorithms by investigating the regret of the updated policy, which unveils the impact of "teammate delay" issue on cooperative policy learning.
- Furthermore, we introduce a practical model-based MARL algorithm explicitly designed to address the challenges posed by the "teammate delay" issue. By leveraging insights from our formal analysis, our algorithm aims to enhance cooperative policy learning.
- To validate the effectiveness of our proposed approach, we conduct empirical studies on various benchmarks. These benchmarks include complex problems with continuous action spaces, as well as challenging multi-agent cooperative tasks. The empirical results unequivocally demonstrate the superiority of our method, showcasing its ability to outperform existing approaches and handle diverse scenarios with impressive performance gains.

2 Preliminaries

2.1 Single-Agent Policy Gradient

In single-agent setting, the sequential decision-making problem can be formalized as a Markov Decision Process (MDP) that can be defined as a tuple $(\mathcal{S}, \mathcal{A}, \mathcal{P}, \mathcal{R}, \gamma)$. At each timestep, the agent receives the current state $s \in \mathcal{S}$ and selects an action $a \in \mathcal{A}$ according to the agent policy $\pi(\cdot|s)$. The environment will return the next state $s' \in \mathcal{S}$ and reward r according to $\mathcal{P}(\cdot|s, a)$ and $\mathcal{R}(s, a)$. Besides, the γ denotes the discount factor.

The goal of reinforcement learning is to maximize the discounted return $\eta(\pi)$ of the agent policy π, which according to the performance discrepancy lemma Kakade & Langford (2002) equals to:

$$\eta(\pi) = \eta(\pi^k) + \sum_{s \in \mathcal{S}} \rho_\pi(s) \left[\sum_{a \in \mathcal{A}} \pi(a|s) A_{\pi^k}(s,a) \right],\ A_{\pi^k}(s,a) = Q_{\pi^k}(s,a) - V_{\pi^k}(s), \tag{1}$$

where π^k is the k-th round agent policy, $\rho_\pi(s)$ means the state distribution derived by π and $A_{\pi^k}(s,a)$ denotes the advantage function. More details about the notations are listed in Appendix A.1. As it is hard to sample trajectories corresponding to the state distribution $\rho_\pi(s)$, in practice, we typically use π^k to sample trajectories instead. This implies that the actual learning objective is:

$$J(\pi) = \eta(\pi^k) + \sum_{s \in \mathcal{S}} \rho_{\pi^k}(s) \left[\sum_{a \in \mathcal{A}} \pi(a|s) A_{\pi^k}(s,a) \right]. \tag{2}$$

In fact, $J(\pi)$ is related to π^k, but for brevity we omit it in input. The same applies to the following context. Due to the state distribution change, π can not be updated too far away from π^k, for which traditional actor-critic algorithms, e.g., A3C Mnih et al. (2016), conduct only a few policy gradient ascend while trust-region algorithms, such as PPO Schulman et al. (2017), conforms to the trust-region optimization.

2.2 Multi-Agent Policy Gradient

When it comes to the multi-agent setting, the problem can be defined as a tuple $(N, \mathcal{S}, \boldsymbol{\mathcal{A}}, \mathcal{P}, \mathcal{R}, \gamma)$, where N is the number of agents. For the sake of simplicity and without loss of generality, we have omitted the partial observability in notations above, where an agent needs to make decisions based on its local observations. Moreover, we assume that the joint policy $\boldsymbol{\pi}$ can be decomposed into the product of individual policies $\boldsymbol{\pi}(\boldsymbol{a}|s) = \prod_{i=1}^N \pi_i(a_i|s)$, where π_i is the individual policy for agent i and the joint action $\boldsymbol{a} = [a_1, a_2, \cdots, a_N] \in \boldsymbol{\mathcal{A}}$ is decomposed of individual actions $\{a_i\}_{i=1}^N$.

In this case, the learning objective for each agent in multi-agent policy gradient methods is typically defined as:

$$\begin{aligned} &J_i(\pi_i|\{\pi_j^k\}_{j\neq i}) \\ &= \eta(\boldsymbol{\pi}^k) + \sum_{s \in \mathcal{S}} \rho_{\boldsymbol{\pi}^k}(s) \Bigg[\sum_{\boldsymbol{a} \in \boldsymbol{\mathcal{A}}} \pi_i(a_i|s) \prod_{j \neq i} \pi_j^k(a_j|s) A_{\boldsymbol{\pi}^k}(s, \boldsymbol{a}) \Bigg],\ i \in \{1, 2, \cdots, N\}. \end{aligned} \tag{3}$$

Compared with that in single-agent setting, the data distribution here is also influenced by the teammate policies. In other words, the i-th agent updates its policy associated with the current teammates $\{\pi_j^k\}_{j\neq i}$ in this learning objective. Totally, the learning objective for the joint policy can be formalized as:

$$J(\boldsymbol{\pi}) = \eta(\boldsymbol{\pi}^k) + \sum_{s \in \mathcal{S}} \rho_{\boldsymbol{\pi}^k}(s) \Bigg[\frac{1}{N} \sum_{i=1}^N \sum_{\boldsymbol{a} \in \boldsymbol{\mathcal{A}}} \pi_i(a_i|s) \prod_{j \neq i} \pi_j^k(a_j|s) A_{\boldsymbol{\pi}^k}(s, \boldsymbol{a}) \Bigg]. \tag{4}$$

3 Method

In this work, we identify the teammate delay phenomenon in the common practice of multi-agent policy gradient methods. The direct negative impact of this issue can be analyzed and how to solve this issue deserves further study. In this section, we firstly discuss how the teammate delay issue can cause a negative impact on the cooperative policy learning through analyzing the regret of the updated joint policy at the next round. Motivated by this analysis, we then propose a practical algorithm that exploits the future teammate information to facilitate the cooperation learning.

3.1 Analysis Motivates Predicting Future Teammates

From Equation (4), we know that in typical multi-agent policy gradient methods, the learning objective of the agent policy involves computing an expectation with respect to the current teammate policies $\{\pi_j^k\}_{j\neq i}$.

Consequently, the current policy distribution of the teammates will have an impact on the policy update. In order to provide further analysis on this impact, we replace the teammate policies with a general notation $\{\mu_j\}_{j\neq i}$, which means that the trajectories are sampled associated with a sampling policy $\boldsymbol{\mu}$. In this way, the learning objective is transformed into:

$$J(\boldsymbol{\pi}, \boldsymbol{\mu}) = \eta(\boldsymbol{\pi}^k) + \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}}(s) \left[\frac{1}{N}\sum_{i=1}^{N}\sum_{\boldsymbol{a}\in\boldsymbol{\mathcal{A}}} \pi_i(a_i|s)\prod_{j\neq i}\mu_j(a_j|s)A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a})\right], \tag{5}$$

where $\boldsymbol{\pi}^k$ still denotes the joint policy at the k-th round. In existing multi-agent policy-gradient methods, the sampling policy $\boldsymbol{\mu}$ is typically selected to be $\boldsymbol{\pi}^k$, which means that we expect π_i to collaborate well with the k-th round teammate policies through maximizing $\sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\pi}^k}(s)\sum_{\boldsymbol{a}\in\boldsymbol{\mathcal{A}}} \pi_i(a_i|s)\prod_{j\neq i}\pi_j^k(a_j|s)A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a})$.

We wonder what would happen when we adjust $\boldsymbol{\mu}$ from $\boldsymbol{\pi}^k$ to other distributions. To answer this question, we firstly propose the following lemma that estimates the upper bound of discrepancy between the learning objective $J(\boldsymbol{\pi}, \boldsymbol{\mu})$ and the actual policy return $\eta(\boldsymbol{\pi})$.

Lemma 1 *Assume that we update the joint policy $\boldsymbol{\pi}^k$ to $\boldsymbol{\pi}^{k+1}$ with sampling policy $\boldsymbol{\mu}$. Given the measurement of distance between sampling policy $\boldsymbol{\mu}$ and the updated policy $\boldsymbol{\pi}^{k+1}$ as $\alpha_i = \max_s D_{\mathrm{TV}}\left(\pi_i^{k+1}(\cdot|s)\|\mu_i(\cdot|s)\right)$ [1], we have:*

$$|J(\boldsymbol{\pi}^{k+1}, \boldsymbol{\mu}) - \eta(\boldsymbol{\pi}^{k+1})| \leq \frac{4\epsilon\gamma}{(1-\gamma)^2}\left(\sum_{i=1}^{N}\alpha_i\right)^2 + \frac{2\epsilon(N-1)}{N}\sum_{i=1}^{N}\alpha_i, \tag{6}$$

where γ is the discount factor and $\epsilon = \max_{s,\boldsymbol{a}}|A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a})|$.

For proof see Appendix A.2. The estimated upper bound of the discrepancy between $J(\boldsymbol{\pi}^{k+1}, \boldsymbol{\mu})$ and $\eta(\boldsymbol{\pi}^{k+1})$ in Lemma 1 can aid us in analyzing the regret of $\boldsymbol{\pi}^{k+1}$, leading to the following theorem:

Theorem 1 *Suppose that we update joint policy $\boldsymbol{\pi}^k$ to $\boldsymbol{\pi}^{k+1}$ with sampling policy $\boldsymbol{\mu}$, then the regret of the updated joint policy $\boldsymbol{\pi}^{k+1}$ has the following upper bound:*

$$\eta(\boldsymbol{\pi}^*) - \eta(\boldsymbol{\pi}^{k+1}) \leq \eta(\boldsymbol{\pi}^*) - J(\boldsymbol{\pi}^{k+1}, \boldsymbol{\mu}) + \underbrace{\frac{4\epsilon\gamma}{(1-\gamma)^2}\left(\sum_{i=1}^{N}\alpha_i\right)^2 + \frac{2\epsilon(N-1)}{N}\sum_{i=1}^{N}\alpha_i}_{(c)}. \tag{7}$$

For proof see Appendix A.2. The right hand side of Inequality (7) sheds light on the elements that can influence the cooperative policy learning. Totally, we expect to minimize the regret of the updated policy via minimizing the overall upper bound expression. Other than the first term $\eta(\boldsymbol{\pi}^*)$ that is a constant value, the upper bound is composed of $-J(\boldsymbol{\pi}^{k+1}, \boldsymbol{\mu})$ and one extra term (c). In fact, the second term $-J(\boldsymbol{\pi}^{k+1}, \boldsymbol{\mu})$ is exactly the loss function that the algorithm aims to minimize at each update round, which typically serves as a surrogate function for the regret $\eta(\boldsymbol{\pi}^*) - \eta(\boldsymbol{\pi}^{k+1})$. However, Inequality (7) reveals that the regret can not be bounded by $-J(\boldsymbol{\pi}^{k+1}, \boldsymbol{\mu})$ alone, and an extra term (c) relatively captures the gap between this surrogate function and the actual regret.

This extra term (c), a function of the sampling policy $\boldsymbol{\mu}$ and the updated policy $\boldsymbol{\pi}^{k+1}$, can not be optimized by the previous learning algorithms, but it can have an impact on the cooperation learning. When given a large term (c), the surrogate function would be far from the actual regret, which can result in low learning efficiency. In fact, it is easy to observe that term (c) will be reduced to zero when $\boldsymbol{\mu}$ is equivalent to $\boldsymbol{\pi}^{k+1}$. That is, the extra term (c) would disappear if we trained the agents with the information of future teammates. This outcome motivates us to replace the sampling policy $\boldsymbol{\mu}$ with an approximation of the future teammates, thus to reduce the regret. A more comprehensive analysis on how approximating future teammates reduces the regret upper bound is provided in Appendix A.3. In Section 3.2 and Section 3.3, we will show how we approximate the future teammates.

[1] The TV distance measures the distance between two distributions via calculating $D_{\mathrm{TV}}(P,Q) = \frac{1}{2}\sum_x |P(x) - Q(x)|$ Cover (1999).

3.2 Future Teammate Approximation

Based on the above analysis, we are motivated to replace the sampling policy $\boldsymbol{\mu}$ with the future teammate policy $\boldsymbol{\pi}^{k+1}$ in each round of policy update. However, achieving this goal is not easy in practice, because in each round of policy update, the updated policy $\boldsymbol{\pi}^{k+1}$ is affected by the sampling policy $\boldsymbol{\mu}$, that is, $\boldsymbol{\pi}^{k+1}$ and $\boldsymbol{\mu}$ are coupled. Thus, to serve this goal, we propose that the future teammate policy can be obtained by solving a bi-level optimization problem below:

Theorem 2 *Let ψ be the policy update operator [2]. The sampling policy $\boldsymbol{\mu}^*$ that can derive the same updated policy, i.e., $\boldsymbol{\mu}^* = \psi(\boldsymbol{\mu}^*, \boldsymbol{\pi}^k)$, is the solution of the following bi-level optimization problem:*

$$\min_{\boldsymbol{\mu}} D_{\mathrm{KL}}(\boldsymbol{\mu} \| \boldsymbol{\pi}^{k+1}), \ \ s.t. \ \boldsymbol{\pi}^{k+1} = \arg\max_{\boldsymbol{\pi}} J(\boldsymbol{\pi}, \boldsymbol{\mu}). \tag{8}$$

Its proof can be found in Appendix A.2. This theorem inspires us that we can obtain the expected $\boldsymbol{\mu}^*$ by solving the consistent bi-level optimization problem. The solution of this problem to some extent contains the information of future teammate policy. However, this problem typically follows a form of Stackelberg Game Friedman (1971), and is not easy to solve.

In this case, we propose to perform one-step approximation of this optimization problem, which means that with $\boldsymbol{\mu}$ initialized as $\boldsymbol{\pi}^k$, we firstly solve the inner-loop optimization with $\boldsymbol{\pi}^{k+1} = \arg\max_{\boldsymbol{\pi}} J(\boldsymbol{\pi}, \boldsymbol{\mu})$ and then we assign the obtained $\boldsymbol{\pi}^{k+1}$ to the sampling policy $\boldsymbol{\mu}$, thus obtaining the approximation of the solution $\boldsymbol{\mu}^*$. This one-step approximation is commonly utilized for stackelberg-game-like problems, and it achieves a trade-off between the solution accuracy and the computation cost. In brief, for feasible future teammate approximation, we perform an additional round of optimization before each algorithm iteration, using the previous round's policy $\boldsymbol{\pi}^k$ as the sampling policy, and the obtained policy $\tilde{\boldsymbol{\pi}}^{k+1}$ serves as the approximation of future teammate policy.

3.3 Practical Algorithm Implementation

Model-based Approximation The above analysis motivates us to conduct extra training to estimate the future teammate policy. However, a straight-forward implementation is not practical because it wastes near half of the online samples for estimating the future teammate policy, and those samples are not utilized for the actual policy training, which as a result will lead to very low sample efficiency of the algorithm. To avoid this issue, we propose to learn an environment model, and put the teammate policy estimation process within it, thus avoiding the waste of a large number of online samples.

In specific, we maintain a data buffer to store all the transition data that has been encountered during the training process. In each iteration of the algorithm, we additionally conduct model learning by sampling training data from this buffer. Typically, we update the model parameters through maximizing the likelihood of observing the training data under the environment model. Subsequently, we perform future teammate approximation within the model to derive a lookahead sampling policy denoted as $\tilde{\boldsymbol{\pi}}^{k+1}$. The derived policy is then utilized for actual policy training within the real environment.

Off-policy Value Estimation The intuition of our work is to modify the sampling policy $\boldsymbol{\mu}$ in Equation (5), thus to derive a better optimization objective that can bring a smaller upper bound of the regret for the updated policy. However, term $A_{\boldsymbol{\pi}^k}$ is expected to be maintained which means that we want to estimate the advantage with the policy of the last round. In typical practice, it is easy to achieve because the trajectories are sampled by $\boldsymbol{\pi}^k$ and we can estimate the advantage directly. While in our algorithm design, the sampling policy is replaced with the lookahead policy $\tilde{\boldsymbol{\pi}}^k$, which means that we need to conduct off-policy estimation for $A_{\boldsymbol{\pi}^k}$. In specific, we adopt the V-trace trick to estimate $A_{\boldsymbol{\pi}^k}$ with the trajectories sampled by $\tilde{\boldsymbol{\pi}}^{k+1}$.

Overall Flow of the Algorithm Combining all the algorithmic design techniques that we have raised, we propose a practical algorithm that can enhance the underlying multi-agent policy gradient method. The

[2] $\psi(\boldsymbol{\mu}, \boldsymbol{\pi}^k)$ means the result of one round of policy update starting from $\boldsymbol{\pi}^k$ using $\boldsymbol{\mu}$ as the sampling policy, i.e., $\psi(\boldsymbol{\mu}, \boldsymbol{\pi}^k) = \arg\max_{\boldsymbol{\pi}} J(\boldsymbol{\pi}, \boldsymbol{\mu})$ within the trust region of $\boldsymbol{\pi}^k$ for MAPPO Yu et al. (2022a).

Algorithm 1 Multi-Agent Policy Gradient Learning with Lookahead

Input: The number of agent N, max iteration number K, trajectory batch size M

Output: Obtained multi-agent cooperation policy

1: Initialize replay buffer $\mathcal{B}$;
2: Initialize a joint policy $\boldsymbol{\pi} = \{\pi_i\}_{i=1}^{N}$ randomly;
3: **for** iteration $k = 1$ to K **do**
4: Sample a batch of transitions from $\mathcal{B}$ and update the environment model;
5: Sample a batch of trajectories $\{\tilde{\tau}\}_M$ in the environment model with sampling policy $\boldsymbol{\pi}^k$, and obtain $\tilde{\boldsymbol{\pi}}^{k+1} = \psi(\boldsymbol{\pi}^k, \boldsymbol{\pi}^k)$ using the training trajectories $\{\tilde{\tau}\}_M$;
6: Sample a batch of trajectories $\{\tau\}_M$ in the real environment with sampling policy $\tilde{\boldsymbol{\pi}}^{k+1}$, and obtain $\boldsymbol{\pi}^{k+1} = \psi(\tilde{\boldsymbol{\pi}}^{k+1}, \boldsymbol{\pi}^k)$ using the training trajectories $\{\tau\}_M$;
7: Add trajectories τ to the buffer $\mathcal{B}$;
8: **end for**

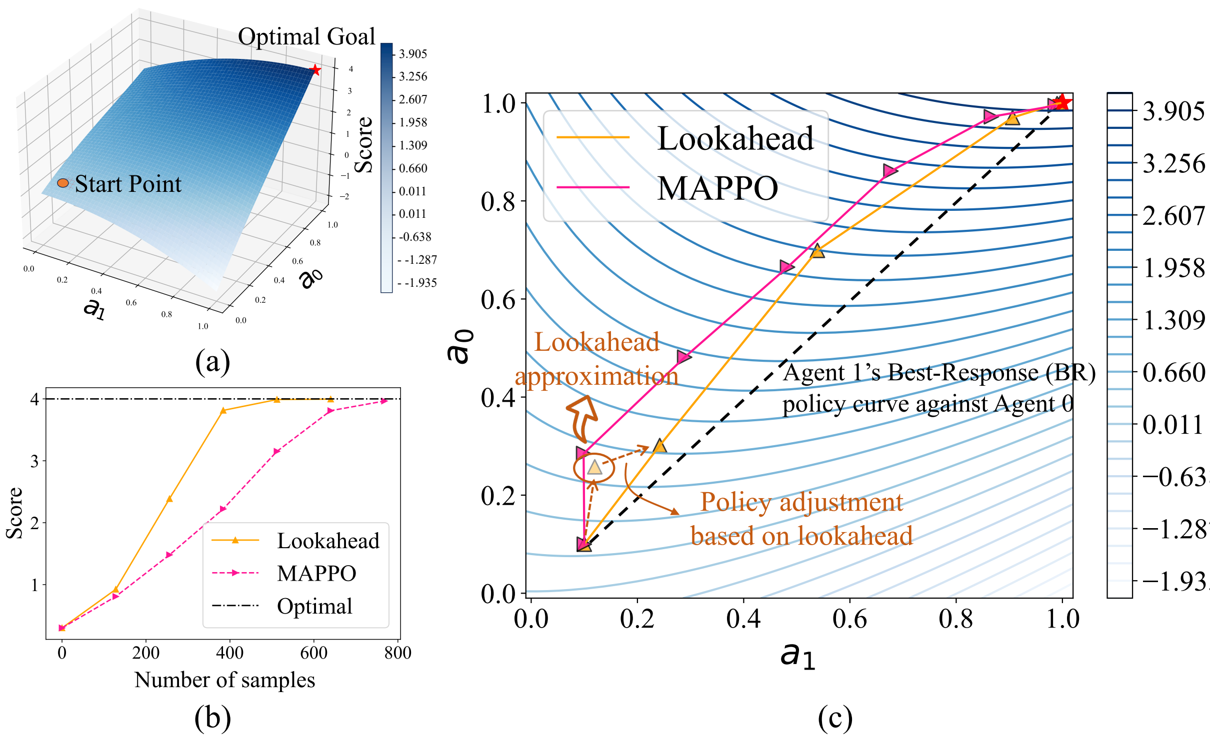
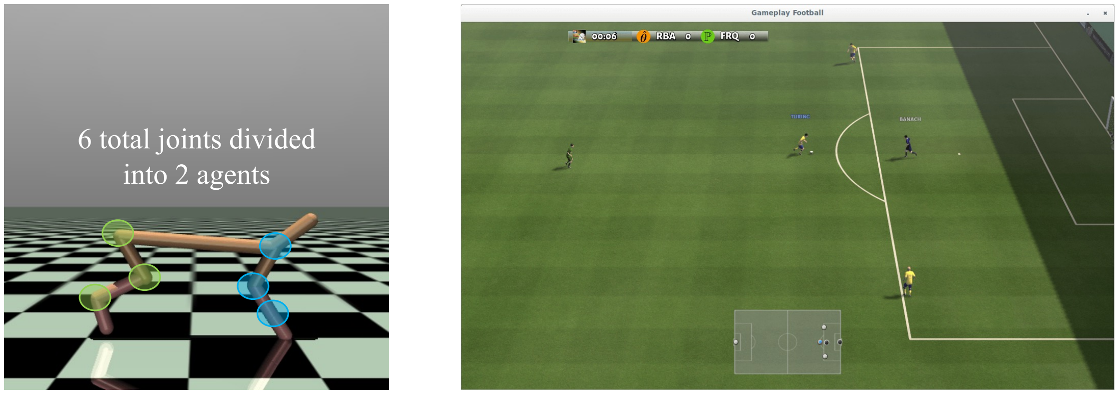


Figure 2: Visualization results on the toy environment. (a) Landscape of the two-variable function, where darker the color is, higher function score the region obtains; (b) Algorithm learning score curve; (c) Optimization process of Lookahead and MAPPO.

overall flow of our algorithm has been presented in Algorithm 1. In line 5, we obtain the estimated future teammate policy $\tilde{\boldsymbol{\pi}}^{k+1}$ within the environment model, while in line 6 we utilize $\tilde{\boldsymbol{\pi}}^{k+1}$ to aid in actually updating the policy in the real environment. Besides, we update the environment model in line 4.

4 Experiments

In this section, we substantiate the efficacy of our proposed approach through empirical validation via experiments conducted on diverse benchmarks. These benchmarks include a toy environment, which serves to illustrate the algorithmic process of our approach, and two intricate cooperative multi-agent scenarios that provide practical validation of our approach's effectiveness. Specifically, we aim to utilize these experimental



(a) 2x3-Agent HalfCheetah (b) academy 3 vs 1 with Keeper

Figure 3: Two cases of Multi-Agent MuJoCo (MA-MuJoCo) and Google Football Research (GRF) environments.

results to investigate the following questions: 1) How does our algorithm work and can we analyze the underlying mechanism through one simple task (Section 4.1)? 2) Can our algorithm actually enhance the cooperation learning in complex multi-agent cooperative tasks (Section 4.2)? 3) Does the phenomenon exhibited by our algorithm in complex cooperative tasks still align with our analysis (Section 4.3)?

4.1 Algorithm Analysis in Toy Environment

To visually reveal how our method works, we devised a toy environment involving a two-variable function optimization problem. As depicted in Figure 2(a), this problem comprises two agents with continuous action spaces in the range $[0, 1]$. Whenever the agents execute a joint action $[a_0, a_1]$, the environment yields reward: $R = a_0^3 - 2(a_0 - a_1)^2 + 3a_0$.

Specifically, we initialize the joint policy as $[0.1, 0.1]$ and both adopt the algorithms of MAPPO and our lookahead strategy to investigate how they converge to the optimal policy $[1, 1]$. As shown in Figure 2(c), without our lookahead strategy, agent 1 always shows a large gap from the Best-Response (BR) against the updated agent 0, revealing the phenomenon of "teammate delay". While our lookahead strategy can help agent 1 predict the updated policy of agent 0, leading to a shorter optimization path. From the learning curve in Figure 2(b), we also find that our lookahead strategy helps converge to the optimal policy using much fewer samples, enhancing the learning efficiency.

The algorithm analysis in this straightforward objective optimization task helps provide an intuitive explanation about the algorithm mechanism and motivation behind our approach. In the subsequent sections, we explore whether the proposed lookahead strategy can indeed enhance the cooperative learning in more complex task scenarios.

4.2 Main Results in Complex Cooperative Tasks

4.2.1 Experiment Setup

To investigate the effectiveness of our approach in more practical task scenarios, this section focuses on two prevalent cooperative benchmark environments, including continuous control tasks from Multi-Agent MuJoCo (MA-MuJoCo) de Witt et al. (2020b) and Google Research Football (GRF) Kurach et al. (2020) games with discrete action spaces. Two cases for these two environments are provided in Figure 3. Below we provide introduction for these two environments:

Table 1: Evaluation results of various methods on MA-MuJoCo tasks, providing average scores across 5 seeds with standard errors. The highest score for each task scenario is **bolded** and the top-2 scores are marked in blue. The average rank denotes the average ranking across all task scenarios of each method.

Algorithm	Ant 2x4	Ant 4x2	HalfCheetah 2x3	HalfCheetah 3x2	Walker2d 2x3	Walker2d 3x2	Average Rank
Lookahead	**3393.39**(336.98)	**2858.22**(540.76)	**3315.83**(346.46)	**3687.10**(304.98)	2048.30(309.27)	2670.71(123.74)	**1.33**
HAPPO	2471.15(201.23)	2120.18(168.48)	2910.18(39.38)	3016.20(80.90)	**2544.62**(272.91)	**2780.65**(76.25)	2.00
TAPPO	2055.21(182.25)	2503.62(207.66)	2154.73(443.24)	3487.52(711.65)	1475.63(215.27)	1445.56(350.34)	3.67
MAPPO	1034.19(18.99)	1002.15(18.30)	2160.29(503.76)	2350.32(477.29)	1852.8(41.48)	1812.54(139.44)	4.33
IPPO	884.93(46.24)	875.8(20.84)	2652.04(635.31)	2477.98(566.12)	2021.89(67.64)	1775.2(122.09)	4.33
MADDPG	1866.08(9.77)	1701.08(13.45)	1553.54(251.6)	1295.5(384.87)	71.68(15.36)	100.72(35.19)	5.33

Table 2: Evaluation results of various methods on GRF tasks. GRF 3vs1, CA(hard) and Corner are respectively short for maps of academy 3 vs 1 with keeper, academy counterattack hard and academy corner in GRF environment.

Algorithm	GRF 3vs1	GRF CA (hard)	GRF Corner	Average Rank
Lookahead	0.82(0.02)	**0.50**(0.07)	**0.63**(0.03)	**1.33**
HAPPO	**0.86**(0.03)	0.46(0.09)	0.49(0.07)	2.00
TAPPO	0.77(0.03)	0.49(0.03)	0.28(0.10)	3.00
MAPPO	0.66(0.04)	0.37(0.08)	0.48(0.11)	3.67
CDS	0.49(0.11)	0.21(0.07)	0.02(0.01)	5.00

Multi-Agent MuJoCo (MA-MuJoCo) The MA-MuJoCo environment is built upon the MuJoCo physics engine to create realistic simulations for MARL research. In specific, MA-MuJoCo partitions the body graph in MuJoCo into disjoint sub-graphs, one for each agent, e.g., 2x4-Agent Ant means dividing the 8 joints in Ant into 2 agents, each controlling 4 joints.

Google Research Football (GRF) The Google Research Football (GRF) is a novel benchmark environment offering simulations of soccer matches, enabling the study of multi-agent behaviors and reinforcement learning. It introduces challenging cooperation learning tasks as it has the property of heterogeneity and sparse rewards.

To thoroughly explore the cooperative performance that our approach can potentially bring about, we integrate our lookahead strategy with HAPPO, one of the current state-of-the-art multi-agent policy gradient algorithms, in all experiments of this section. For comparison, we select several popular multi-agent actor-critic algorithms as baselines. An opponent modeling approach, TAPPO, is also included, which learns teammate representations to incorporate additional policy conditions like in previous methods Papoudakis & Albrecht (2020); Cao et al. (2023). We adopt this baseline to contrast our approach with traditional opponent modeling approaches in mitigating non-stationarity issue arising from teammate co-learning. Moreover, in the GRF environment, we add one additional baseline CDS Li et al. (2021), a value-based MARL algorithm designed specifically for solving GRF games, for a more comprehensive comparison. More details about baselines can be found in Appendix B.1.

4.2.2 Results Analysis

MA-MuJoCo As shown in Table 1, in multiple task scenarios of MA-MuJoCo, our approach Lookahead has achieved superior cooperative performance compared to other baseline algorithms. For tasks of Ant and HalfCheetah, our approach has consistently achieved the highest scores across all methods. These results imply that in these task scenarios, through predicting the potential future policies of other agents controlling their respective joints, our algorithm can help agents learn to manipulate their own joints in coordination with other agents better, finally enhancing the cooperative performance. Despite not achieving the highest

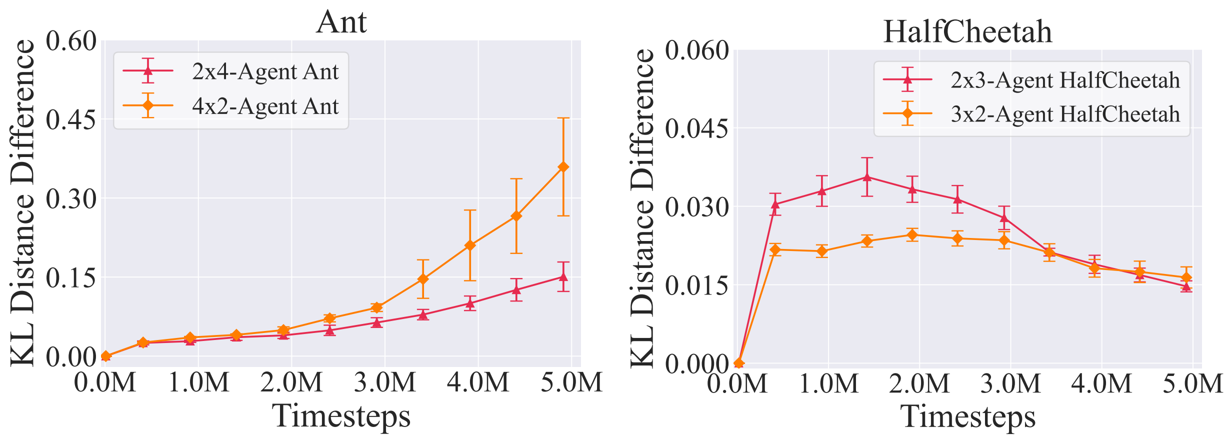


Figure 4: Measuring policy distances in Multi-Agent MuJoCo environments. The y-axis calculates the difference in distances from $\boldsymbol{\pi}^k$ and $\tilde{\boldsymbol{\pi}}^{k+1}$ to $\boldsymbol{\pi}^{k+1}$, i.e., $D_{\mathrm{KL}}(\boldsymbol{\pi}^{k+1}, \boldsymbol{\pi}^k) - D_{\mathrm{KL}}(\boldsymbol{\pi}^{k+1}, \tilde{\boldsymbol{\pi}}^{k+1})$, and the plot illustrates the changes in this metric throughout the policy training process.

score, our approach also attains top-2 performance in the Walker2d scenarios. We hypothesize that the slight performance loss might be due to the nature of the Walker2d task, which requires not only proficient walking but also maintaining the balance of the mechanical legs at all times. The possible failure to maintain the legs' balance may pose great challenges to the learning of the environment model, consequently having a negative impact on the performance of our algorithm. Actually, the selection of environment model learning methods is orthogonal to our algorithm. In the future, we will consider designing better model learning methods to further enhance the performance of our approach.

Google Research Football (GRF) Similar to the results in MA-MuJoCo, the results in Table 2 demonstrate that our approach also achieves superior performance in GRF problems. In particular, our approach is the only one that attains a success rate exceeding 60% in the academy corner scenario, achieving a notable improvement of over 25% compared to the second-best algorithm. Moreover, the average rank of our approach also stands out as the best in the GRF environment, the same as that in MA-MuJoCo.

Ablation Study The comparison in Tables 1 and 2 between the Lookahead and HAPPO algorithms on both benchmark environments can be seen as ablation study to assess the impact of our introduced lookahead strategy. Across the majority of task scenarios, the incorporation of our lookahead strategy results in enhanced cooperative performance compared to the original HAPPO algorithm, e.g., exceeding the second-best algorithm by around 1000 points in 2x4-Agent Ant, which effectively validates the efficacy of the proposed lookahead strategy.

4.3 Analysis of Lookahead Policy in Complex Problems

While we have analyzed the algorithmic mechanism in a toy environment, applying the algorithm in complex tasks is more intricate due to the involvement of model learning. In this section, we measure the policy distances to investigate whether our lookahead approximation still provides right direction information in MA-MuJoCo. In specific, we compute the difference between $D_{\mathrm{KL}}(\boldsymbol{\pi}^{k+1}, \boldsymbol{\pi}^k)$ and $D_{\mathrm{KL}}(\boldsymbol{\pi}^{k+1}, \tilde{\boldsymbol{\pi}}^{k+1})$, which equals to $D_{\mathrm{KL}}(\boldsymbol{\pi}^{k+1}, \boldsymbol{\pi}^k) - D_{\mathrm{KL}}(\boldsymbol{\pi}^{k+1}, \tilde{\boldsymbol{\pi}}^{k+1})$. As we can see from Figure 4 that this metric consistently keep positive throughout the training process, the results reveal that $\tilde{\boldsymbol{\pi}}^{k+1}$ is actually closer to the future teammate policy $\boldsymbol{\pi}^{k+1}$, forming a relatively good approximation. These results support our motivation and more analytical experimental results can be found in Appendix C.

5 Related Work

The related work of this paper mainly covers three aspects: multi-agent policy gradient, multi-agent model learning, and opponent modeling. Below, we provide the introduction to related works in these three aspects respectively.

Multi-Agent Policy Gradient The multi-agent policy gradient algorithms hold better convergence stability compared to the value-based algorithms, and they provide the ability to handle continuous control tasks. IA2C Chu et al. (2019) introduces the A2C method to the multi-agent setting, and adopts an independent learning paradigm. Subsequently, COMA Foerster et al. (2018b) proposes the paradigm of centralized critic with decentralized actors, which tries to conduct credit-assignment for each agent via introducing a counterfactual baseline. MAAC Iqbal & Sha (2019) and DOP Wang et al. (2020) respectively improve the policy gradient methods by introducing the attention mechanism to the critic network and conducting value decomposition for the centralized critic. On the other hand, IPPO de Witt et al. (2020a) and MAPPO Yu et al. (2022a) extend the trust-region policy optimization scheme to the multi-agent setting, and obtain remarkable performance. However, all the policy gradient methods above directly optimize the agent policy associated with the current teammates, and may suffer from the "teammate delay" issue. Recently, HAPPO Kuba et al. (2021) introduces sequential update scheme to the multi-agent policy gradient algorithm, which considers the mutual influences between different agents' policy update. Nevertheless, it adopts importance sampling technique which suffers from high variance, and it is orthogonal to our algorithm. More discussion is provided in Appendix B.2. Besides, there exist algorithms introducing deterministic policy gradient to the multi-agent setting Lowe et al. (2017), while we mainly consider stochastic policy gradient methods in this work.

Multi-Agent Model Learning Model-based reinforcement learning enjoys higher sample efficiency. However, multi-agent model learning faces significant challenges due to the exponential growth of the state-action space and the non-stationary in multi-agent scenarios. Adopting the Dreamer Hafner et al. (2019) architecture, MAMBA Egorov & Shpilman (2022) sustains a world model for each agent with necessary communication, thus to scale gracefully with the number of agents. Another work Mahajan et al. (2021) shows utilizing tensor decomposition in multi-agent model learning can significantly improve the sample efficiency when the environment transition and reward functions are of low CP-rank. Krupnik Krupnik et al. (2020) adopts generative models to learn a multi-step world model which can consider the delayed effects of the previous actions. Besides, considering the characteristics of multi-agent settings, AORPO Zhang et al. (2021) and CTRL Park et al. (2019) incorporate the opponent modeling into the model learning in order to roll-out opponent-wise trajectories. When the dynamic model has been obtained, dyna-style algorithms Zhang et al. (2022); Willemsen et al. (2021) conduct data augmentation to enhance policy learning. MBVD Xu et al. (2022) evaluates the current state value via imagining future states within the model. Han Han et al. (2022) conducts credit assignment by computing the shapley value Winter (2002) using the samples roll-outed in the model. In this work, we pay little attention to designing model learning techniques, instead we focus on approximating the future teammates within the model.

Opponent Modeling Opponent modeling is a well-studied topic in the field of MARL. Some previous works utilize opponent modeling to alleviate the non-stationarity issue in MARL. Among them, some works Hong et al. (2018); Papoudakis & Albrecht (2020); Xie et al. (2021); Cao et al. (2023) involve utilizing the opponent representations as additional inputs to the policy network, thereby enhancing the policy learning. While AMS-A3C and AFS-A3C Hernandez-Leal et al. (2019) treat the opponent modeling as an auxiliary task to guide the network optimization. Besides, another series of works assume that opponents are uncertain or may change, and they aim to help recognize and adapt to the opponents. DPN-BPR+ Zheng et al. (2018) and MBOM Yu et al. (2022b) estimate the most probable types of opponents from a statistical perspective, while Fastap Zhang et al. (2023) further considers that the changes of teammates may happen within one episode and learn a instantaneous representation to achieve fast recognition of teammate changes. Moreover, there exist other series of works Foerster et al. (2018a); Willi et al. (2022); Lu et al. (2022) that propose a better update operator for general-sum games by modeling the influences of agents' policies on the other agent. However, these methods are limited to two-player simple problems, while our work focuses on complex cooperative tasks.

6 Closing Remarks

This paper introduces a pioneering approach to enhance cooperative MARL by anticipating future teammate policies. Alleviating the prevalent issue of "teammate delay", our proposed lookahead strategy bridges the gap between the learning objective and the real evaluation scenario, significantly boosting the learning efficiency. Through seamless integration with existing gradient-based MARL methods, our approach surpasses state-of-the-art algorithms, exhibiting good performance in complex cooperative multi-agent benchmarks. Currently, our method mainly relies on the environment model to predict the future teammates. Thus, the practical algorithm performance is to some extent limited by the model learning error. How to better estimate the future teammates and whether there exist other ways to harness the predicted information of future teammates deserve further investigation. We believe researches in this topic can bring great advancement in the MARL domain.

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Appendix

A Notations and Theoretical Analysis

A.1 Notations

In Table 3, we list the main notations in our paper.

Table 3: Notation list.

Symbol	Meaning
$\mathcal{S}, s$	$\mathcal{S}$ denotes the state space for either the single-agent problem or multi-agent problem, while $s \in \mathcal{S}$ is an instance of the state.
$\mathcal{A}, a$	$\mathcal{A}$ denotes the action space for the single-agent problem, while a is an instance of the action.
N	Number of the agents in multi-agent problems.
$\boldsymbol{\mathcal{A}}, \{\mathcal{A}_i\}_{i=1}^N$	$\boldsymbol{\mathcal{A}}$ is the joint action space for the multi-agent problem, $\mathcal{A}_i$ is the action space for agent i.
$\boldsymbol{a}, \{a_i\}_{i=1}^N$	$\boldsymbol{a} = [a_1, a_2, \cdots, a_N]$ is an instance of the joint action, where a_i is the action for agent i.
$\mathcal{P}$	Transition function for either the single-agent problem or multi-agent problem.
$\mathcal{R}$	Reward function for either the single-agent problem or multi-agent problem.
γ	Discount factor.
π	π denotes the policy for single-agent problems, where $\pi(a\|s)$ means the probability of taking action a under state s.
$\boldsymbol{\pi}, \{\pi_i\}_{i=1}^N$	$\boldsymbol{\pi}$ denotes the joint policy for multi-agent problems, while π_i indicates the policy for agent i. $\boldsymbol{\pi}(\boldsymbol{a}\|s) = \prod_{i=1}^N \pi_i(a_i\|s)$ means the probability of taking action $\boldsymbol{a}$ under state s.
$\boldsymbol{\pi}^k$	The obtained joint policy after the k-th round of policy update.
$\eta(\boldsymbol{\pi})$	The discounted return of joint policy $\boldsymbol{\pi}$ in multi-agent problems.
$\rho_{\boldsymbol{\pi}}(s)$	The stationary state distribution derived by the joint policy $\boldsymbol{\pi}$.
$Q_{\pi^k}(s,a), Q_{\boldsymbol{\pi}^k}(s,\boldsymbol{a})$	$Q_{\pi^k}(s,a)$ represents the Q-function in single-agent problems, defined as the expected cumulative reward obtained by taking action a in state s and then following policy π^k thereafter, i.e., $Q_{\pi^k}(s,a) = \mathbb{E}_{\pi^k}\left[\sum_{t=0}^{\infty} \gamma^t r_t \| s_0 = s, a_0 = a\right]$. $Q_{\boldsymbol{\pi}^k}(s,\boldsymbol{a})$ is for multi-agent problems.
$V_{\pi^k}(s), V_{\boldsymbol{\pi}^k}(s)$	$V_{\pi^k}(s)$ represents the state value function in single-agent problems, indicating the expected cumulative reward starting from state s and following policy π thereafter, i.e., $V_{\pi^k}(s) = \mathbb{E}_{\pi^k}\left[\sum_{t=0}^{\infty} \gamma^t r_t \| s_0 = s\right]$. $V_{\boldsymbol{\pi}^k}(s)$ is for multi-agent problems.
α_i	$\alpha_i = \max_s D_{\mathrm{TV}}\left(\pi_i^{k+1}(\cdot\|s) \\| \mu_i(\cdot\|s)\right)$ is utilized to denote the distance between the sampling policy and the updated policy (the policy at the next round).

A.2 Proofs of Main Theoretical Results

In this section, we provide the proofs of the main theoretical results in our paper. In specific, we begin by outlining the primary theoretical results below, followed by their respective proofs one-by-one. Among them, Lemma 1, Theorem 1, and Theorem 2 are introduced in the main text, while Theorem 3 is introduced in the supplementary discussion in Appendix A.3.

Lemma 1 *Assume that we update the joint policy $\boldsymbol{\pi}^k$ to $\boldsymbol{\pi}^{k+1}$ with sampling policy $\boldsymbol{\mu}$. Given the measurement of distance between sampling policy $\boldsymbol{\mu}$ and the updated policy $\boldsymbol{\pi}^{k+1}$ as $\alpha_i = \max_s D_{\mathrm{TV}}\left(\pi_i^{k+1}(\cdot|s)\|\mu_i(\cdot|s)\right)$, we have:*

$$|J(\boldsymbol{\pi}^{k+1},\boldsymbol{\mu})-\eta(\boldsymbol{\pi}^{k+1})| \leq \frac{4\epsilon\gamma}{(1-\gamma)^2}\left(\sum_{i=1}^{N}\alpha_i\right)^2+\frac{2\epsilon(N-1)}{N}\sum_{i=1}^{N}\alpha_i, \tag{9}$$

where γ is the discount factor and $\epsilon = \max_{s,\boldsymbol{a}}|A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a})|$.

Theorem 1 *Suppose that we update joint policy $\boldsymbol{\pi}^k$ to $\boldsymbol{\pi}^{k+1}$ with sampling policy $\boldsymbol{\mu}$, then the regret of the updated joint policy $\boldsymbol{\pi}^{k+1}$ has the following upper bound:*

$$\eta(\boldsymbol{\pi}^*)-\eta(\boldsymbol{\pi}^{k+1}) \leq \eta(\boldsymbol{\pi}^*)-J(\boldsymbol{\pi}^{k+1},\boldsymbol{\mu})+\frac{4\epsilon\gamma}{(1-\gamma)^2}\left(\sum_{i=1}^{N}\alpha_i\right)^2+\frac{2\epsilon(N-1)}{N}\sum_{i=1}^{N}\alpha_i. \tag{10}$$

Theorem 2 *Let ψ be the policy update operator [3]. The sampling policy $\boldsymbol{\mu}^*$ that can derive the same updated policy, i.e., $\boldsymbol{\mu}^* = \psi(\boldsymbol{\mu}^*,\boldsymbol{\pi}^k)$, is the solution of the following bi-level optimization problem:*

$$\min_{\boldsymbol{\mu}} D_{\mathrm{KL}}(\boldsymbol{\mu}\|\boldsymbol{\pi}^{k+1}),\ \textit{s.t. } \boldsymbol{\pi}^{k+1}=\arg\max_{\boldsymbol{\pi}} J(\boldsymbol{\pi},\boldsymbol{\mu}). \tag{11}$$

Theorem 3 *Let ϕ be the ego-max-operator [4]. We suppose that $\boldsymbol{\mu}^*$ denotes the lookahead policy which means that it can derive the same updated policy, i.e., $\boldsymbol{\mu}^* = \psi(\boldsymbol{\mu}^*,\boldsymbol{\pi}^k)$; and $\boldsymbol{\pi'} = \psi(\boldsymbol{\pi}^k,\boldsymbol{\pi}^k)$ denotes the updated policy when using $\boldsymbol{\pi}^k$ as the sampling policy. We express the trust region as that $D_{\mathrm{TV}}\left(\pi_i'(\cdot|s)\|\pi_i^k(\cdot|s)\right) \leq \beta_i$. In this case, when $\beta_i \leq \frac{\sum_{s\in\mathcal{S}}\rho_{\boldsymbol{\mu}^*}(s)\phi(s,A_{\boldsymbol{\pi}^k})}{2\sum_{s\in\mathcal{S}}\rho_{\boldsymbol{\pi}^k}(s)\phi(s,|A_{\boldsymbol{\pi}^k}|)}$, we have $J(\boldsymbol{\mu}^*,\boldsymbol{\mu}^*) \geq J(\boldsymbol{\pi'},\boldsymbol{\pi}^k)$.*

Below are proofs.

Lemma 1 *Assume that we update the joint policy $\boldsymbol{\pi}^k$ to $\boldsymbol{\pi}^{k+1}$ with sampling policy $\boldsymbol{\mu}$. Given the measurement of distance between sampling policy $\boldsymbol{\mu}$ and the updated policy $\boldsymbol{\pi}^{k+1}$ as $\alpha_i = \max_s D_{\mathrm{TV}}\left(\pi_i^{k+1}(\cdot|s)\|\mu_i(\cdot|s)\right)$, we have:*

$$|J(\boldsymbol{\pi}^{k+1},\boldsymbol{\mu})-\eta(\boldsymbol{\pi}^{k+1})| \leq \frac{4\epsilon\gamma}{(1-\gamma)^2}\left(\sum_{i=1}^{N}\alpha_i\right)^2+\frac{2\epsilon(N-1)}{N}\sum_{i=1}^{N}\alpha_i, \tag{12}$$

where γ is the discount factor and $\epsilon = \max_{s,\boldsymbol{a}}|A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a})|$.

[3] $\psi(\boldsymbol{\mu},\boldsymbol{\pi}^k)$ means the result of one round of policy update starting from $\boldsymbol{\pi}^k$ using $\boldsymbol{\mu}$ as the sampling policy, i.e., $\psi(\boldsymbol{\mu},\boldsymbol{\pi}^k) = \arg\max_{\boldsymbol{\pi}} J(\boldsymbol{\pi},\boldsymbol{\mu})$ within the trust region of $\boldsymbol{\pi}^k$ for MAPPO.

[4] Assuming f is a function defined over the state and joint action space, the ego-max-operator ϕ is defined as $\phi(f,s) = \frac{1}{N}\sum_{i=1}^{N}\max_{a_i\in\mathcal{A}}\sum_{a_{-i}\in\mathcal{A}}\prod_{j\neq i}\pi_j^k(a_j|s)f(s,\boldsymbol{a})$.

Proof. Firstly, according to the *performance difference lemma* Kakade & Langford (2002), we have:

$$\begin{aligned}
&\eta(\boldsymbol{\pi}^{k+1}) - J(\boldsymbol{\pi}^{k+1}, \boldsymbol{\mu}) \\
=& \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\pi}^{k+1}}(s) \sum_{\boldsymbol{a}\in\boldsymbol{\mathcal{A}}} \boldsymbol{\pi}^{k+1}(\boldsymbol{a}|s) A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a}) \\
&\qquad - \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}}(s) \left[\frac{1}{N}\sum_{i=1}^{N}\sum_{\boldsymbol{a}\in\boldsymbol{\mathcal{A}}} \pi_i(a_i|s)\prod_{j\neq i}\mu_j(a_j|s) A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a})\right] \\
=& \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\pi}^{k+1}}(s) \sum_{\boldsymbol{a}\in\boldsymbol{\mathcal{A}}} \boldsymbol{\pi}^{k+1}(\boldsymbol{a}|s) A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a}) - \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}}(s) \sum_{\boldsymbol{a}\in\boldsymbol{\mathcal{A}}} \boldsymbol{\pi}^{k+1}(\boldsymbol{a}|s) A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a}) \\
&\qquad + \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}}(s) \sum_{\boldsymbol{a}\in\boldsymbol{\mathcal{A}}} \boldsymbol{\pi}^{k+1}(\boldsymbol{a}|s) A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a}) \\
&\qquad - \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}}(s) \left[\frac{1}{N}\sum_{i=1}^{N}\sum_{\boldsymbol{a}\in\boldsymbol{\mathcal{A}}} \pi_i(a_i|s)\prod_{j\neq i}\mu_j(a_j|s) A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a})\right] \\
\leq& \left|\sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\pi}^{k+1}}(s) \sum_{\boldsymbol{a}\in\boldsymbol{\mathcal{A}}} \boldsymbol{\pi}^{k+1}(\boldsymbol{a}|s) A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a}) - \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}}(s) \sum_{\boldsymbol{a}\in\boldsymbol{\mathcal{A}}} \boldsymbol{\pi}^{k+1}(\boldsymbol{a}|s) A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a})\right| \\
&\qquad + \Bigg|\sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}}(s) \sum_{\boldsymbol{a}\in\boldsymbol{\mathcal{A}}} \boldsymbol{\pi}^{k+1}(\boldsymbol{a}|s) A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a}) \\
&\qquad - \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}}(s) \left[\frac{1}{N}\sum_{i=1}^{N}\sum_{\boldsymbol{a}\in\boldsymbol{\mathcal{A}}} \pi_i(a_i|s)\prod_{j\neq i}\mu_j(a_j|s) A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a})\right]\Bigg| \\
\overset{\text{(I)}}{\leq}& \frac{4\epsilon\gamma}{(1-\gamma)^2}\alpha^2 + \Bigg|\sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}}(s) \sum_{\boldsymbol{a}\in\boldsymbol{\mathcal{A}}} \boldsymbol{\pi}^{k+1}(\boldsymbol{a}|s) A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a}) \\
&\qquad - \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}}(s) \left[\frac{1}{N}\sum_{i=1}^{N}\sum_{\boldsymbol{a}\in\boldsymbol{\mathcal{A}}} \pi_i(a_i|s)\prod_{j\neq i}\mu_j(a_j|s) A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a})\right]\Bigg|,
\end{aligned} \tag{13}$$

where (I) holds because of the conclusion that has already been obtained in TRPO Schulman et al. (2015) (see Theorem 1). Besides, we further have:

$$\begin{aligned}
&\Bigg|\sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}}(s) \sum_{\boldsymbol{a}\in\boldsymbol{\mathcal{A}}} \boldsymbol{\pi}^{k+1}(\boldsymbol{a}|s) A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a}) \\
&\qquad - \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}}(s) \left[\frac{1}{N}\sum_{i=1}^{N}\sum_{\boldsymbol{a}\in\boldsymbol{\mathcal{A}}} \pi_i^{k+1}(a_i|s)\prod_{j\neq i}\mu_j(a_j|s) A_{\boldsymbol{\pi}^k}(s,\boldsymbol{a})\right]\Bigg| \\
\leq& \left|\epsilon \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}}(s)\frac{1}{N}\sum_{i=1}^{N}\sum_{a_i\in\mathcal{A}_i} \pi_i^{k+1}(a_i|s) \sum_{a_{-i}\in\mathcal{A}_{-i}} \left(\prod_{j\neq i}\mu_j(a_j|s) - \prod_{j\neq i}\pi_j^{k+1}(a_j|s)\right)\right| \\
\overset{\text{(II)}}{=}& \epsilon \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}}(s)\frac{2}{N}\sum_{i=1}^{N}\sum_{a_i\in\mathcal{A}_i} \pi_i^{k+1}(a_i|s) D_{\mathrm{TV}}\left(\pi_{-i}^{k+1}(\cdot|s)\|\mu_{-i}(\cdot|s)\right) \\
=& \frac{2\epsilon}{N}\sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}}(s)\sum_{i=1}^{N} D_{\mathrm{TV}}\left(\pi_{-i}^{k+1}(\cdot|s)\|\mu_{-i}(\cdot|s)\right) \\
\leq& \frac{2\epsilon}{N}\sum_{i=1}^{N}\max_s D_{\mathrm{TV}}\left(\pi_{-i}^{k+1}(\cdot|s)\|\mu_{-i}(\cdot|s)\right),
\end{aligned} \tag{14}$$

where (II) holds according to the definition of TV distance. Thus, we finally have:

$$
\begin{aligned}
\eta(\boldsymbol{\pi}^{k+1}) - J(\boldsymbol{\pi}^{k+1}, \boldsymbol{\mu}) &\leq \frac{4\epsilon\gamma}{(1-\gamma)^2}\alpha^2 + \frac{2\epsilon}{N}\sum_{i=1}^{N}\max_s D_{\mathrm{TV}}\left(\pi_{-i}^{k+1}(\cdot|s)\|\mu_{-i}(\cdot|s)\right) \\
&= \frac{4\epsilon\gamma}{(1-\gamma)^2}\alpha^2 + \frac{2\epsilon(N-1)}{N}\sum_{i=1}^{N}\alpha_i \\
&\overset{\text{(III)}}{\leq} \underbrace{\frac{4\epsilon\gamma}{(1-\gamma)^2}\left(\sum_{i=1}^{N}\alpha_i\right)^2}_{(a)} + \underbrace{\frac{2\epsilon(N-1)}{N}\sum_{i=1}^{N}\alpha_i}_{(b)},
\end{aligned}
\tag{15}
$$

where (III) is because $\alpha \leq \sum_{i=1}^{N}\alpha_i$. Specifically, term (a) in the final upper bound is due to the state distribution mismatch of the training trajectories, while term (b) reveals the impact of the "teammate delay" phenomenon on the learning objective.
□

Theorem 1 *Suppose that we update joint policy $\boldsymbol{\pi}^k$ to $\boldsymbol{\pi}^{k+1}$ with sampling policy $\boldsymbol{\mu}$, then the regret of the updated joint policy $\boldsymbol{\pi}^{k+1}$ has the following upper bound:*

$$
\eta(\boldsymbol{\pi}^*) - \eta(\boldsymbol{\pi}^{k+1}) \leq \eta(\boldsymbol{\pi}^*) - J(\boldsymbol{\pi}^{k+1}, \boldsymbol{\mu}) + \frac{4\epsilon\gamma}{(1-\gamma)^2}\left(\sum_{i=1}^{N}\alpha_i\right)^2 + \frac{2\epsilon(N-1)}{N}\sum_{i=1}^{N}\alpha_i. \tag{16}
$$

Proof.

$$
\begin{aligned}
&\eta(\boldsymbol{\pi}^*) - \eta(\boldsymbol{\pi}^{k+1}) \\
&= \eta(\boldsymbol{\pi}^*) - J(\boldsymbol{\pi}^{k+1}, \boldsymbol{\mu}) + J(\boldsymbol{\pi}^{k+1}, \boldsymbol{\mu}) - \eta(\boldsymbol{\pi}^{k+1}) \\
&\leq \eta(\boldsymbol{\pi}^*) - J(\boldsymbol{\pi}^{k+1}, \boldsymbol{\mu}) + \left|J(\boldsymbol{\pi}^{k+1}, \boldsymbol{\mu}) - \eta(\boldsymbol{\pi}^{k+1})\right| \\
&\overset{\text{(IV)}}{\leq} \eta(\boldsymbol{\pi}^*) - J(\boldsymbol{\pi}^{k+1}, \boldsymbol{\mu}) + \frac{4\epsilon\gamma}{(1-\gamma)^2}\left(\sum_{i=1}^{N}\alpha_i\right)^2 + \frac{2\epsilon(N-1)}{N}\sum_{i=1}^{N}\alpha_i,
\end{aligned}
\tag{17}
$$

where (IV) is obtained due to *Lemma 1*.
□

Theorem 2 *Let ψ be the policy update operator. The sampling policy $\boldsymbol{\mu}^*$ that can derive the same updated policy, i.e., $\boldsymbol{\mu}^* = \psi(\boldsymbol{\mu}^*, \boldsymbol{\pi}^k)$, is the solution of the following bi-level optimization problem:*

$$
\min_{\boldsymbol{\mu}} D_{\mathrm{KL}}(\boldsymbol{\mu}\|\boldsymbol{\pi}^{k+1}), \ \textit{s.t.}\ \boldsymbol{\pi}^{k+1} = \arg\max_{\boldsymbol{\pi}} J(\boldsymbol{\pi}, \boldsymbol{\mu}). \tag{18}
$$

Proof. This bi-level optimization problem can be viewed as a constrained optimization problem, where we want to find a pair of $\boldsymbol{\mu}$ and $\boldsymbol{\pi}^{k+1}$ that minimizes the $D_{\mathrm{KL}}(\boldsymbol{\mu}\|\boldsymbol{\pi}^{k+1})$, while satisfying the condition that $\boldsymbol{\pi}^{k+1} = \arg\max_{\boldsymbol{\pi}} J(\boldsymbol{\pi}, \boldsymbol{\mu})$. For lookahead policy $\boldsymbol{\mu}^*$, if we set $\boldsymbol{\mu} = \boldsymbol{\mu}^*$, we can define a $\boldsymbol{\pi}^{k+1}$ as $\boldsymbol{\pi}^{k+1} = \boldsymbol{\mu}^*$. Then, as we know $\boldsymbol{\mu}^* = \psi(\boldsymbol{\mu}^*, \boldsymbol{\pi}^k)$, and $\psi(\boldsymbol{\mu}, \boldsymbol{\pi}^k)$ typically means $\arg\max_{\boldsymbol{\pi}} J(\boldsymbol{\pi}, \boldsymbol{\mu})$ with some conditions, we have that the pair of $(\boldsymbol{\mu}, \boldsymbol{\pi}^{k+1})$ we find satisfies the constraint of this optimization problem. Moreover, as we set $\boldsymbol{\pi}^{k+1} = \boldsymbol{\mu}^*$, we know that $D_{\mathrm{KL}}(\boldsymbol{\mu}\|\boldsymbol{\pi}^{k+1})$ equals to zero for $\boldsymbol{\mu} = \boldsymbol{\pi}^{k+1} = \boldsymbol{\mu}^*$, while D_{KL} for two distributions is always greater or equals to zero. Thus, we know $\boldsymbol{\mu}^*$ is the solution of this bi-level optimization problem.
□

Theorem 3 *Let ϕ be the ego-max-operator. We suppose that $\boldsymbol{\mu}^*$ denotes the lookahead policy which means that it can derive the same updated policy, i.e., $\boldsymbol{\mu}^* = \psi(\boldsymbol{\mu}^*, \boldsymbol{\pi}^k)$; and $\boldsymbol{\pi'} = \psi(\boldsymbol{\pi}^k, \boldsymbol{\pi}^k)$ denotes the updated policy when using $\boldsymbol{\pi}^k$ as the sampling policy. We express the trust region as that $D_{\mathrm{TV}}\left(\pi'_i(\cdot|s)||\pi_i^k(\cdot|s)\right) \leq \beta_i$. In this case, when $\beta_i \leq \frac{\sum_{s\in\mathcal{S}}\rho_{\boldsymbol{\mu}^*}(s)\phi(s,A_{\boldsymbol{\pi}^k})}{2\sum_{s\in\mathcal{S}}\rho_{\boldsymbol{\pi}^k}(s)\phi(s,|A_{\boldsymbol{\pi}^k}|)}$, we have $J(\boldsymbol{\mu}^*, \boldsymbol{\mu}^*) \geq J(\boldsymbol{\pi'}, \boldsymbol{\pi}^k)$.*

Proof. To begin with, for the updated policy $\boldsymbol{\pi'} = \psi(\boldsymbol{\pi}^k, \boldsymbol{\pi}^k)$ using $\boldsymbol{\pi}^k$ as the sampling policy, we have:

$$\begin{aligned}
J(\boldsymbol{\pi'}, \boldsymbol{\pi}^k) &= \eta(\boldsymbol{\pi}^k) + \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\pi}^k}(s) \left[\frac{1}{N} \sum_{i=1}^{N} \sum_{a\in\mathcal{A}} \pi'_i(a_i|s) \prod_{j\neq i} \pi_j^k(a_j|s) A_{\boldsymbol{\pi}^k}(s,a) \right] \\
\implies & |J(\boldsymbol{\pi'}, \boldsymbol{\pi}^k) - J(\boldsymbol{\pi}^k, \boldsymbol{\pi}^k)| \\
&\leq \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\pi}^k}(s) \left[\frac{1}{N} \sum_{i=1}^{N} \sum_{a\in\mathcal{A}} \left| \left(\pi'_i(a_i|s) - \pi_i^k(a_i|s)\right) \prod_{j\neq i} \pi_j^k(a_j|s) A_{\boldsymbol{\pi}^k}(s,a) \right| \right] \\
&= \sum_{s\in\mathcal{S}} \frac{\rho_{\boldsymbol{\pi}^k}(s)}{N} \sum_{i=1}^{N} \sum_{a\in\mathcal{A}} |\pi'_i(a_i|s) - \pi_i^k(a_i|s)| \prod_{j\neq i} \pi_j^k(a_j|s) |A_{\boldsymbol{\pi}^k}(s,a)| \\
&\leq \sum_{s\in\mathcal{S}} \frac{2\rho_{\boldsymbol{\pi}^k}(s)}{N} \sum_{i=1}^{N} D_{\mathrm{TV}}(\pi'_i(\cdot|s) \| \pi_i^k(\cdot|s)) \max_{a_i\in\mathcal{A}} \sum_{a_{-i}\in\mathcal{A}} \prod_{j\neq i} \pi_j^k(a_j|s) |A_{\boldsymbol{\pi}^k}(s,a)|.
\end{aligned} \tag{19}$$

We have trust region condition that $\forall s \in \mathcal{S}, D_{\mathrm{TV}}(\pi'_i(\cdot|s) \| \pi_i^k(\cdot|s)) \leq \beta_i$. We assume β_i has an upper bound ζ for each agent i, then we further have:

$$\begin{aligned}
|J(\boldsymbol{\pi'}, \boldsymbol{\pi}^k) - J(\boldsymbol{\pi}^k, \boldsymbol{\pi}^k)| &\leq 2\zeta \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\pi}^k}(s) \left[\frac{1}{N} \sum_{i=1}^{N} \max_{a_i\in\mathcal{A}} \sum_{a_{-i}\in\mathcal{A}} \prod_{j\neq i} \pi_j^k(a_j|s) |A_{\boldsymbol{\pi}^k}(s,a)| \right] \\
\to J(\boldsymbol{\pi'}, \boldsymbol{\pi}^k) &\leq J(\boldsymbol{\pi}^k, \boldsymbol{\pi}^k) + 2\zeta \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\pi}^k}(s) \left[\frac{1}{N} \sum_{i=1}^{N} \max_{a_i\in\mathcal{A}} \sum_{a_{-i}\in\mathcal{A}} \prod_{j\neq i} \pi_j^k(a_j|s) |A_{\boldsymbol{\pi}^k}(s,a)| \right] \\
\to J(\boldsymbol{\pi'}, \boldsymbol{\pi}^k) &\leq \eta(\boldsymbol{\pi}^k) + 2\zeta \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\pi}^k}(s) \left[\frac{1}{N} \sum_{i=1}^{N} \max_{a_i\in\mathcal{A}} \sum_{a_{-i}\in\mathcal{A}} \prod_{j\neq i} \pi_j^k(a_j|s) |A_{\boldsymbol{\pi}^k}(s,a)| \right].
\end{aligned} \tag{20}$$

We know that $J(\boldsymbol{\mu}^*, \boldsymbol{\mu}^*) = \arg\max_{\boldsymbol{\pi}\in \mathrm{Ball}(\boldsymbol{\mu}^*)} J(\boldsymbol{\pi}, \boldsymbol{\mu}^*)$, where $\mathrm{Ball}(\boldsymbol{\mu}^*)$ means the trust region of $\boldsymbol{\mu}^*$. Further, this optimization problem means that:

$$\arg\max_{\pi\in \mathrm{Ball}(\mu)} J(\boldsymbol{\pi}, \boldsymbol{\mu}^*) = \eta(\boldsymbol{\pi}^k) + \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}^*}(s) \left[\frac{1}{N} \sum_{i=1}^{N} \sum_{a\in\mathcal{A}} \pi_i(a_i|s) \prod_{j\neq i} \mu_j^*(a_j|s) A_{\boldsymbol{\pi}^k}(s,a) \right]. \tag{21}$$

Thus, we are actually to optimize $\frac{1}{N}\sum_{i=1}^{N} \sum_{a\in\mathcal{A}} \pi_i(a_i|s) \prod_{j\neq i} \mu_j^*(a_j|s) A_{\boldsymbol{\pi}^k}(s,a)$ for each $s \in \mathcal{S}$; and when we find the optimized results are actually μ, it means that for each $s \in \mathcal{S}$, $\mu(\cdot|s)$ is a nash equilibrium for the cooperative game where the utility of action a is defined as $A_{\boldsymbol{\pi}^k}(s,a)$. With proper updating scheme, it is reasonable that we can obtain equilibrium that satisfies:

$$\begin{aligned}
\sum_{a\in\mathcal{A}} \mu_i^*(a_i|s) \prod_{j\neq i} \mu_j^*(a_j|s) A_{\boldsymbol{\pi}^k}(s,a) &= \sum_{a_i\in\mathcal{A}} \mu_i^*(a_i|s) \sum_{a_{-i}\in\mathcal{A}} \prod_{j\neq i} \mu_j^*(a_j|s) A_{\boldsymbol{\pi}^k}(s,a) \\
&\geq \max_{a_i\in\mathcal{A}} \sum_{a_{-i}\in\mathcal{A}} \prod_{j\neq i} \pi_j^k(a_j|s) A_{\boldsymbol{\pi}^k}(s,a).
\end{aligned} \tag{22}$$

Thus we have that:

$$\begin{aligned}
J(\boldsymbol{\mu}^*, \boldsymbol{\mu}^*) &= \eta(\boldsymbol{\pi}^k) + \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}^*}(s) \left[\frac{1}{N} \sum_{i=1}^{N} \sum_{a\in\mathcal{A}} \mu_i^*(a_i|s) \prod_{j\neq i} \mu_j^*(a_j|s) A_{\boldsymbol{\pi}^k}(s,a) \right] \\
&\geq \eta(\boldsymbol{\pi}^k) + \sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}^*}(s) \left[\frac{1}{N} \sum_{i=1}^{N} \max_{a_i\in\mathcal{A}} \sum_{a_{-i}\in\mathcal{A}} \prod_{j\neq i} \pi_j^k(a_j|s) A_{\boldsymbol{\pi}^k}(s,a) \right].
\end{aligned} \tag{23}$$

We define $\phi(f, s) = \frac{1}{N}\sum_{i=1}^{N} \max_{a_i\in\mathcal{A}} \sum_{a_{-i}\in\mathcal{A}} \prod_{j\neq i} \pi_j^k(a_j|s) f(s, \boldsymbol{a})$. Then when $\beta_i \leq \zeta \leq \frac{\sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}^*}(s)\phi(s, A_{\boldsymbol{\pi}^k})}{2\sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\pi}^k}(s)\phi(s, |A_{\boldsymbol{\pi}^k}|)}$, according to Equation (20) and Equation (23), it is obvious that $J(\boldsymbol{\mu}^*, \boldsymbol{\mu}^*) \geq J(\boldsymbol{\pi}', \boldsymbol{\pi}^k)$.
□

A.3 Extra Analysis on Upper Bound

Theorem 1 has told us that when the extra term (c) in the upper bound disappears when we train the agents with future teammate information, which motivates us to predict future teammates. However, we still retrain a question whether eliminating term (c) can indeed reduce the overall upper bound. For this question, one potential risk is that eliminating term (c) might influence the optimization of $-J(\boldsymbol{\pi}, \boldsymbol{\mu})$, thus making the second term $-J(\boldsymbol{\pi}^{k+1}, \boldsymbol{\mu})$ larger. To solve this concern, we prove that under certain conditions it is at least better than the previous algorithms, as described below.

Theorem 3 *To begin with, we introduce the policy update operator ψ* [5] *and ego-max-operator ϕ* [6]*. We suppose that $\boldsymbol{\mu}^*$ denotes the lookahead policy which means that it can derive the same updated policy, i.e., $\boldsymbol{\mu}^* = \psi(\boldsymbol{\mu}^*, \boldsymbol{\pi}^k)$; and $\boldsymbol{\pi}' = \psi(\boldsymbol{\pi}^k, \boldsymbol{\pi}^k)$ denotes the updated policy when using $\boldsymbol{\pi}^k$ as the sampling policy. We express the trust region as that $D_{\mathrm{TV}}\left(\pi_i'(\cdot|s)||\pi_i^k(\cdot|s)\right) \leq \beta_i$. In this case, when $\beta_i \leq \frac{\sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\mu}^*}(s)\phi(s, A_{\boldsymbol{\pi}^k})}{2\sum_{s\in\mathcal{S}} \rho_{\boldsymbol{\pi}^k}(s)\phi(s, |A_{\boldsymbol{\pi}^k}|)}$, we have $J(\boldsymbol{\mu}^*, \boldsymbol{\mu}^*) \geq J(\boldsymbol{\pi}', \boldsymbol{\pi}^k)$.*

For proof see Appendix A.2. This theorem shows that when we replace $\boldsymbol{\mu}$ with an approximation of future teammate policies, under certain conditions we can at least obtain a smaller upper bound compared to the previous typical algorithms. Specifically, the required conditions are relevant to the trust-region setting.

B More Implementation Details

B.1 More Details about Baselines

To conduct performance comparison in our experiments, we firstly select the main multi-agent actor-critic algorithms as baselines, including MADDPG Lowe et al. (2017), IPPO de Witt et al. (2020a), MAPPO Yu et al. (2022a) and HAPPO Kuba et al. (2021). Besides, we additionally design an opponent modeling algorithm TAPPO (abbreviated for Teammate-Aware MAPPO) to further compare our approach with traditional opponent modeling techniques. In specific, TAPPO learns teammate representations for extra policy conditions like in previous works Papoudakis & Albrecht (2020); Cao et al. (2023) and is incorporated into MAPPO. Furthermore, in the GRF environment, we additionally include the CDS algorithm Li et al. (2021), which is a value-based algorithm specifically designed for the GRF problems. It mainly designs mechanism to enhance policy diversity among agents and surpasses typical value-based algorithms in the GRF environment in its experiments.

B.2 Incorporating Lookahead Strategy into HAPPO

Heterogeneous-Agent Proximal Policy Optimisation (HAPPO) Kuba et al. (2021) is a recent work that introduced the *sequential policy update scheme* to the multi-agent policy gradient algorithm. It provides a monotonic improvement guarantee in theory based on the finding of the *multi-agent advantage decomposition lemma*. The core idea of this work is to update the agents' policies in sequence. This approach empowers subsequent agents to adapt their policies based on the updated strategies of preceding agents, thereby mitigating to some extent the impact of the "teammate delay" phenomenon. However, it has two main issues that might impact its effectiveness:

[5] $\psi(\boldsymbol{\mu}, \boldsymbol{\pi}^k)$ means the result of one round of policy update starting from $\boldsymbol{\pi}^k$ using $\boldsymbol{\mu}$ as the sampling policy, i.e., $\psi(\boldsymbol{\mu}, \boldsymbol{\pi}^k) = \arg\max_{\boldsymbol{\pi}} J(\boldsymbol{\pi}, \boldsymbol{\mu})$ within the trust region of $\boldsymbol{\pi}^k$ for MAPPO.

[6] Assuming f is a function defined over the state and joint action space, the ego-max-operator ϕ is defined as $\phi(f, s) = \frac{1}{N}\sum_{i=1}^{N} \max_{a_i\in\mathcal{A}} \sum_{a_{-i}\in\mathcal{A}} \prod_{j\neq i} \pi_j^k(a_j|s) f(s, \boldsymbol{a})$.

Table 4: Common hyper-parameters used across task scenarios of multi-agent MuJoCo. Note that lka is short for Lookahead, mlearn is short for "model learning", and ppo stands for Proximal Policy Optimization (PPO) algorithm.

hyper-parameter	value	hyper-parameter	value	hyper-parameter	value
critic lr	3e-4	max grad norm	10	lka episode length	20
actor lr	3e-4	num rollouts	40	lka num mini-batches	10
gamma γ	0.99	ppo num mini-batches	10	lka entropy coef	0.001
optimizer	Adam	entropy coef	0.01	mlearn batch size	512
optim eps	1e-5	stacked-frames	1		

1) Despite the sequential policy update scheme, the preceding agents in the sequence still learn to cooperate with the previous round of teammates, which means the teammate delay issue persists for the preceding agents. This results in a critical importance placed on the order of agents' update (e.g., for the example in the Introduction section, if the order is Cook first, the updates are more efficient; otherwise, sequential update yields no benefits). However, HAPPO adopts random update orders, which poses a significant limitation.

2) Since in practice, the training trajectories are sampled by the policy of the previous round, HAPPO adopts Importance Sampling to help the subsequent agents learn to cooperate with updated previous agents. This approach can lead to a higher variance in the policy gradients as we need to multiply it by an importance sampling ratio to correct the objective. This issue becomes exacerbated when dealing with a larger number of agents, as we need to accumulate the product of importance ratios for all preceding agents.

Due to these two main issues, the effectiveness of HAPPO in practice may be influenced and it can not fully resolve the "teammate delay" issue . Actually, in practice, our lookahead strategy can be seamlessly integrated with HAPPO, further enhancing its effectiveness, which has been validated by our empirical experiments. The detailed process is introduced in the Algorithm 2, where the text highlighted in red emphasizes the uniqueness introduced by HAPPO.

Algorithm 2 Heterogeneous-Agent Proximal Policy Optimisation with Lookahead

Input: The Number of agent N

Output: A cooperation policy for a multi-agent system

1: Initialize a replay buffer $\mathcal{B}$;
2: Initialize a policy $\boldsymbol{\pi}$ randomly;
3: **for** each iteration k **do**
4: Sample a batch of transitions from $\mathcal{B}$ and update the environment model;
5: Sample a batch of trajectories $\tilde{\tau}$ in the environment model with sampling policy $\boldsymbol{\pi}^k$, and obtain $\tilde{\boldsymbol{\pi}}^{k+1}$ via maximizing $J(\boldsymbol{\pi}, \boldsymbol{\pi}^k)$ within trust region in a sequential update scheme using the training trajectories $\tilde{\tau}$;
6: Sample a batch of trajectories τ in the real environment with sampling policy $\tilde{\boldsymbol{\pi}}^{k+1}$, and obtain $\boldsymbol{\pi}^{k+1}$ via maximizing $J(\boldsymbol{\pi}, \tilde{\boldsymbol{\pi}}^{k+1})$ within trust region in a sequential update scheme using the training trajectories τ;
7: Add trajectories τ to the buffer $\mathcal{B}$;
8: **end for**

B.3 Details about Hyper-parameters

In this section, we firstly introduce the hyper-parameter configurations of our method in the experiments, and then we illustrate how we tune the hyper-parameters.

B.3.1 Hyper-parameter configuration

Here, we list the configuration of hyper-parameters that was utilized in our experiments to facilitate reproducing our experimental results. **Note** that for the common hyper-parameters, both the Lookahead algorithm and HAPPO adopted the same value in our experiments. Hence, the hyper-parameter configurations provided in this section are also applicable to our experimental results of the HAPPO algorithm.

Multi-agent MuJoCo For hyper-parameters that were set to the same values across all task scenarios, the configuration is provided in Table 4. Additionally, the varying hyper-parameter configurations across different tasks are provided in Table 5.

Table 5: Different hyper-parameters used across task scenarios of multi-agent MuJoCo. Note that lka is short for Lookahead, mlearn is short for "model learning", and ppo stands for Proximal Policy Optimization (PPO) algorithm.

hyper-parameter	Ant	HalfCheetah	Walker2d
episode length	200	400	200
ppo num epochs	10	20	10
lka num rollouts	2000	4000	2000
lka num epochs	10	20	10
mlearn num epochs	4000	2000	2000

Google Research Football (GRF) In the three task scenarios of Google Research Football (GRF), we employed identical hyper-parameter configurations, which are detailed in Table 6.

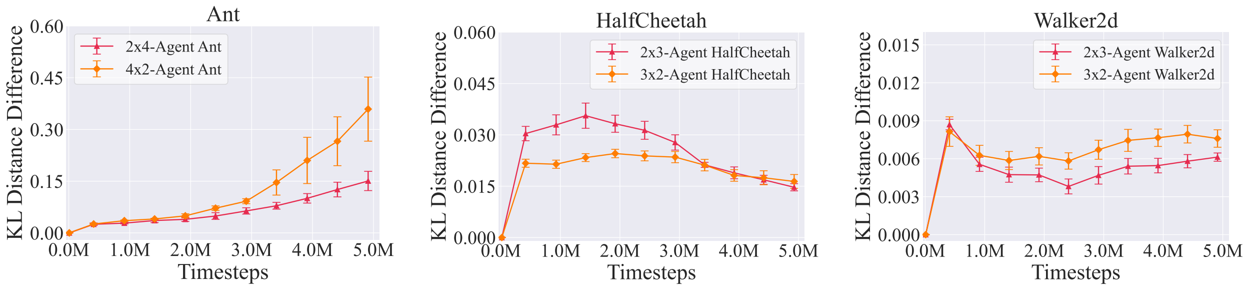
Table 6: Common hyper-parameters used across task scenarios of Google Research Football (GRF). Note that lka is short for Lookahead, mlearn is short for "model learning", and ppo stands for Proximal Policy Optimization (PPO) algorithm.

hyper-parameter	value	hyper-parameter	value	hyper-parameter	value
critic lr	5e-4	episode length	100	lka num rollouts	100
actor lr	5e-4	num rollouts	10	lka num mini-batches	1
gamma γ	0.99	ppo num mini-batches	1	lka num epochs	15
optimizer	Adam	ppo num epochs	15	lka entropy coef	0
optim eps	1e-5	entropy coef	5e-3	mlearn batch size	1024
max grad norm	10	lka episode length	100	mlearn num epochs	800

B.3.2 Hyper-parameter tuning strategy

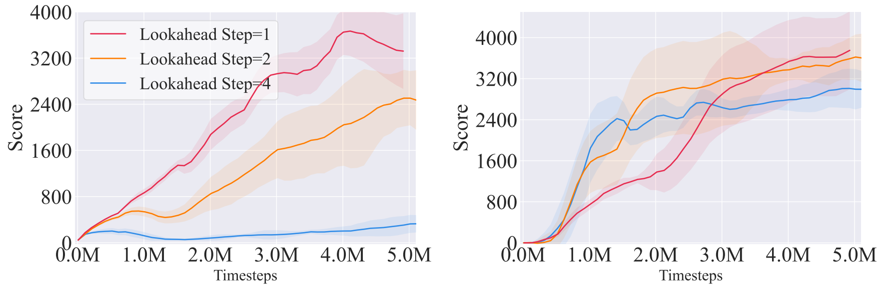
Multi-agent MuJoCo For the practical implementation efficiency of the algorithm, we employed JAX to implement our Lookahead algorithm. Additionally, to ensure a fair and effective comparison of the efficacy of our added lookahead strategy, the underlying HAPPO algorithm also utilized the same codebase. Furthermore, the fundamental hyper-parameters for both Lookahead and HAPPO were kept consistent. Consequently, we mainly tune the hyper-parameters to align the performance of the HAPPO algorithm of our codebase with that disclosed in the original paper.

Google Research Football (GRF) Similar to the case in multi-agent MuJoCo, to ensure a fair comparison, we maintained consistent foundational hyper-parameters for both Lookahead and the underlying HAPPO algorithm. While tuning these hyper-parameters, we conducted a search within certain ranges to fine-tune the underlying HAPPO algorithm for reasonably good performance results. Specifically, we explored learning rate `lr` (including `critic_lr` and `actor_lr`) within the range of `{1e-4, 5e-4, 1e-3}`, number of learning epochs `ppo_num_epochs` within `{10, 15, 20}`, and entropy regularization coefficient `entropy_coef` within `{1e-3, 5e-3}`.



(a) Ant Task (b) HalfCheetah Task (c) Walker2d Task

Figure 5: Measuring policy distances in multi-agent MuJoCo environment.



(a) 2x4-Agent Ant (b) 2x3-Agent HalfCheetah

Figure 6: Experimental results for study about multiple steps of lookahead approximation.

C More Experimental Results

C.1 More Results about Lookahead Policy Analysis

In Section 4.3, we measure the KL distance difference of policies on Ant and HalfCheetah tasks of multi-agent MuJoCo. Here, we additionally provide the results on the Walker2d task. As we can see, the results on three different types of tasks all validate that our approach can empirically obtain positive results for $D_{\mathrm{KL}}(\boldsymbol{\pi}^{k+1}, \boldsymbol{\pi}^{k}) - D_{\mathrm{KL}}(\boldsymbol{\pi}^{k+1}, \tilde{\boldsymbol{\pi}}^{k+1})$, which means that $\tilde{\boldsymbol{\pi}}^{k+1}$ can to some extent provide the direction information of future teammate policy $\boldsymbol{\pi}^{k+1}$ and is relatively a good approximation.

C.2 Study about Multiple Steps of Lookahead Approximation

In the practical implementation of the algorithm in this work, we employ a one-step approximation to estimate future teammate policies. We wonder whether we can obtain a better approximation of future teammates through more rounds of lookahead training. To answer this question, we conduct additional experiments, comparing with the baselines that perform more rounds of policy update when obtaining the lookahead policy. The results are depicted in Figure 6, where "Lookahead Step" represents the number of policy update rounds conducted for approximating future teammates, i.e., "Lookahead Step=1" corresponds to the results in the maintext.

From the results, we can see that when we increase the Lookahead Step, the quality of the lookahead approximation does not increase and we obtain lower performance. It is reasonable because when we conduct more iterations for lookahead training within the model, the newly updated policy would appear unfamiliar to the model, as the environmental model has been trained on data sampled from the old policies. This necessitates refraining from employing excessively off-policy policies for trajectory rollout within the model. However, despite achieving lower convergence performance, it seems to learn faster in the early stage in the task of 2x3-Agent HalfCheetah when we increase the Lookahead Step. This encourages us to design better model learning algorithm in the future, thus to further improve the effectiveness of our approach.