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Graphon Mean-Field Control for Cooperative Multi-Agent Reinforcement Learning

Yuanquan Hu, Xiaoli Wei∗ , Junji Yan, Hengxi Zhang

Abstract

The marriage between mean-field theory and reinforcement learning has shown a great capacity to solve large-scale control problems with homogeneous agents. To break the homogeneity restriction of mean-field theory, a recent interest is to introduce graphon theory to the mean-field paradigm. In this paper, we propose a graphon mean-field control (GMFC) framework to approximate cooperative heterogeneous multi-agent reinforcement learning (MARL) with nonuniform interactions and heterogeneous reward functions and state transition functions among agents and show that the approximate order is of $\mathcal{O}(\frac{1}{\sqrt{l}})$ $\frac{1}{N}$), with N the number of agents. By discretizing the graphon index of GMFC, we further introduce a smaller class of GMFC called block GMFC, which is shown to well approximate cooperative MARL in terms of the value function and the policy. Finally, we design a Proximal Policy Optimization based algorithm for block GMFC that converges to the optimal policy of cooperative MARL. Our empirical studies on several examples demonstrate that our GMFC approach is comparable with the state-of-art MARL algorithms while enjoying better scalability.

Keywords:

Cooperative Multi-Agent Reinforcement Learning, Graphon Theory, Graphon Mean-Field Control, Proximal Policy Optimization 2000 MSC: 60J20, 91A13

¹ 1. Introduction

 Multi-agent reinforcement learning (MARL) has found various applications in the field of transportation and simulation $[50, 1]$, stock price analysis and trading $[32, 31]$, wireless communication networks [12, 11, 13], and learning behaviors in social dilemmas [33, 28, 34]. MARL, however, becomes intractable due to the complex interactions among agents as the number of agents increases.

⁷ A recent tractable approach is a mean-field approach by considering MARL in the regime ⁸ with a large number of homogeneous agents under weak interactions [20]. According to the

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 number of agents and learning goals, there are three subtle types of mean-field theories for MARL. The first one is called mean-field MARL (MF-MARL), which refers to the empirical average of the states or actions of a finite population. For example, [52] proposes to approx- imate interactions within the population of agents by averaging the actions of the overall population or neighboring agents. [35] proposes a mean-field proximal policy optimization algorithm for a class of MARL with permutation invariance. The second one is called mean- field game (MFG), which describes the asymptotic limit of non-cooperative stochastic games as the number of agents goes to infinity [30, 27, 8]. Recently, a rapidly growing literature studies MFG for noncooperative MARL either in a model-based way [53, 6, 26] or by a model-free approach [25, 48, 18, 14, 44]. The third one is called mean-field control (MFC), which is closely related to MFG yet different from MFG in terms of learning goals. For cooperative MFC, the Bellman equation for the value function is defined on an enlarged space of probability measures, and MFC is always reformulated as a new Markov decision process (MDP) with continuous state-action space. [9] shows the existence of optimal poli- cies for MFC in the form of mean-field MDP and adapts classical reinforcement learning (RL) methods to the mean-field setups. [23] approximates MARL by a MFC approach, and proposes a model-free kernel-based Q-learning algorithm (MFC-K-Q) that enjoys a linear convergence rate and is independent of the number of agents. [44] presents a model-based RL algorithm M3-UCRL for MFC with a general regret bound. [2] proposes a unified two- timescale learning framework for MFG and MFC by tuning the ratio of learning rates of Q function and the population state distribution. Under the framework of MFC, [41] proposes locally executable policies such that the resulting discounted sum of average rewards well approximates the optimal value function over all policies with theoretical guarantee.

 One restriction of the mean-field theory is that it eliminates the difference among agents and interactions between agents are assumed to be uniform. However, in many real world scenarios, strategic interactions between agents are not always uniform and rely on the relative positions of agents. To develop scalable learning algorithms for multi-agent systems with heterogeneous agents, one approach is to exploit the local network structure of agents [45, 37]. Another approach is to consider mean-field systems on large graphs and their asymptotic limits, which leads to graphon mean-field theory [39]. So far, most existing works on graphon mean-field theory consider either diffusion processes without learning in continuous time or non-cooperative graphon mean-field game (GMFG) in discrete time. [3] considers uncontrolled graphon mean-field systems in continuous time. [17] studies MFG on an Erdös-Rényi graph. [19] studies the convergence of weighted empirical measures described by stochastic differential equations. [4] studies propagation of chaos of weakly interacting particles on general graph sequences. [5] considers general GMFG and studies ϵ -Nash equilibria of the multi-agent system by a PDE approach in continuous time. [29] studies stochastic games on large graphs and their graphon limits. It shows that GMFG is viewed as a special case of MFG by viewing the label of agents as a component of the state process. [21, 22] study continuous-time cooperative graphon mean-field systems with linear dynamics. On the other hand, [7] studies static finite-agent network games and their associated graphon games. [49] provides a sequential decomposition algorithm to find Nash equilibria of discrete-time GMFG. [15] constructs a discrete-time learning GMFG framework

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 to analyze approximate Nash equilibria for MARL with nonuniform interactions. However, little is focused on learning cooperative graphon mean-field systems in discrete time, except for [42, 43] on particular forms of nonuniform interactions among agents. [43] proves that when the reward is affine in the state distribution and action distribution, MARL with nonuniform interactions can still be approximated by classic MFC. [42] considers multi- class MARL, where agents belonging to the same class are homogeneous. In contrast, we consider a general discrete-time GMFC framework under which agents are allowed to be fully heterogeneous and interact non-uniformly on any network captured by a graphon.

 ω *Our Work.* In this work, we propose a general discrete-time GMFC framework to approx- imate cooperative heterogeneous MARL on large graphs by combining classical MFC and network games. Theoretically, we first show that GMFC can be reformulated as a new MDP with deterministic dynamics and infinite-dimensional state-action space, hence the Bellman equation for Q function is established on the space of probability measure ensem- bles. It shows that GMFC approximates cooperative MARL well in terms of both value function and optimal policies. The approximation error is at order $\mathcal{O}(1/\sqrt{N})$, where N is the number of agents. Furthermore, instead of learning infinite-dimensional GMFC directly, we introduce a smaller class called block GMFC by discretizing the graphon index, which can be recast as a new MDP with deterministic dynamic and finite-dimensional continuous state-action space. We show that the optimal policy ensemble learned from block GMFC is near optimal for cooperative MARL. Using the approach in [38], we develop a proximal policy optimization (PPO) based algorithm for block GMFC, which, together with approxi- mation result between block GMFC and cooperative MARL, shows that the proposed PPO algorithm converges to the optimal policy of MARL with the sample complexity guarantee. Empirically, our experiments in Section 5 demonstrate that when the number of agents be- comes large, the mean episode reward of MARL becomes increasingly close to that of block GMFC, which verifies our theoretical findings. Furthermore, our block GMFC approach achieves comparable performances with other popular existing MARL algorithms in the finite-agent setting.

 Outline. The rest of the paper is organized as follows. Section 2 recalls basic notations of graphons and introduces the setup of cooperative MARL with nonuniform interactions and its asymptotic limit called GMFC. Section 3 connects cooperative MARL and GMFC, introduces block GMFC for efficient algorithm design, and builds its connection with coop- erative MARL. The main theoretical proofs are presented in Section 4. Section 5 tests the performance of block GMFC experimentally.

2. Mean-Field MARL on Dense Graphs

2.1. Preliminary: Graphon Theory

 In the following, we consider a cooperative multi-agent system and its associated mean- field limit. In this system, each agent is affected by all others, with different agents exerting \bullet different effects on her. This multi-agent system with N agents can be described by a 91 weighted graph $G_N = (\mathcal{V}_N, \mathcal{E}_N)$, where the vertex set $\mathcal{V}_N = \{1, \ldots, N\}$ and the edge set \mathcal{E}_N

⁹² represent agents and the interactions between agents, respectively. The adjacency matrix of G_N is represented as $\{\xi_{i,j}^N\}_{1\leq i,j\leq N}$. To study the limit of the multi-agent system as N 94 goes to infinity, we adopt the graphon theory introduced in [39] used to characterize the ⁹⁵ limit behavior of dense graph sequences. Therefore, throughout the paper, we assume the 96 graph G_N is dense and leave sparse graphs for future study.

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 97 In general, a graphon is represented by a bounded symmetric measurable function W : 98 $\mathcal{I} \times \mathcal{I} \to \mathcal{I}$, with $\mathcal{I} = [0, 1]$. We denote by W the space of all graphons and equip the space 99 W with the cut norm $\|\cdot\|_{\Box}$

$$
||W||_{\square} = \sup_{S,T \subset \mathcal{I}} \left| \int_{S \times T} W(\alpha, \beta) d\alpha d\beta \right|.
$$

100 For each weighted graph $G_N = (\mathcal{V}_N, \mathcal{E}_N)$, we consider the correspondence between the 101 adjacency matrix $\{\xi_{i,j}^N\}$ and a function on $\mathcal{I} \times \mathcal{I}$ with constant value $\xi_{i,j}^N$ on each block $\left(\frac{i-1}{N},\frac{i}{N}\right]\times\left(\frac{j-1}{N},\frac{j}{N}\right)$ 102 $(\frac{i-1}{N}, \frac{i}{N}] \times (\frac{j-1}{N}, \frac{j}{N}]$. We make the following condition on the strength of interaction $\xi_{i,j}^N$ 103 between agents i and j and the associated W_N .

$_{104}\;$ Condition on W_N and $\xi_{i,j}^N$

105 1) W_N is a step graphon, that is, $0 \leq W_N \leq 1$ and W_N is a constant on each block $\left(\frac{i-1}{N},\frac{i}{N}\right] \times \left(\frac{j-1}{N},\frac{j}{N}\right)$ 106 $\left(\frac{i-1}{N},\frac{i}{N}\right] \times \left(\frac{j-1}{N},\frac{j}{N}\right]$:

$$
W_N(\alpha, \beta) = W_N\left(\frac{i}{N}, \frac{j}{N}\right), \text{ if } \alpha \in \left(\frac{i-1}{N}, \frac{i}{N}\right], \ \beta \in \left(\frac{j-1}{N}, \frac{j}{N}\right].\tag{2.1}
$$

2) $\xi_{i,j}^{N}$ is taken as either

$$
\xi_{i,j}^N = W_N(\frac{i}{N}, \frac{j}{N})
$$
\n(C1)

or

$$
\xi_{i,j}^N \sim \text{Bernoulli}\big(W_N(\frac{i}{N}, \frac{j}{N})\big). \tag{C2}
$$

107 We further assume that the sequence of W_N converges to a graphon W in cut norm as 108 the number of agents N goes to infinity, which is crucial for the convergence analysis of ¹⁰⁹ cooperative MARL in Section 3.

110 Assumption 2.1 The sequence $(W_N)_{N \in \mathbb{N}}$ converges in cut norm to some graphon $W \in \mathcal{W}$ ¹¹¹ such that

$$
||W_N - W||_{\square} \to 0.
$$

¹¹² Some common examples of graphons include

113 1) Erdős Rényi: $W(\alpha, \beta) = p, 0 \le p \le 1, \alpha, \beta \in \mathcal{I};$

¹¹⁴ 2) Stochastic block model:

$$
W(\alpha, \beta) = \begin{cases} p & \text{if } 0 \leq \alpha, \beta \leq 0.5 \text{ or } 0.5 \leq \alpha, \beta \leq 1, \\ q & \text{otherwise,} \end{cases}
$$

115 where p represents the intra-community interaction and q the inter-community inter-¹¹⁶ action;

117 3) Random geometric graphon: $W(\alpha, \beta) = f(\min(|\beta-\alpha|, 1-|\beta-\alpha|))$, where $f : [0, 0.5] \rightarrow$ $[0, 1]$ is a non-increasing function.

¹¹⁹ 2.2. Cooperative Heterogeneous MARL

¹²⁰ In this section, we facilitate the analysis of MARL by considering a particular class of ¹²¹ MARL with nonuniform interactions, where each agent interacts with all other agents via ¹²² the aggregated weighted mean-field effect of the population of all agents.

123 Recall that we use the weighted graph $G_N = (\mathcal{V}_N, \mathcal{E}_N)$ to represent the multi-agent ¹²⁴ system, in which agents are cooperative and coordinated by a central controller. They 125 share a finite state space S and take actions from a finite action space A . We denote by 126 $\mathcal{P}(\mathcal{S})$ and $\mathcal{P}(\mathcal{A})$ the space of all probability measures on S and $\overline{\mathcal{A}}$, respectively. Furthermore, 127 denote by $\mathcal{B}(\mathcal{S})$ the space of all Borel measures on \mathcal{S} .

 128 For each agent i, the *neighborhood empirical measure* is given by

l

$$
\mu_t^{i,W_N}(\cdot) := \frac{1}{N} \sum_{j \in \mathcal{V}_N} \xi_{i,j}^N \delta_{s_t^j}(\cdot),\tag{2.2}
$$

129 where $\delta_{s_t^j}$ denotes Dirac measure at s_t^j , and (See [15] for more details).

130 At each step $t = 0, 1, \dots$, if agent $i, i \in [N]$ at state $s_t^i \in \mathcal{S}$ takes an action $a_t^i \in \mathcal{A}$, then ¹³¹ she will receive a reward

$$
r^i\left(s^i_t, \mu^{i,W_N}_t, a^i_t\right), \quad i \in [N], \tag{2.3}
$$

132 where $r^i : \mathcal{S} \times \mathcal{B}(\mathcal{S}) \times \mathcal{A} \to \mathbb{R}, i \in [N]$, and she will change to a new state s_{t+1}^i according to ¹³³ a transition probability such that

$$
s_{t+1}^i \sim P^i \left(\cdot \middle| s_t^i, \mu_t^{i,W_N}, a_t^i \right), \quad i \in [N], s_0^i \sim \mu \in \mathcal{P}(\mathcal{S}), \tag{2.4}
$$

134 where $P^i : \mathcal{S} \times \mathcal{B}(\mathcal{S}) \times \mathcal{A} \to \mathcal{P}(\mathcal{S}), i \in [N]$.

 $(2.3)-(2.4)$ indicate that the reward and the transition probability of agent i at time 136 t depend on both her individual information (s_t^i, a_t^i) and neighborhood empirical measure 137 $\mu_t^{i,W_N}.$

¹³⁸ Furthermore, the policy is assumed to be stationary for simplicity and takes the Marko-¹³⁹ vian form

$$
a_t^i \sim \pi^i \left(\cdot | s_t^i, \mu_t^{i, W_N} \right) \in \mathcal{P}(\mathcal{A}), \quad i \in [N], \tag{2.5}
$$

140 which maps agent is state to a randomized action. (2.5) is called global policy since the $_{141}$ policy of agent i depends on both her own state and the aggregate information of the whole 142 population. For each agent i, the space of all global policies is denoted as Π .

 Remark 2.2 It is computationally expensive to collect the aggregate information of the whole population in many practical scenarios. Considering the costly collection of the ag- gregation information of the whole population, one can restrict the policy to be in a local manner, that is, the policy that the agent i can execute depends solely on her own state information:

$$
a_t^i \sim \pi^i \left(\cdot | s_t^i \right) \in \mathcal{P}(\mathcal{A}), \quad i \in [N].
$$

148 This has been studied in [41] for standard MFC. Precisely, [41] designs locally executable ¹⁴⁹ policies such that the resulting discounted sum of average rewards well approximates the ¹⁵⁰ optimal value function over all policies. We expect that a similar result holds for GMFC.

151 Remark 2.3 When $\xi_{ij}^N \equiv 1$, $r^i \equiv r$, $P^i \equiv P$, $i, j \in [N]$, it corresponds to classical mean-¹⁵² field theory with uniform interactions [9, 23]. Furthermore, our framework is flexible enough 153 to include the nonuniform interactions of actions via $\nu_t^{i,W_N} = \frac{1}{N} \sum_{j \in \mathcal{V}_N} \xi_{i,j}^N \delta_{a_i^j}(\cdot)$.

154 The expected discounted accumulated reward of agent i is

l

$$
J_{N,i}(\mu, \pi^1, \dots, \pi^N) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t r^i (s_t^i, \ \mu_t^{i, W_N}, \ a_t^i) \ \middle| \ s_0^i \sim \mu, a_t^i \sim \pi^i(\cdot | s_t^i, \mu_t^{i, W_N})\right], \quad (2.6)
$$

155 subject to (2.2) - (2.5) with a discount factor $\gamma \in (0,1)$.

156 The objective of this cooperative multi-agent system $(2.2)-(2.5)$ is to find Pareto opti-¹⁵⁷ mality given in the Definition 2.4 below.

158 Definition 2.4 (Pareto Optimality) $(\pi^{1,*}, \ldots, \pi^{N,*}) \in \Pi^N$ is called Pareto optimality 159 for the multi-agent system (2.2) - (2.5) if there does not exist $(\pi^1, \ldots, \pi^N) \in \Pi^N$ such that

$$
\forall 1 \leq i \leq N, J_{N,i}(\mu, \pi^1, \dots, \pi^N) \geq J_{N,i}(\mu, \pi^{1,*}, \dots, \pi^{N,*}),
$$

$$
\exists 1 \leq i \leq N, J_{N,i}(\mu, \pi^1, \dots, \pi^N) > J_{N,i}(\mu, \pi^{1,*}, \dots, \pi^{N,*}).
$$

¹⁶⁰ To study Pareto optimality, we introduce the expected discounted accumulated reward ¹⁶¹ averaged over all agents, i.e.,

$$
V_N(\mu) = \sup_{(\pi^1, ..., \pi^N) \in \Pi^N} J_N(\mu, \pi^1, ..., \pi^N)
$$

 :=
$$
\sup_{(\pi^1, ..., \pi^N) \in \Pi^N} \frac{1}{N} \sum_{i=1}^N J_{N,i}(\mu, \pi^1, ..., \pi^N),
$$
 (2.7)

subject to (2.2) - (2.5) . Let $(\pi^{1,*}, \dots, \pi^{N,*}) \in \mathbb{R}$ arg max $(\pi^1,...,\pi^N)\in\Pi^N$ 162 subject to $(2.2)-(2.5)$. Let $(\pi^{1,*}, \ldots, \pi^{N,*}) \in \arg \max J_N(\mu, \pi^1, \ldots, \pi^N)$, then $(\pi^{1,*}, \ldots, \pi^{N,*})$

 is shown to be a Pareto optimality in Definition 2.4. Therefore, searching for Pareto opti- mality of cooperative MARL amounts to solving the optimal policy of (2.7). However, it is always difficult to exactly obtain the optimal policy of cooperative MARL. We consider a 166 weak notion of $ε$ -Pareto optimality.

167 **Definition 2.5** (ε -Pareto Optimality) $(\pi^{1,*}_{\varepsilon}, \ldots, \pi^{N,*}_{\varepsilon}) \in \Pi^{N}$ is called ε -Pareto optimality for the multi-agent system (2.2)-(2.5) if there does not exist (π 1 , . . . , π^N) [∈] ^Π^N ¹⁶⁸ such ¹⁶⁹ that

$$
\forall 1 \leq i \leq N, J_{N,i}(\mu, \pi^1, \dots, \pi^N) \geq J_{N,i}(\mu, \pi_{\varepsilon}^{1,*}, \dots, \pi_{\varepsilon}^{N,*}) + \varepsilon,
$$

$$
\exists 1 \leq i \leq N, J_{N,i}(\mu, \pi^1, \dots, \pi^N) > J_{N,i}(\mu, \pi_{\varepsilon}^{1,*}, \dots, \pi_{\varepsilon}^{N,*}) + \varepsilon.
$$

170 For any $\varepsilon > 0$, let $(\pi_{\varepsilon}^{1,*}, \ldots, \pi_{\varepsilon}^{N,*}) \in \Pi^N$ such that

l

$$
J_N(\mu, \pi_\varepsilon^{1,*}, \dots, \pi_\varepsilon^{N,*}) \ge \sup_{(\pi^1, \dots, \pi^N) \in \Pi^N} J_N(\mu, \pi^1, \dots, \pi^N) - \varepsilon,
$$
\n(2.8)

171 then $(\pi_{\varepsilon}^{1,*}, \ldots, \pi_{\varepsilon}^{N,*}) \in \Pi^N$ is an ε -Pareto Optimality in Definition 2.5.

¹⁷² 2.3. Graphon Mean-Field Control

173 We expect the cooperative MARL $(2.2)-(2.7)$ to become a GMFC problem as $N \to \infty$. 174 In GMFC, there is a continuum of agents $\alpha \in \mathcal{I}$, and each agent with the index $\alpha \in \mathcal{I}$ ¹⁷⁵ follows $\overline{\mathbf{A}}$

$$
s_0^{\alpha} \sim \mu^{\alpha}, \quad a_t^{\alpha} \sim \pi^{\alpha}(\cdot | s_t^{\alpha}, \mu_t^{\alpha, W}), \quad s_{t+1}^{\alpha} \sim P^{\alpha}(\cdot | s_t^{\alpha}, \mu_t^{\alpha, W}, a_t^{\alpha}), \tag{2.9}
$$

176 where $\mu_t^{\alpha} = \mathcal{L}(s_t^{\alpha}), \alpha \in \mathcal{I}$ denotes the probability distribution of s_t^{α} , and $\mu_t^{\alpha, W}$ is defined as 177 the neighborhood mean-field measure of agent α :

$$
\mu_t^{\alpha, W} = \int_{\mathcal{I}} W(\alpha, \beta) \mu_t^{\beta} d\beta \in \mathcal{B}(\mathcal{S}), \tag{2.10}
$$

 178 with the graphon W given in Assumption 2.1.

179 To ease the sequel analysis, define the space of state distribution ensembles \mathcal{M} := 180 $\mathcal{P}(\mathcal{S})^{\mathcal{I}} := \{f : \mathcal{I} \to \mathcal{P}(\mathcal{S})\}$ and the space of policy ensembles $\Pi := \mathcal{P}(\mathcal{A})^{\mathcal{S} \times \mathcal{I}}$. Then 181 $\boldsymbol{\mu} := (\mu^{\alpha})_{\alpha \in \mathcal{I}}$ and $\boldsymbol{\pi} := (\pi^{\alpha})_{\alpha \in \mathcal{I}}$ are elements in $\boldsymbol{\mathcal{M}}$ and $\boldsymbol{\Pi}$, respectively.

¹⁸² The objective of GMFC is to maximize the expected discounted accumulated reward 183 averaged over all agents $\alpha \in \mathcal{I}$

$$
V(\mu) : = \sup_{\pi \in \Pi} J(\mu, \pi)
$$
\n
$$
= \sup_{\pi \in \Pi} \int_{\mathcal{I}} \mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^t r^{\alpha} (s_t^{\alpha}, \mu_t^{\alpha, W}, a_t^{\alpha}) \middle| s_0^{\alpha} \sim \mu^{\alpha}, a_t^{\alpha} \sim \pi^{\alpha}(\cdot | s_t^{\alpha}, \mu_t^{\alpha, W}) \right] d\alpha.
$$
\n(2.11)

¹⁸⁴ 3. Main Results

¹⁸⁵ 3.1. Reformulation of GMFC

186 In this section, we show that GMFC $(2.9)-(2.11)$ can be reformulated as a MDP with 187 deterministic dynamics and continuous state-action space $\mathcal{M} \times \Pi$.

188 Theorem 3.1 GMFC (2.9) - (2.11) can be reformulated as

l

$$
V(\boldsymbol{\mu}) = \sup_{\boldsymbol{\pi} \in \Pi} \sum_{t=0}^{\infty} \gamma^t R(\boldsymbol{\mu}_t, \boldsymbol{\pi}(\boldsymbol{\mu}_t)),
$$
\n(3.1)

¹⁸⁹ subject to

$$
\mu_{t+1}^{\alpha}(\cdot) = \mathbf{\Phi}^{\alpha}(\boldsymbol{\mu}_t, \boldsymbol{\pi}(\boldsymbol{\mu}_t))(\cdot), \ t \in \mathbb{N}, \ \mu_0^{\alpha} = \mu^{\alpha}, \ \alpha \in \mathcal{I}, \tag{3.2}
$$

190 where the aggregated reward $R : \mathcal{M} \times \Pi \to \mathbb{R}$ and the aggregated transition dynamics Φ : 191 $\mathcal{M} \times \Pi \rightarrow \mathcal{M}$ are given by

$$
R(\boldsymbol{\mu}, \boldsymbol{\pi}(\boldsymbol{\mu})) = \int_{\mathcal{I}} \sum_{s \in \mathcal{S}} \sum_{a \in \mathcal{A}} r^{\alpha}(s, a, \mu^{\alpha, W}) \pi^{\alpha}(a|s, \mu^{\alpha, W}) \mu^{\alpha}(s) d\alpha,
$$
 (3.3)

$$
\Phi^{\alpha}(\boldsymbol{\mu}, \boldsymbol{\pi}(\boldsymbol{\mu}))(\cdot) = \sum_{s \in \mathcal{S}} \sum_{a \in \mathcal{A}} P^{\alpha}(\cdot | s, \mu^{\alpha, W}, a) \pi^{\alpha}(a | s, \mu^{\alpha, W}) \mu^{\alpha}(s).
$$
(3.4)

192 The proof of Theorem 3.1 is similar to the proof of Lemma 2.2 in [24]. So we omit it here. 193 (3.4) and (3.2) indicate the evolution of the state distribution ensemble μ_t over time. 194 That is, under the fixed policy ensemble π , the state distribution μ_{t+1}^{α} of agent α at time $t+1$ 195 is fully determined by the policy ensemble π and the state distribution ensemble μ_t at time ¹⁹⁶ t. Note that the change of population state distribution ensemble will affect neighborhood ¹⁹⁷ mean-field measure. In turn, the change of neighborhood mean-field measure will have an ¹⁹⁸ influence on population state distribution ensemble.

199 With the reformulation in Theorem 3.1, the associated Q function starting from $(\mu, \pi) \in$ 200 $\mathcal{M} \times \Pi$ is defined as

$$
Q(\boldsymbol{\mu}, \boldsymbol{\pi}) = R(\boldsymbol{\mu}, \boldsymbol{\pi}(\boldsymbol{\mu})) + \sup_{\boldsymbol{\pi}' \in \Pi} \left[\sum_{t=1}^{\infty} \gamma^t R(\boldsymbol{\mu}_t, \boldsymbol{\pi}'(\boldsymbol{\mu}_t)) \middle| s_0^{\alpha} \sim \mu^{\alpha}, a_0^{\alpha} \sim \pi^{\alpha}(\cdot | s_0^{\alpha}, \mu^{\alpha, W}) \right]
$$
(3.5)

²⁰¹ Hence its Bellman equation is given by

$$
Q(\boldsymbol{\mu}, \boldsymbol{\pi}) = R(\boldsymbol{\mu}, \boldsymbol{\pi}(\boldsymbol{\mu})) + \gamma \sup_{\boldsymbol{\pi}' \in \Pi} Q(\boldsymbol{\Phi}(\boldsymbol{\mu}, \boldsymbol{\pi}(\boldsymbol{\mu})), \boldsymbol{\pi}'). \tag{3.6}
$$

202 Remark 3.2 (Label-state formulation) GMFC (2.9) - (2.11) can be viewed as a classical MFC $_{203}$ with extended state space $\mathcal{S}\times\mathcal{I}$, action space \mathcal{A} , policy $\tilde{\pi}\in\mathcal{P}(\mathcal{A})^{\mathcal{S}\times\mathcal{I}}$, mean-field information 204 $\tilde{\mu} \in \mathcal{P}(\mathcal{S} \times \mathcal{I}),$ reward $\tilde{r}((s, \alpha), \tilde{\mu}, a) := r((s, \alpha), \int_{\mathcal{I}} W(\alpha, \beta) \tilde{\mu}(\cdot, \beta) d\beta, a),$ transition dynamics 205 of (\tilde{s}_t, α_t) such that

$$
\tilde{s}_{t+1} \sim P(\cdot | (\tilde{s}_t, \alpha_t), \tilde{a}_t, \int_{\mathcal{I}} W(\alpha_t, \beta) \tilde{\mu}_t(\cdot, \beta) d\beta), \ \alpha_{t+1} = \alpha_t, \ \tilde{a}_t \sim \tilde{\pi}(\cdot | \tilde{s}_t, \alpha_t, \int_{\mathcal{I}} W(\alpha_t, \beta) \tilde{\mu}_t(\cdot, \beta) d\beta),
$$

206 with the initial condition $\tilde{s}_0 \sim \mu_0$, $\tilde{\alpha}_0 \sim Unif(0,1)$. It is worth pointing out such a label-²⁰⁷ state formulation has also been studied in GMFG [29, 15].

²⁰⁸ 3.2. Approximation

209 In this section, we show that GMFC $(2.9)-(2.11)$ provides a good approximation for the 210 cooperative multi-agent system $(2.2)-(2.7)$ in terms of the value function and the optimal 211 policy ensemble. To do this, the following assumptions on W , P , r , and π are needed.

212 **Assumption 3.3 (graphon** W) There exists $L_W > 0$ such that for all $\alpha, \alpha', \beta, \beta' \in \mathcal{I}$

$$
|W(\alpha, \beta) - W(\alpha', \beta')| \le L_W \cdot (|\alpha - \alpha'| + |\beta - \beta'|).
$$

²¹³ Assumption 3.3 is common in graphon mean-field theory [21, 15, 29]. Indeed, the Lips- $_{214}$ chitz continuity assumption on W in Assumption 3.3 can be relaxed to piecewise Lipschitz ²¹⁵ continuity on W.

216 Assumption 3.4 (transition probability P) There exists $L_P > 0$ and $\tilde{L}_P > 0$ such that 217 for any $\alpha, \beta \in \mathcal{I}$, all $s \in \mathcal{S}$, $a \in \mathcal{A}$, $\mu_1, \mu_2 \in \mathcal{B}(\mathcal{S})$

$$
||P^{\alpha}(\cdot|s,\mu_1,a)-P^{\beta}(\cdot|s,\mu_2,a)||_1 \leq L_P \cdot ||\mu_1-\mu_2||_1 + \tilde{L}_P \cdot |\alpha-\beta|,
$$

218 where $\|\cdot\|_1$ denotes L^1 norm here and throughout the paper.

l

Assumption 3.5 (reward r) There exist $M_r > 0$, $L_r > 0$ and $\tilde{L}_r > 0$ such that for all 220 $s \in \mathcal{S}, a \in \mathcal{A}, \mu_1, \mu_2 \in \mathcal{B}(\mathcal{S}),$

$$
|r^{\alpha}(s,\mu,a)| \le M_r, \ |r^{\alpha}(s,\mu_1,a) - r^{\beta}(s,\mu_2,a)| \le L_r \cdot ||\mu_1 - \mu_2||_1 + \tilde{L}_r \cdot |\alpha - \beta|.
$$

Assumption 3.6 (policy π) There exists $L_{\text{II}} > 0$ and $\tilde{L}_{\text{II}} > 0$ such that for any policy \mathbf{z}_{222} ensemble $\boldsymbol{\pi} := (\pi^{\alpha})_{\alpha \in \mathcal{I}} \in \mathbf{\Pi}$ is Lipschitz continuous, that is, for any $\alpha, \beta \in \mathcal{I}$ and $\mu_1, \mu_2 \in \mathcal{I}$ 223 $\mathcal{B}(\mathcal{S}),$

$$
\max_{s \in \mathcal{S}} \|\pi^{\alpha}(\cdot|s,\mu_1) - \pi^{\beta}(\cdot|s,\mu_2)\|_1 \le L_{\mathbf{\Pi}} \cdot ||\mu_1 - \mu_2||_1 + \tilde{L}_{\mathbf{\Pi}} \cdot \alpha - \beta|.
$$

224 Assumptions 3.3-3.6 state that W, P, r and π are Lipschitz continuous with respect to ²²⁵ both the index of the agent and the neighborhood mean-field measure. The distance between 226 indexes $|\alpha - \beta|$ measures the similarity of agents. If P, r and π are identical, Assumptions ²²⁷ 3.4-3.6 are commonly used to bridge the multi-agent system and classical mean-field theory ²²⁸ [23, 41, 42, 43].

²²⁹ To show approximation properties of GMFC in the large-scale multi-agent system, we ²³⁰ need to relate policy ensembles of GMFC to policies of the multi-agent system. On one 231 hand, one can see that any $\pi \in \Pi$ leads to a N-agent policy tuple $(\pi^1, \ldots, \pi^N) \in \Pi^N$ with

$$
\Gamma^{N}: \mathbf{\Pi} \ni \boldsymbol{\pi} \mapsto (\pi^{1}, \dots, \pi^{N}) \in \Pi^{N}, \quad \text{with } \pi^{i} := \boldsymbol{\pi}^{\frac{i}{N}}.
$$
 (3.7)

232 On the other hand, any N-agent policy tuple $(\pi^1, \ldots, \pi^N) \in \Pi^N$ can be seen as a step 233 policy ensemble $\boldsymbol{\pi}^N$ in $\boldsymbol{\Pi}$:

$$
\boldsymbol{\pi}^{N,\alpha} := \sum_{i=1}^{N} \pi^i \mathbf{1}_{\alpha \in \left(\frac{i-1}{N}, \frac{i}{N}\right]} \in \boldsymbol{\Pi}.
$$
\n(3.8)

234 Similarly, any N-agent reward tuple (r^1, \ldots, r^N) can be regarded as a step reward function ²³⁵ of GMFC:

l

$$
r^{N,\alpha} := \sum_{i=1}^{N} r^i \mathbf{1}_{\alpha \in (\frac{i-1}{N}, \frac{i}{N}]}.
$$
\n(3.9)

236

²³⁷ Theorem 3.7 (Approximate Pareto Property) Assume Assumptions 2.1, 3.3, 3.4, 3.5 238 and 3.6. Then under either the condition $(C1)$ or $(C2)$, we have for any initial distribution 239 $\mu \in \mathcal{P}(\mathcal{S})$

$$
|V_N(\mu) - V(\mu)| \to 0, \quad \text{as } N \to \infty. \tag{3.10}
$$

Moreover, if the graphon convergence in Assumption 2.1 is at rate $\mathcal{O}(\frac{1}{\sqrt{N}})$ 240 Moreover, if the graphon convergence in Assumption 2.1 is at rate $\mathcal{O}(\frac{1}{\sqrt{N}})$, then $|V_N(\mu) |V(\mu)|\,=\, {\cal O}(\frac{1}{\sqrt{N}})$ 241 $|V(\mu)| = \mathcal{O}(\frac{1}{\sqrt{N}})$. As a consequence, for any $\varepsilon > 0$, there exists an integer N_{ε} such that 242 when $N \geq N_{\varepsilon}$, the optimal policy ensemble of GMFC denoted as π^* (if it exists) provides 243 an ε -Pareto optimality $(\pi^{1,*}, \ldots, \pi^{N,*}) := \Gamma^N(\pi^*)$ for the multi-agent system (2.7) , with Γ^N 244 *defined in* (3.7) .

 Theorem 3.7 implies that if we could compute an algorithm to learn the optimal policy ensemble of GMFC, then the learned optimal policy ensemble is close to the optimal policy of MARL. Directly learning the optimal policy of GMFC, however, will lead to high complexity 248 due to the infinite-dimensional feature of μ and π . Instead, we will introduce a smaller class of GMFC with a lower dimension in the next section, which enables a scalable algorithm.

²⁵⁰ 3.3. Algorithm Design and Convergence Analysis

251 This section will show that discretizing the graphon index $\alpha \in \mathcal{I}$ of GMFC enables to 252 approximate Q function in (3.6) by an approximated Q function in (3.11) below defined on ²⁵³ a smaller space, which is critical for designing efficient learning algorithms.

Precisely, we choose uniform grids $\alpha_m \in \mathcal{I}_M := \{\frac{m}{M}, 0 \leq m \leq M\}$ for simplicity, and 255 approximate each agent $\alpha \in \mathcal{I}$ by the nearest $\alpha_m \in \mathcal{I}_M$ close to it. Introduce $\widetilde{\mathcal{M}}_M :=$ 256 $\mathcal{P}(\mathcal{S})^{\mathcal{I}_M}$, $\overline{\mathbf{\Pi}}_M := \mathcal{P}(\mathcal{A})^{\mathcal{S} \times \mathcal{I}_M}$. Meanwhile, $\tilde{\boldsymbol{\mu}} := (\tilde{\mu}^{\alpha_m})_{m \in [M]} \in \mathcal{M}_M$ and $\tilde{\boldsymbol{\pi}} := (\tilde{\pi}^{\alpha_m})_{m \in [M]} \in$ \mathbf{I}_{M} can be viewed as a piecewise constant state distribution ensemble in **M** and a piecewise 258 constant policy ensemble in Π , respectively. Our arguments can be easily generalized to ²⁵⁹ nonuniform grids.

 Consequently, instead of performing algorithms according to (3.6) with a continuum of $_{261}$ graphon labels directly, we work with GMFC with M blocks called **block GMFC**, in which agents in the same block are homogeneous. The Bellman equation for Q function of block GMFC is given by

$$
\widetilde{Q}(\widetilde{\boldsymbol{\mu}}, \widetilde{\boldsymbol{\pi}}) = \widetilde{R}(\widetilde{\boldsymbol{\mu}}, \widetilde{\boldsymbol{\pi}}(\widetilde{\boldsymbol{\mu}})) + \gamma \sup_{\widetilde{\boldsymbol{\pi}}' \in \widetilde{\mathbf{\Pi}}_M} \widetilde{Q}(\widetilde{\boldsymbol{\Phi}}(\widetilde{\boldsymbol{\mu}}, \widetilde{\boldsymbol{\pi}}(\widetilde{\boldsymbol{\mu}})), \widetilde{\boldsymbol{\pi}}'), \tag{3.11}
$$

264 where the neighborhood mean-field measure, the aggregated reward $\tilde{R}: \tilde{M}_M \times \tilde{\Pi}_M \to \mathbb{R}$ 265 and the aggregated transition dynamics $\tilde{\Phi}: \mathcal{M}_M \times \Pi_M \to \mathcal{M}_M$ are given by

l

$$
\tilde{\mu}^{\alpha_m, W} = \frac{1}{M} \sum_{m'=0}^{M-1} W(\alpha_m, \alpha_{m'}) \tilde{\mu}^{\alpha_{m'}}, m \in [M],
$$
\n(3.12)

$$
\widetilde{R}(\widetilde{\boldsymbol{\mu}}, \widetilde{\boldsymbol{\pi}}(\widetilde{\boldsymbol{\mu}})) = \frac{1}{M} \sum_{m=0}^{M-1} \sum_{s \in \mathcal{S}} \sum_{a \in \mathcal{A}} r^{\alpha_m}(s, a, \widetilde{\mu}^{\alpha_m, W}) \widetilde{\mu}^{\alpha_m}(s) \widetilde{\pi}^{\alpha_m}(a|s, \widetilde{\mu}^{\alpha_m, W}), (3.13)
$$

$$
\widetilde{\Phi}^{\alpha_m}(\widetilde{\boldsymbol{\mu}}, \widetilde{\boldsymbol{\pi}}(\widetilde{\boldsymbol{\mu}})) (\cdot) = \sum_{s \in \mathcal{S}} \sum_{a \in \mathcal{A}} P^{\alpha_m}(\cdot | s, a, \widetilde{\mu}^{\alpha_m, W}) \widetilde{\mu}^{\alpha_m}(s) \widetilde{\pi}^{\alpha_m}(a | s, \widetilde{\mu}^{\alpha_m, W}). \tag{3.14}
$$

266 We see from (3.11) that block GMFC is a MDP with deterministic dynamics $\widetilde{\Phi}$ and ²⁶⁷ continuous state-action space $\mathcal{M}_M \times \Pi_M$. The following Theorem shows that there exists 268 an optimal policy ensemble of block GMFC in $\overline{\mathbf{\Pi}}_M$.

²⁶⁹ Theorem 3.8 (Existence of Optimal Policy Ensemble) Given Assumptions 3.4, 3.5, $_2$ zo assume $\gamma\cdot(1+L_P+L_{\Pi})<\infty,$ then for any fixed integer $M>0,$ there exists an $\tilde{\bm{\pi}}^*\in \bm{\Pi}_M$ 271 that maximize $\widetilde{Q}(\widetilde{\boldsymbol{\mu}}, \widetilde{\boldsymbol{\pi}})$ in (3.11) for any $\widetilde{\boldsymbol{\mu}} \in \mathcal{M}_M$.

 272 Furthermore, we show that with sufficiently fine partitions of the graphon index \mathcal{I} , i.e., 273 M is sufficiently large, block GMFC $(3.11)-(3.14)$ well approximates the multi-agent system ²⁷⁴ in Section 2.2.

275 **Theorem 3.9** Assume $\gamma \cdot (1 + L_P + L_{\Pi}) < \infty$ and Assumptions 2.1, 3.3, 3.4, 3.5 and 276 3.6. Under either (C1) or (C2), for any $\varepsilon > 0$, there exists N_{ε} , M_{ε} such that for $N \ge N_{\varepsilon}$, $_{{\tt s}77}$ the optimal policy ensemble $\tilde{\bm{\pi}}^*$ of block GMFC (3.11) with M_ε blocks provides an ε-Pareto 278 optimality $(\tilde{\pi}^{1,*}, \ldots, \tilde{\pi}^{N,*}) := \Gamma^N(\tilde{\pi}^*)$ for the multi-agent system (2.7) with N agents.

 Theorem 3.9 shows that the optimal policy ensemble of block GMFC is near-optimal for all sufficiently large multi-agent systems, meaning that block GMFC provides a good approximation for the multi-agent system. Therefore, If we could develop an algorithm for block GMFC to extract an optimal policy ensemble of block GMFC, then the extracted policy is near optimal for MARL.

284 When model parameters P^{α}, r^{α} and W are known, one can easily extract the optimal 285 policy based on Bellman equation. If any of these model parameters P^{α}, r^{α} and W is ²⁸⁶ unknown, we take a model-free approach. The key issue is to handle population state 287 distribution ensemble $\tilde{\mu}$, which is an input of Q function in (3.11). We assume that we 288 have a block GMFC simulator $\mathcal{G}(\tilde{\mu}, \tilde{\pi}) = (\tilde{\mu}', R)$. That is, for any pair of population state distribution ensemble and policy ensemble $(\tilde{\mu}, \tilde{\pi})$, we can sample the aggregated reward \tilde{R} 290 and the next population state distribution ensemble $\tilde{\mu}'$. To learn the optimal policy of block ²⁹¹ GMFC, one can adopt any existing techniques for standard MFC, such as a kernel-based Q ²⁹² learning method in [23] and a uniform discretization method in [9].

293 Remark 3.10 If we can only observe the state of agent $\alpha_m \in \mathcal{I}_M$ and do not have access to 294 population state distribution ensemble, we can estimate $\tilde{\mu}^{\alpha_m}$ following [2] or [42]. However, 295 different from [2] and [42], we also need to estimate $\tilde{\mu}^{\alpha_m,W}$ due to the graphon structure W ²⁹⁶ and leave it for future study.

 We choose to adapt DRL algorithm neural Proximal Policy Optimization (PPO) [47, 38] to block GMFC given in Algorithm 1. Following Corollary 4.11 in [38], together with Theorem 3.9, we can state the global convergence of neural PPO for block GMFC. Since assumptions that make the result hold are similar as [38], we do not state these assumptions ³⁰¹ here.

Algorithm 1 Neural PPO for block GMFC

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Input Width of neural network M, radius of constraint R, number of SGD and TD iterations T, number of PPO iteration K, penalty parameter β Initialize for $k = 0$ to $K - 1$ do set temperature parameter $\tau_{k+1} \leftarrow \frac{\beta \sqrt{K}}{k+1}$ and penalty parameter $\beta_k \leftarrow \beta \sqrt{K}$. Sample $(\tilde{\boldsymbol{\mu}}_t, \tilde{\boldsymbol{\pi}}_t, \tilde{\boldsymbol{\mu}}_t', \tilde{\boldsymbol{\pi}}_t')_{t=1}^T$ with $\tilde{\boldsymbol{\pi}}_0 \sim \Pi^0(\cdot | \tilde{\boldsymbol{\mu}})$, $\tilde{\boldsymbol{\mu}}_t' = \tilde{\boldsymbol{\Phi}}(\tilde{\boldsymbol{\mu}}_t, \tilde{\boldsymbol{\pi}}_t)$, $\tilde{\boldsymbol{\pi}}_t \sim \Pi^{\theta_k}(\cdot | \tilde{\boldsymbol{\mu}}_t)$. Solve for Q function parameterized by neural network $Q_{\omega_k} = NN(\omega_k, M)$ using the TD update. Solve for energy function parameterized by neural network $f_{\theta_{k+1}} = NN(\theta_{k+1}, M)$

using the SGD update.

Update policy: $\Pi^{\theta_k} \propto \exp(\tau_{k+1}^{-1} f_{\theta_{k+1}}).$ end for

Theorem 3.11 Suppose that Assumptions 2.1, 3.3, 3.4, 3.5 and 3.6 hold. Further assume $\gamma \cdot (1 + L_{\Pi} + L_P) < 1$. Furthermore, suppose that the width of neural network is sufficiently large. For any $\varepsilon > 0$, there exists M_{ε} and N_{ε} such that for any $M \geq M_{\varepsilon}$ and $N \geq N_{\varepsilon}$, and the policy attained by Algorithm 1 denoted as π_{PPO}

$$
|J_N(\mu; \pi^{1, *}, \dots, \pi^{N, *}) - \tilde{J}^M(\mu; \pi_{PPO})| \le \frac{C}{\sqrt{K}} + \bar{C}\varepsilon,
$$
\n(3.15)

302 where J_N and \tilde{J}^M are given in (2.7) and (4.7) respectively, K is the number of iteration, C 303 and \bar{C} are constants.

By setting $K = \frac{C}{c^2}$ 304 By setting $K = \frac{C}{\epsilon^2}$, the optimal empirical value function of MARL is approximated by the 305 value function of block GMFC under the learned policy in Algorithm 1 with the error $\mathcal{O}(\varepsilon)$. In other words, Theorem 3.11 states that, with a sample complexity of $\mathcal{O}(\frac{1}{\varepsilon^2})$ 306 In other words, Theorem 3.11 states that, with a sample complexity of $\mathcal{O}(\frac{1}{\varepsilon^2})$, Algorithm 1 307 generates a $\mathcal{O}(\varepsilon)$ -Pareto optimality of cooperative MARL.

³⁰⁸ To evaluate the performance of Algorithm 1 and to validate our theoretical findings, we ³⁰⁹ describe the deployment of block GMFC in the multi-agent system in Algorithm 2, which ³¹⁰ we call it N-agent GMFC.

Algorithm 2 N-agent GMFC

Input Initial state distribution μ_0 , number of agents N, episode length T, the learned policy $\tilde{\pi} \in \Pi_M$ learned by PPO Initialize $s_0^i \sim \mu_0, i \in [N]$ for $t = 1$ to T do for $i = 1$ to N do Choose $m(i) = \arg \min_{i} |\frac{i}{N} - \frac{m}{M}|$ $m \in [M]$ Sample action $a_t^i \sim \tilde{\pi}^{\alpha_{m(i)}}(\cdot | s_t^i)$, observe reward r_t^i and new state s_{t+1}^i end for end for

³¹¹ 4. Proofs of Main Results

³¹² In this section, we will provide proofs of Theorems 3.7-3.9.

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³¹³ 4.1. Proof of Theorem 3.7

³¹⁴ To prove Theorem 3.7, we need the following two Lemmas. We start by defining the 315 step state distribution $\boldsymbol{\mu}_t^N := (\mu_t^{N,\alpha})_{\alpha \in \mathcal{I}}$ for notational simplicity

$$
\mu_t^{N,\alpha}(\cdot) = \sum_{i \in \mathcal{V}_N} \delta_{s_t^i}(\cdot) \mathbf{1}_{\alpha \in (\frac{i-1}{N}, \frac{i}{N}]}.
$$
\n(4.1)

³¹⁶ Lemma 4.1 shows the convergence of the neighborhood empirical measure to the neigh-³¹⁷ borhood mean-field measure.

³¹⁸ Lemma 4.1 Assume Assumptions 2.1, 3.3, 3.4 and 3.6. Under either condition (C1) or 319 (C2), for any policy ensemble $\pi \in \Pi$, we have

$$
\sum_{i=1}^{N} \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \mathbb{E}\big[\|\mu_t^{i, W_N} - \mu_t^{\alpha, W}\|_1\big] d\alpha \to 0, \quad \text{as } N \to \infty,
$$
\n(4.2)

320 where $\mu_t^i = \mu_t^{\alpha} \equiv \mu \in \mathcal{P}(\mathcal{S})$.

Moreover, if the graphon convergence in Assumption 2.1 is at rate $\mathcal{O}(\frac{1}{\sqrt{l}})$ $\frac{1}{\overline{N}}$, then

$$
\sum_{i=1}^N\int_{(\frac{i-1}{N},\frac{i}{N}]}\mathbb{E}\big[\|\mu^{i,W_N}_t-\mu_t^{\alpha,W}\|_1\big]d\alpha=\mathcal O(\frac{1}{\sqrt{N}}).
$$

321 **Proof of Lemma 4.1** We first prove (4.2) under the condition (Cl) and then show (4.2) 322 also holds under the condition $(C2)$.

Case 1: $\xi_{i,j}^N = W_N(\frac{i}{N},\frac{j}{N})$ 323 **Case 1:** $\xi_{i,j}^N = W_N(\frac{i}{N}, \frac{j}{N})$. Note that under the condition (C1), $\mu_t^{i,W_N} = \int_{\mathcal{I}} W_N(\frac{i}{N}, \beta) \mu_t^{N, \beta} d\beta$ ³²⁴ by the definition of $\mu_t^{N,\alpha}$ in (4.1). Then

l

$$
\begin{array}{lcl} & \displaystyle \sum_{i=1}^{N}\int_{(\frac{i-1}{N},\frac{i}{N}]} \mathbb{E}\big[\|\mu^{i,W_N}_t - \mu^{ \alpha,W}_t\|_1\big] d\alpha \\ \\ & = & \displaystyle \sum_{i=1}^{N}\int_{(\frac{i-1}{N},\frac{i}{N}]} \mathbb{E}\Big[\Big\|\int_{\mathcal{I}} W_N(\frac{i}{N},\beta)\mu^{N,\beta}_t d\beta - \int_{\mathcal{I}} W(\alpha,\beta)\mu^{\beta}_t d\beta\Big\|_1\Big] d\alpha \\ \\ & \leq & \displaystyle \sum_{i=1}^{N}\int_{(\frac{i-1}{N},\frac{i}{N}]} \mathbb{E}\Big[\Big\|\int_{\mathcal{I}} W_N(\frac{i}{N},\beta)\mu^{N,\beta}_t d\beta - \int_{\mathcal{I}} W_N(\frac{i}{N},\beta)\mu^{\beta}_t d\beta\Big\|_1\Big] d\alpha \\ & & + \displaystyle \sum_{i=1}^{N}\int_{(\frac{i-1}{N},\frac{i}{N}]} \mathbb{E}\Big[\Big\|\int_{\mathcal{I}} W_N(\frac{i}{N},\beta)\mu^{\beta}_t d\beta - \int_{\mathcal{I}} W(\alpha,\beta)\mu^{\beta}_t d\beta\Big\|_1\Big] d\alpha \\ \\ & = & : I_1 + I_2. \end{array}
$$

 325 For the term I_1 , we adapt Theorem 2 that works with local policy in [15] to our setting of 326 global policy and have that under the policy ensemble π and N-agent policy $(\pi^1, \ldots, \pi^N) :=$ 327 $\Gamma_N(\pi)$, with Γ_N defined in (3.7)

$$
I_1=\mathbb{E}\Big[\Big\|\int_\mathcal{I}W_N(\frac{i}{N},\beta)\mu_t^{N,\beta}d\beta-\int_\mathcal{I}W_N(\frac{i}{N},\beta)\mu_t^\beta d\beta\Big\|_1\Big]\rightarrow 0, \text{ as } N\rightarrow\infty.
$$

Moreover, if the graphon convergence in Assumption 2.1 is at rate $\mathcal{O}(\frac{1}{\sqrt{N}})$ 328 Moreover, if the graphon convergence in Assumption 2.1 is at rate $\mathcal{O}(\frac{1}{\sqrt{N}})$, then the term I_1 is also at rate $\mathcal{O}(\frac{1}{\sqrt{l}})$ 329 I_1 is also at rate $\mathcal{O}(\frac{1}{\sqrt{N}})$.

330 By noting that $W_N(\alpha, \beta) = W_N\left(\frac{\lceil N\alpha \rceil}{N}, \frac{\lceil N\beta \rceil}{N}\right),$

∢

$$
I_2 = \sum_{i=1}^N \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \left\| \int_{\mathcal{I}} W_N\left(\frac{[N\alpha]}{N}, \beta\right) \mu_t^{\beta} d\beta - \int_{\mathcal{I}} W(\alpha, \beta) \mu_t^{\beta} d\beta \right\|_1 d\alpha
$$

\n
$$
= \sum_{i=1}^N \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \left\| \int_{\mathcal{I}} W_N(\alpha, \beta) \mu_t^{\beta} d\beta - \int_{\mathcal{I}} W(\alpha, \beta) \mu_t^{\beta} d\beta \right\|_1 d\alpha
$$

\n
$$
= \int_{\mathcal{I}} \left\| \int_{\mathcal{I}} W_N(\alpha, \beta) \mu_t^{\beta} d\beta - \int_{\mathcal{I}} W(\alpha, \beta) \mu_t^{\beta} d\beta \right\|_1 d\alpha
$$

\n
$$
= \sum_{s \in \mathcal{S}} \int_{\mathcal{I}} \left| \int_{\mathcal{I}} W_N(\alpha, \beta) \mu_t^{\beta}(s) d\beta - \int_{\mathcal{I}} W(\alpha, \beta) \mu_t^{\beta}(s) d\beta \right| d\alpha
$$

\n
$$
\rightarrow 0,
$$

where the last inequality is from the fact in [39] that the convergence of $||W_N - W||_{\square} \to 0$ is equivalent to the convergence of

$$
||W_N - W||_{L_{\infty} \to L_1} := \sup_{||g||_{\infty} \le 1} \int_{\mathcal{I}} \left| \int_{\mathcal{I}} \left(W_N(\alpha, \beta) - W(\alpha, \beta) \right) g(\beta) d\beta \right| d\alpha \to 0.
$$

331 Combining I_1 and I_2 , we prove (4.2) under the condition $(C1)$.

l

Case 2: $\xi_{i,j}^N$ are random variables with Bernoulli $(W_N(\frac{i}{N},\frac{j}{N}))$ 1 \quad \quad \quad \quad \quad \qquad \qquad

$$
\begin{array}{lcl} & \displaystyle \sum_{i=1}^{N}\int_{(\frac{i-1}{N},\frac{i}{N}]} \mathbb{E}\|\mu_{t}^{i,W_{N}}-\mu_{t}^{\alpha,W}\|_{1}d\alpha\\[2mm] & = & \displaystyle \sum_{i=1}^{N}\int_{(\frac{i-1}{N},\frac{i}{N}]} \mathbb{E}\|\frac{1}{N}\sum_{j=1}^{N}\xi_{ij}^{N}\delta_{s_{t}^{j}}-\int_{\mathcal{I}}W(\alpha,\beta)\mu_{t}^{\beta}d\beta\|_{1}d\alpha\\[2mm] & \leq & \displaystyle \sum_{i=1}^{N}\int_{(\frac{i-1}{N},\frac{i}{N}]} \mathbb{E}\|\frac{1}{N}\sum_{j=1}^{N}\xi_{ij}^{N}\delta_{s_{t}^{j}}-\int_{\mathcal{I}}W_{N}(\frac{i}{N},\beta)\mu_{t}^{N,\beta}d\beta\|_{1}d\alpha\\[2mm] & & +\displaystyle \sum_{i=1}^{N}\int_{(\frac{i-1}{N},\frac{i}{N}]} \mathbb{E}\|\int_{\mathcal{I}}W_{N}(\frac{i}{N},\beta)\mu_{t}^{N,\beta}d\beta-\int_{\mathcal{I}}W(\alpha,\beta)\mu_{t}^{\beta}d\beta\|_{1}d\alpha\\[2mm] & =: & I_{1}+I_{2}. \end{array}
$$

Note from **Case 1** that $I_2 \to 0$ as $N \to \infty$ and $I_2 = \mathcal{O}(\frac{1}{\sqrt{N}})$ 333 Note from **Case 1** that $I_2 \to 0$ as $N \to \infty$ and $I_2 = \mathcal{O}(\frac{1}{\sqrt{N}})$ if the graphon convergence in Assumption 2.1 is at rate $\mathcal{O}(\frac{1}{\sqrt{l}})$ 334 Assumption 2.1 is at rate $\mathcal{O}(\frac{1}{\sqrt{N}})$. Therefore, it is enough to estimate I_1 .

$$
I_1 = \mathbb{E} \Big\| \frac{1}{N} \sum_{j=1}^N \xi_{ij}^N \delta_{s_t^j} - \int_{\mathcal{I}} W_N(\frac{i}{N}, \beta) \mu_t^{N, \beta} d\beta \Big\|_1
$$

$$
\leq \mathbb{E} \Big[\mathbb{E} \Big[\sup_{f: \mathcal{S} \to \{-1, 1\}} \Big\{ \frac{1}{N} \sum_{j=1}^N \xi_{ij}^N f(s_t^j) - \frac{1}{N} \sum_{j=1}^N W_N(\frac{i}{N}, \frac{j}{N}) f(s_t^j) \Big\} \Big| s_t^1, \dots, s_t^N \Big] \Big].
$$

³³⁵ We proceed the same argument as in the proof of Theorem 6.3 in [23]. Precisely, conditioned on s_t^1, \ldots, s_t^N , $\left\{ \xi_{ij}^N f(s_t^j) - W_N(\frac{i}{N}, \frac{j}{N}) \right\}$ $\frac{j}{N}$) $f(s_t^j)$ $\Big\}_{i=1}^N$ 336 on $s_t^1,\ldots,s_t^N, \; \left\{\xi_{ij}^Nf(s_t^j)-W_N(\frac{v}{N},\frac{j}{N})f(s_t^j)\right\}_{j=1}$ is a sequence of independent mean-zero random variables bounded in [-1, 1] due to $\mathbb{E}[\xi_{i,j}^N] = W_N(\frac{i}{N}, \frac{j}{N})$ 337 random variables bounded in $[-1, 1]$ due to $\mathbb{E}[\xi_{i,j}^N] = W_N(\frac{i}{N}, \frac{j}{N})$. This implies that each $\xi_{ij}^N f(s_t^j) - W_N(\frac{i}{N}, \frac{j}{N})$ 338 $\xi_{ij}^N f(s_t^j) - W_N(\frac{i}{N}, \frac{j}{N}) f(s_t^j)$ is a sub-Gaussian with variance bounded by 4. As a result, conditioned on s_t^1, \ldots, s_t^N , $\left\{ \frac{1}{N} \sum_{j=1}^N \xi_{ij}^N f(s_t^j) - \frac{1}{N} \sum_{j=1}^N W_N(\frac{i}{N}, \frac{j}{N}) \right\}$ $\frac{j}{N}$) $f(s_t^j)$ $\Big\}_{i=1}^N$ 339 conditioned on $s_t^1, \ldots, s_t^N, \left\{\frac{1}{N}\sum_{j=1}^N \xi_{ij}^N f(s_t^j) - \frac{1}{N}\sum_{j=1}^N W_N(\frac{i}{N}, \frac{j}{N}) f(s_t^j)\right\}_{i=1}$ is a mean-zero $\frac{4}{N}$. By the equation (2.66) in [51], we have

$$
I_1 \leq \mathbb{E}\Big[\mathbb{E}\Big[\sup_{f:\mathcal{S}\to\{-1,1\}}\Big\{\frac{1}{N}\sum_{j=1}^N\xi_{ij}^Nf(s_t^j) - \frac{1}{N}\sum_{j=1}^NW_N(\frac{i}{N},\frac{j}{N})f(s_t^j)\Big\}\Big|s_t^1,\ldots,s_t^N\Big]\Big] \leq \frac{\sqrt{8\ln(2)|\mathcal{S}|}}{\sqrt{N}}.
$$

341 Therefore, combining I_1 and I_2 in **Case 2**, we show that when $\xi_{i,j}^N$ are random variables with Bernoulli $(W_N(\frac{i}{N}, \frac{j}{N}))$ 342 with Bernoulli $(W_N(\frac{i}{N}, \frac{j}{N}))$, (4.2) holds under the condition (C2).

³⁴³ Lemma 4.2 shows the convergence of the state distribution of N-agent game to the state ³⁴⁴ distribution of GMFC.

³⁴⁵ Lemma 4.2 Assume Assumptions 2.1, 3.3, 3.4 and 3.6. For any uniformly bounded family 346 G of functions $g^{\alpha}: \mathcal{S} \to \mathbb{R}$, we have

l

$$
\sup_{\{g^{\alpha}\}_{\alpha\in\mathcal{I}}\in\mathcal{G}}\sum_{i=1}^{N}\int_{(\frac{i-1}{N},\frac{i}{N}]} \left| \mathbb{E}[g^{\alpha}(s_i^i) - g^{\alpha}(s_i^{\alpha})] \right| d\alpha \to 0,
$$
\n(4.3)

where $s_0^i \sim \mu_0$, $s_0^{\alpha} \sim \mu_0$. Moreover, if the graphon convergence in Assumption 2.1 is at rate $\mathcal{O}(\frac{1}{\sqrt{l}}$ $\frac{1}{\overline{N}}$), then

$$
\sup_{\{g^{\alpha}\}_{\alpha\in\mathcal{I}}\in\mathcal{G}}\sum_{i=1}^{N}\int_{(\frac{i-1}{N},\frac{i}{N}]} \left|\mathbb{E}[g^{\alpha}(s_t^i)-g^{\alpha}(s_t^{\alpha})]\right|d\alpha=\mathcal{O}(\frac{1}{\sqrt{N}}).
$$

347 Proof of Lemma 4.2 The proof is by induction as follows. To do this, first introduce

$$
l_{g^{\alpha}}^{\beta}(s,\mu,\pi) := \sum_{a \in \mathcal{A}} \sum_{s' \in \mathcal{S}} g^{\alpha}(s') P^{\beta}(s'|s,\mu,a)\pi(a|s,\mu).
$$

348 (4.3) holds obviously at $t = 0$. Suppose that (4.3) holds at t. Then for any uniformly 349 bounded function g^{α} with $|g^{\alpha}| \leq M_g$ at $t + 1$

$$
\sum_{i=1}^{N} \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \left| \mathbb{E}[g^{\alpha}(s_{t+1}^{i}) - g^{\alpha}(s_{t+1}^{\alpha})] \right| d\alpha
$$
\n
$$
= \sum_{i=1}^{N} \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \left| \mathbb{E}\left[l_{g^{\alpha}}^{\frac{i}{N}}(s_{t}^{i}, \mu_{t}^{i, W_{N}}, \pi^{i})\right] - \mathbb{E}\left[l_{g^{\alpha}}^{\alpha}(s_{t}^{\alpha}, \mu_{t}^{\alpha, W}, \pi^{\alpha})\right] \right| d\alpha
$$
\n
$$
\leq \sum_{i=1}^{N} \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \left| \mathbb{E}\left[l_{g^{\alpha}}^{\frac{i}{N}}(s_{t}^{i}, \mu_{t}^{i, W_{N}}, \pi^{i})\right] - \mathbb{E}\left[l_{g^{\alpha}}^{\alpha}(s_{t}^{i}, \mu_{t}^{\alpha, W}, \pi^{i})\right] \right| d\alpha
$$
\n
$$
+ \sum_{i=1}^{N} \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \left| \mathbb{E}\left[l_{g^{\alpha}}^{\alpha}(s_{t}^{i}, \mu_{t}^{\alpha, W}, \pi^{i})\right] - \mathbb{E}\left[l_{g^{\alpha}}^{\alpha}(s_{t}^{\alpha}, \mu_{t}^{\alpha, W}, \pi^{i})\right] \right| d\alpha
$$
\n
$$
+ \sum_{i=1}^{N} \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \left| \mathbb{E}\left[l_{g^{\alpha}}^{\alpha}(s_{t}^{\alpha}, \mu_{t}^{\alpha, W}, \pi^{i})\right] - \mathbb{E}\left[l_{g^{\alpha}}^{\alpha}(s_{t}^{\alpha}, \mu_{t}^{\alpha, W}, \pi^{\alpha})\right] \right| d\alpha
$$
\n
$$
= : I + II + III,
$$
\n(4.4)

³⁵⁰ where the first equality is by the law of total expectation.

 λ

First term of (4.4) .

$$
\begin{array}{lcl} I & = & \displaystyle \sum_{i=1}^N \int_{(\frac{i-1}{N}, \frac{i}{N}]} \bigg| \mathbb{E} \big[l_{g^{\alpha}}^{\frac{i}{N}}(s_t^i, \mu_t^{i, W_N}, \pi^i) \big] - \mathbb{E} \big[l_{g^{\alpha}}^{\alpha}(s_t^i, \mu_t^{\alpha, W}, \pi^i) \big] \bigg| d\alpha \\ \\ & \leq & M_g \Big(L_P \sum_{i=1}^N \int_{(\frac{i-1}{N}, \frac{i}{N}]} \mathbb{E} \big[\| \mu_t^{i, W_N} - \mu_t^{\alpha, W} \|_1 \big] d\alpha + \tilde{L}_P \sum_{i=1}^N \int_{(\frac{i-1}{N}, \frac{i}{N}]} |\alpha - \frac{i}{N}| d\alpha \Big) \\ \\ & \to & 0, \quad \text{as } N \to \infty \end{array}
$$

 351 where the second inequality is from the continuity of P , and the last inequality is from ³⁵² Lemma 4.1.

353 Second term of (4.4). One can view $l_{g}^{\alpha}(s, \mu_t^{\alpha,W}, \pi^i)$ as a function of $s \in S$ for any fixed 354 $\mu_t^{\alpha,W}$ and $\pi^i, \alpha \in \mathcal{I}$. Note that $|l_{g^{\alpha}}^{\alpha}(s, \mu_t^{\alpha,W}, \pi^i)| \leq M_g$, where M_g is a constant independent 355 of $\mu_t^{\alpha,W}$, π^i . Since (4.3) holds at t, then

l

$$
\begin{array}{rcl}\nII & = & \displaystyle \sum_{i=1}^{N} \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \left| \mathbb{E} \left[l^{\alpha}_{g^{\alpha}}(s_t^i, \mu_t^{\alpha, W}, \pi^i) \right] - \mathbb{E} \left[l^{\alpha}_{g^{\alpha}}(s_t^{\alpha}, \mu_t^{\alpha, W}, \pi^i) \right] \right| d\alpha \\
& \to & 0, \quad \text{as } N \to \infty.\n\end{array}
$$

Third term of (4.4).

$$
\begin{array}{lcl} III & = & \displaystyle \sum_{i=1}^N \int_{(\frac{i-1}{N}, \frac{i}{N}]} \left| \mathbb{E} \big[l^{\alpha}_{g^{\alpha}}(s^{\alpha}_t, \mu^{\alpha, W}_t, \pi^i) \big] - \mathbb{E} \big[l^{\alpha}_{g^{\alpha}}(s^{\alpha}_t, \mu^{\alpha, W}_t, \pi^{\alpha}) \big] \right| d\alpha \\ \\ & \leq & M_g \sum_{i=1}^N \int_{(\frac{i-1}{N}, \frac{i}{N}]} \mathbb{E} \big[\| \pi^i(s^{\alpha}_t) - \pi^{\alpha}(s^{\alpha}_t) \|_1 \big] d\alpha \\ \\ & \leq & M_g L_\Pi \sum_{i=1}^N \int_{(\frac{i-1}{N}, \frac{i}{N}]} \max_{\alpha \in (\frac{i-1}{N}, \frac{i}{N}]} |\frac{i}{N} - \alpha| d\alpha \\ \\ & = & \mathcal{O}(\frac{1}{N}), \end{array}
$$

 356 where the second inequality is by the uniform boundedness of g and the third inequality is 357 from Assumption 3.6.

Now we are ready to prove Theorem 3.7. We start by defining \hat{r}^{α} the aggregated reward 359 over all possible actions under the policy π

$$
\widehat{r}^{\alpha}(s,\mu,\pi) := \sum_{a \in \mathcal{A}} r^{\alpha}(s,\mu,a)\pi(a|s,\mu).
$$

l

Proof of Theorem 3.7

$$
|V_{N}(\mu) - V(\mu)|
$$
\n
$$
= \left| \sup_{\Pi^{N}} \frac{1}{N} \sum_{i=1}^{N} \mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^{t} r^{i} (s_{t}^{i}, \mu_{t}^{i, W_{N}}, a_{t}^{i}) \right] - \sup_{\pi \in \Pi} \int_{\mathcal{I}} \mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^{t} r^{\alpha} (s_{t}^{\alpha}, \mu_{t}^{\alpha, W}, a_{t}^{\alpha}) \right] d\alpha \right|
$$
\n
$$
\leq \sup_{\pi \in \Pi} \left| \frac{1}{N} \sum_{i=1}^{N} \mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^{t} r^{i} (s_{t}^{i}, \mu_{t}^{i, W_{N}}, a_{t}^{i}) \right] - \int_{\mathcal{I}} \mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^{t} r^{\alpha} (s_{t}^{\alpha}, \mu_{t}^{\alpha, W}, a_{t}^{\alpha}) \right] d\alpha \right|
$$
\n
$$
= \sup_{\pi \in \Pi} \left| \sum_{t=0}^{\infty} \gamma^{t} \sum_{i=1}^{N} \int_{(\frac{i-1}{N}, \frac{i}{N}]} \left(\mathbb{E} [\tilde{r}^{i} (s_{t}^{i}, \mu_{t}^{i, W_{N}}, \pi^{i})] - \mathbb{E} [\tilde{r}^{\alpha} (s_{t}^{\alpha}, \mu_{t}^{\alpha, W}, \pi^{\alpha})] \right) d\alpha \right|
$$
\n
$$
\leq \sup_{\pi \in \Pi} \left| \sum_{t=0}^{\infty} \gamma^{t} \sum_{i=1}^{N} \int_{(\frac{i-1}{N}, \frac{i}{N}]} \left(\mathbb{E} [\tilde{r}^{i} (s_{t}^{i}, \mu_{t}^{i, W_{N}}, \pi^{i})] - \mathbb{E} [\tilde{r}^{\alpha} (s_{t}^{i}, \mu_{t}^{\alpha, W}, \pi^{i})] \right) d\alpha \right|
$$
\n
$$
+ \sup_{\pi \in \Pi} \left| \sum_{t=0}^{\infty} \gamma^{t} \sum_{i=1}
$$

360 where we use (3.8) in the second inequality.

First term of (4.5) .

$$
I = \sup_{\pi \in \mathbf{\Pi}} \Big| \sum_{t=0}^{\infty} \gamma^{t} \sum_{i=1}^{N} \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \mathbb{E} \Big[\hat{r}^{i}(s_{t}^{i}, \mu_{t}^{i,W_{N}}, \pi^{i}) \Big] - \mathbb{E} \Big[\hat{r}^{\alpha}(s_{t}^{i}, \mu_{t}^{\alpha,W}, \pi^{i}) \Big] \Big) d\alpha \Big|
$$

\n
$$
= \sup_{\pi \in \mathbf{\Pi}} \Big| \sum_{t=0}^{\infty} \gamma^{t} \sum_{i=1}^{N} \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \left(\mathbb{E} \Big[\hat{r}^{i}(s_{t}^{i}, \mu_{t}^{i,W_{N}}, \pi^{i}) \Big] - \mathbb{E} \Big[\hat{r}^{i}(s_{t}^{i}, \mu_{t}^{\alpha,W}, \pi^{i}) \Big] \Big) d\alpha \Big|
$$

\n
$$
+ \sup_{\pi \in \mathbf{\Pi}} \Big| \sum_{t=0}^{\infty} \gamma^{t} \sum_{i=1}^{N} \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \left(\mathbb{E} \Big[\hat{r}^{i}(s_{t}^{i}, \mu_{t}^{\alpha,W}, \pi^{i}) \Big] - \mathbb{E} \Big[\hat{r}^{\alpha}(s_{t}^{i}, \mu_{t}^{\alpha,W}, \pi^{i}) \Big] \right) d\alpha \Big|
$$

\n
$$
\leq \sup_{\pi} L_{r} \sum_{t=0}^{\infty} \gamma^{t} \sum_{i=1}^{N} \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \mathbb{E} \Big[\mu_{t}^{i,W_{N}} - \mu_{t}^{\alpha,W} \Big|_{1} d\alpha + \sup_{\pi} \tilde{L}_{r} \sum_{t=0}^{\infty} \gamma^{t} \sum_{i=1}^{N} \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \Big| \frac{i}{N} - \alpha | d\alpha \Big|
$$

\n
$$
= \mathcal{O}(\frac{1}{\sqrt{N}}), \tag{4.6}
$$

³⁶¹ where the last equality is from Lemma 4.1 when the convergence in Assumption 2.1 is at 362 rate $\mathcal{O}(1/\sqrt{N}).$

Second term of (4.5). From Lemma 4.2, we have $II = \mathcal{O}(\frac{1}{\sqrt{I}})$ 363 Second term of (4.5). From Lemma 4.2, we have $II = \mathcal{O}(\frac{1}{\sqrt{N}})$. Third term of (4.5).

$$
III \leq \sup_{\pi} L_r \sum_{t=0}^{\infty} \gamma^t \sum_{i=1}^N \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \max_{s \in S} \|\pi^i(s) - \pi^{\alpha}(s)\|_1 d\alpha
$$

$$
\leq L_r \tilde{L}_{\Pi} \sup_{\pi} \sum_{t=0}^{\infty} \gamma^t \sum_{i=1}^N \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \left|\frac{i}{N} - \alpha\right| d\alpha
$$

$$
= O(\frac{1}{N}).
$$

 364 Therefore, combining I, II and III yields the desired result. \Box

l

³⁶⁵ 4.2. Proof of Theorem 3.8

³⁶⁶ First, we see that (3.11) corresponds to the following optimal control problem

$$
\widetilde{V}^{M}(\widetilde{\mu}) := \sup_{\widetilde{\pi} \in \widetilde{\Pi}_{M}} \widetilde{J}^{M}(\widetilde{\mu}, \widetilde{\pi})
$$
\n
$$
= \sup_{\widetilde{\pi} \in \widetilde{\Pi}_{M}} \frac{1}{M} \sum_{m=1}^{M} \mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^{t} r\left(\widetilde{s}_{t}^{\alpha_{m}}, \widetilde{\mu}_{t}^{\alpha_{m}, W}, \widetilde{a}_{t}^{\alpha_{m}}\right) \Big| \widetilde{s}_{0}^{\alpha_{m}} \sim \widetilde{\mu}^{\alpha_{m}}, \widetilde{a}_{t}^{\alpha_{m}} \sim \widetilde{\pi}^{\alpha_{m}}(\cdot | \widetilde{s}_{t}^{\alpha_{m}}) \right] (4.7)
$$

 367 The associated Q function of (4.7) is defined as

$$
\tilde{Q}(\tilde{\boldsymbol{\mu}}, \tilde{\boldsymbol{\pi}}) = \sup_{\tilde{\boldsymbol{\pi}}'} \frac{1}{M} \sum_{m=1}^{M} \mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^{t} r(\tilde{s}_{t}^{\alpha_{m}}, \tilde{\mu}_{t}^{\alpha_{m}, W}, \tilde{a}_{t}^{\alpha_{m}}) \middle| \tilde{s}_{0}^{\alpha_{m}} \sim \tilde{\mu}^{\alpha_{m}}, \tilde{a}_{0}^{\alpha_{m}} \sim \tilde{\pi}^{\alpha_{m}}(\cdot | \tilde{s}_{t}^{\alpha_{m}}) \right]
$$
\n
$$
= R(\tilde{\boldsymbol{\mu}}, \tilde{\boldsymbol{\pi}}) + \sup_{\tilde{\boldsymbol{\pi}}' \in \tilde{\Pi}_{M}} \sum_{t=1}^{\infty} \gamma^{t} \tilde{R}(\tilde{\boldsymbol{\mu}}_{t}, \tilde{\boldsymbol{\pi}}'), \qquad (4.8)
$$

368 subject to $\tilde{\boldsymbol{\mu}}_{t+1} = \boldsymbol{\Phi}(\tilde{\boldsymbol{\mu}}_t, \tilde{\boldsymbol{\pi}}), \tilde{\boldsymbol{\mu}}_0 = \tilde{\boldsymbol{\mu}}.$

We first show the verification result and then prove the continuity property of \tilde{Q} in (4.8), ³⁷⁰ which thus leads to Theorem 3.8.

371 Lemma 4.3 (Verification) Assume Assumption 3.5. Then \tilde{Q} in (4.8) is the unique func t tion satisfying the Bellman equation (3.11). Furthermore, if there exists $\tilde{\pi}^* \in \arg\max_{\widetilde{\Pi}_M} \tilde{Q}(\tilde{\mu}, \tilde{\pi})$ 373 for each $\tilde{\mu} \in \mathcal{M}_M$, then $\tilde{\pi}^* \in \Pi_M$ is an optimal stationary policy ensemble.

³⁷⁴ The proof of Lemma 4.3 is standard and very similar to the proof of Proposition 3.3 in 375 $[23]$.

376 Proof of Lemma 4.3 First, define $\frac{M_r}{1-\gamma}$ -bounded function space $\mathcal{Q} := \{f : \mathcal{M}_M \times \mathbf{\tilde{H}}_M \to \mathbb{R}^3 \}$ 377 $[-\frac{M_r}{1-\gamma}, \frac{M_r}{1-\gamma}]\}$. Then we define a Bellman operator $B: \mathcal{Q} \to \mathcal{Q}$

$$
(Bq)(\tilde{\boldsymbol{\mu}}, \tilde{\boldsymbol{\pi}}) := \tilde{R}(\tilde{\boldsymbol{\mu}}, \tilde{\boldsymbol{\pi}}) + \gamma \sup_{\tilde{\boldsymbol{\pi}}' \in \tilde{\mathbf{\Pi}}_M} q(\tilde{\boldsymbol{\Phi}}(\tilde{\boldsymbol{\mu}}, \tilde{\boldsymbol{\pi}}), \tilde{\boldsymbol{\pi}}'),
$$

378 One can show that B is a contraction operator with the module-γ. By Banach fixed point σ_1 are theorem, B admits a unique fixed point. As \tilde{Q} function of (4.8) satisfies $B\tilde{Q} = \tilde{Q}, \tilde{Q}$ is ³⁸⁰ unique solution of (3.11).

381 We next define $B^{\tilde{\pi}'}: \mathcal{Q} \to \mathcal{Q}$ under the policy ensemble $\tilde{\pi}' \in \tilde{\Pi}_M$ with

l

$$
(B^{\tilde{\boldsymbol{\pi}}'}q)(\tilde{\boldsymbol{\mu}},\tilde{\boldsymbol{\pi}}):=\widetilde{R}(\tilde{\boldsymbol{\mu}},\tilde{\boldsymbol{\pi}})+\gamma q(\widetilde{\boldsymbol{\Phi}}(\tilde{\boldsymbol{\mu}},\tilde{\boldsymbol{\pi}}),\tilde{\boldsymbol{\pi}}').
$$

382 Similarly, we can show that $B^{\tilde{\pi}'}$ is a contraction map with the module- γ and thus admits a 383 unique fixed point, which is denoted as $\tilde{Q}^{\tilde{\pi}'}$. From this, we have

$$
\begin{array}{rcl}\tilde{Q}^{\tilde{\boldsymbol{\pi}}^*}(\tilde{\boldsymbol{\mu}},\tilde{\boldsymbol{\pi}})&=&\widetilde{R}(\tilde{\boldsymbol{\mu}},\tilde{\boldsymbol{\pi}})+\gamma\tilde{Q}^{\tilde{\boldsymbol{\pi}}^*}(\tilde{\boldsymbol{\Phi}}(\tilde{\boldsymbol{\mu}},\tilde{\boldsymbol{\pi}}),\tilde{\boldsymbol{\pi}}^*)\\&=&\widetilde{R}(\tilde{\boldsymbol{\mu}},\tilde{\boldsymbol{\pi}})+\gamma\sup_{\tilde{\boldsymbol{\pi}}'\in\widetilde{\mathbf{H}}_M}\tilde{Q}(\tilde{\boldsymbol{\Phi}}(\tilde{\boldsymbol{\mu}},\tilde{\boldsymbol{\pi}}),\tilde{\boldsymbol{\pi}}')=\tilde{Q}(\tilde{\boldsymbol{\mu}},\tilde{\boldsymbol{\pi}}),\end{array}
$$

 \mathbf{a}^* which implies $\tilde{\boldsymbol{\pi}}^*$ is an optimal policy ensemble.

385 Lemma 4.4 Let Assumptions 3.4, 3.5 hold. Assume further $\gamma \cdot (1 + L_P + L_{\Pi}) < 1$. Then
386 \tilde{Q} in (4.8) is continuous. \tilde{Q} in (4.8) is continuous.

387 Proof of Lemma 4.4 We will show that as $\tilde{\mu}_n \to \tilde{\mu}, \tilde{\pi}_n \to \tilde{\pi}$ in the sense that $\frac{1}{M} \sum_{m=0}^{M-1} \|\tilde{\mu}^{\alpha_m} - \tilde{\mu}\|_2^2$ 388 $\|\tilde{\mu}_n^{\alpha_m}\|_1 + \frac{1}{M} \sum_{m=0}^{M-1} \max_{s \in \mathcal{S}} \|\tilde{\pi}^{\alpha_m}(\tilde{\mu}_n^{\alpha_m,W}) - \tilde{\pi}_n^{\alpha_m}(\tilde{\mu}_n^{\alpha_m,W})\|_1 \to 0,$

$$
\tilde{Q}(\tilde{\boldsymbol{\mu}}_n, \tilde{\boldsymbol{\pi}}_n(\tilde{\boldsymbol{\mu}}_n)) \to \tilde{Q}(\tilde{\boldsymbol{\mu}}, \tilde{\boldsymbol{\pi}}(\tilde{\boldsymbol{\mu}})).
$$

³⁸⁹ From (4.8) and (3.13),

$$
\begin{split}\n&\|\tilde{Q}(\tilde{\mu}_{n},\tilde{\pi}_{n})-\tilde{Q}(\tilde{\mu},\tilde{\pi})\| \\
&\leq \|\tilde{R}(\tilde{\mu},\tilde{\pi}(\tilde{\mu}))+\sup_{\tilde{\pi}'\in\tilde{\Pi}_{M}}\sum_{t=1}^{\infty}\gamma^{t}\tilde{R}(\tilde{\mu}_{t},\tilde{\pi}'(\tilde{\mu}_{t}))-\tilde{R}(\tilde{\mu}_{n},\tilde{\pi}_{n}(\tilde{\mu}_{n})))+\sup_{\tilde{\pi}'\in\tilde{\Pi}_{M}}\sum_{t=1}^{\infty}\gamma^{t}\tilde{R}(\tilde{\mu}_{n,t},\tilde{\pi}'(\tilde{\mu}_{n,t}))\| \\
&\leq \|\tilde{R}(\tilde{\mu},\tilde{\pi}(\tilde{\mu}))-\tilde{R}(\tilde{\mu}_{n},\tilde{\pi}_{n}(\tilde{\mu}_{n}))\|+\sup_{\tilde{\pi}'\in\tilde{\Pi}_{M}}\sum_{t=1}^{\infty}\gamma^{t}\left|\tilde{R}(\tilde{\mu}_{n,t},\tilde{\pi}'(\tilde{\mu}_{n,t}))-\tilde{R}(\tilde{\mu}_{t},\tilde{\pi}'(\tilde{\mu}_{t}))\right| \\
&\leq L_{r} \cdot \frac{1}{M} \sum_{m=0}^{M-1}\|\tilde{\mu}^{c_{m},W}-\tilde{\mu}_{n}^{c_{m},W}\|_{1}+M_{r} \cdot \frac{1}{M} \sum_{m=0}^{M-1}\|\tilde{\mu}^{c_{m}}-\tilde{\mu}_{n}^{c_{m}}\|_{1}d\alpha \\
&+M_{r} \cdot \frac{1}{M} \sum_{m=0}^{M-1}\max_{s\in\mathcal{S}}\|\tilde{\pi}^{\alpha}(\tilde{\mu}^{c_{m},W})-\tilde{\pi}_{n}^{\alpha}(\tilde{\mu}_{n}^{c_{m},W})\|_{1}d\alpha \\
&+\sup_{\tilde{\pi}'\in\tilde{\Pi}_{M}}\sum_{t=1}^{\infty}\gamma^{t} \cdot \left((L_{r}+L_{\Pi})\cdot \frac{1}{M} \sum_{m=0}^{M-1}\|\tilde{\mu}_{t}^{c_{m},W}-\tilde{\mu}_{n,t}^{c_{m},W}\|_{1}+M_{r} \cdot \frac{1}{M} \sum_{m=0}^{M-1}\|\tilde{\mu}_{t
$$

l

³⁹⁰ By induction, we obtain

$$
\frac{1}{M} \sum_{m=0}^{M-1} \|\tilde{\mu}_{t}^{\alpha_{m}} - \tilde{\mu}_{n,t}^{\alpha_{m}}\|_{1}
$$
\n
$$
= \frac{1}{M} \sum_{m=0}^{M-1} \sum_{s' \in S} \sum_{s \in S} \sum_{a \in A} P^{\alpha_{m}}(s'|s, a, \tilde{\mu}_{t-1}^{\alpha_{m}, W}) \tilde{\mu}_{t-1}^{\alpha_{m}}(s) \tilde{\pi}(\alpha|s, \tilde{\mu}_{t-1}^{\alpha_{m}, W})
$$
\n
$$
- \sum_{s \in S} \sum_{a \in A} P^{\alpha_{m}}(s'|s, a, \tilde{\mu}_{n,t-1}^{\alpha_{m}, W}) \tilde{\mu}_{n,t-1}^{\alpha_{m}}(s) \tilde{\pi}(\alpha|s, \tilde{\mu}_{n,t-1}^{\alpha_{m}, W})|
$$
\n
$$
\leq (L_{P} + L_{\Pi} + 1) \cdot \frac{1}{M} \sum_{m=0}^{M-1} \|\tilde{\mu}_{t-1}^{\alpha} - \tilde{\mu}_{n,t-1}^{\alpha_{m}}\|_{1}
$$
\n
$$
\leq \dots \leq (L_{P} + L_{\Pi} + 1)^{(t-1)} \frac{1}{M} \sum_{m=0}^{M-1} \|\tilde{\mu}_{1}^{\alpha} - \tilde{\mu}_{n,1}^{\alpha}\|_{1}.
$$

391 Therefore, if $\gamma \cdot (1 + L_P + L_{\Pi}) < 1$, then

$$
|\tilde{Q}(\tilde{\boldsymbol{\mu}}_n, \tilde{\boldsymbol{\pi}}_n) - \tilde{Q}(\tilde{\boldsymbol{\mu}}, \tilde{\boldsymbol{\pi}})| \leq C \Big(\frac{1}{M} \sum_{m=0}^{M-1} \|\tilde{\mu}^{\alpha_m} - \tilde{\mu}_n^{\alpha_m}\|_1 + \frac{1}{M} \sum_{m=0}^{M-1} \max_{s \in \mathcal{S}} \|\tilde{\pi}^{\alpha_m}(\tilde{\mu}^{\alpha_m, W}) - \tilde{\pi}_n^{\alpha_m}(\tilde{\mu}_n^{\alpha_m, W})\|_1 \Big).
$$

392 where C is a constant depending on L_r, M_r, L_p, L_{Π} .

³⁹³ Now we prove Theorem 3.8.

Proof of Theorem 3.8 By Lemma 4.4, along with the compactness of $\widetilde{\Pi}_M$, there exists 395 $\tilde{\pi}^* \in \Pi_M$ such that $\tilde{\pi}^* \in \argmax_{\mathbf{\mu}} Q(\tilde{\mu}, \tilde{\pi})$. By Lemma 4.3, there exists an optimal policy $\tilde{\tilde{\pi}} \in \widetilde{\tilde{\Pi}}_M$

$$
\text{as a} \quad \text{ensemble } \tilde{\boldsymbol{\pi}}^* \in \boldsymbol{\Pi}_M. \qquad \qquad \Box
$$

$$
4.3. Proof of Theorem 3.9
$$

³⁹⁸ We first prove the following Lemma, which shows that GMFC and block GMFC become ³⁹⁹ increasingly close to each other as the number of blocks becomes larger.

⁴⁰⁰ Lemma 4.5 Under Assumptions 3.3, 3.4 and 3.6, we have

$$
\begin{split} & \sum_{m=1}^{M} \int_{(\frac{m-1}{M}, \frac{m}{M}]} \| \mu_t^{\alpha, W} - \tilde{\mu}_t^{\alpha_m, W} \|_1 d\alpha \leq \Big[(1 + L_P + L_\Pi)^t - 1 \Big] \frac{\tilde{L}_\Pi + \tilde{L}_P + 2(L_P + L_\Pi) L_W}{M} + \frac{2L_W}{M}, \\ & \sum_{m=1}^{M} \int_{(\frac{m-1}{M}, \frac{m}{M}]} \| \mu_t^{\alpha} - \tilde{\mu}_t^{\alpha_m} \|_1 d\alpha \leq \Big[(1 + L_P + L_\Pi)^t - 1 \Big] \frac{\tilde{L}_\Pi + \tilde{L}_P + 2(L_P + L_\Pi) L_W}{M}. \end{split}
$$

Proof of Lemma 4.5

$$
\sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right)} \|\mu_t^{\alpha, W} - \tilde{\mu}_t^{\alpha_m, W}\|_1 d\alpha \tag{4.9}
$$
\n
$$
\leq \sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right)} \|\mu_t^{\alpha, W} - \mu_t^{\alpha_m, W}\|_1 d\alpha + \frac{1}{M} \sum_{m=1}^{M} \|\mu_t^{\alpha_m, W} - \bar{\mu}_t^{\alpha_m, W}\|_1
$$
\n
$$
+ \frac{1}{M} \sum_{m=1}^{M} \|\bar{\mu}_t^{\alpha_m, W} - \tilde{\mu}_t^{\alpha_m, W}\|_1,
$$
\n(4.9)

401 where $\bar{\mu}^{\alpha_m, W} := \frac{1}{M} \sum_{m'=1}^{M} W(\alpha_m, \alpha_{m'}) \mu^{\alpha_{m'}}$.

l

402 By the definition of $\mu_t^{\alpha, W}, \mu_t^{\alpha_m, W}$ in (2.10), $\tilde{\mu}_t^{\alpha_m, W}$ in (3.12) and $\bar{\mu}^{\alpha_m, W}$, together with the 403 Lipschitz continuity of W in Assumption 3.3,

$$
\sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right]} \|\mu_t^{\alpha, W} - \mu_t^{\alpha, W}\|_1 d\alpha \le \sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right]} \|\mu_t^{\alpha} - \mu_t^{\alpha, m}\|_1 d\alpha + \frac{L_W}{M}, \tag{4.10}
$$

$$
\frac{1}{M} \sum_{m=1}^{\infty} \|\mu_t^{\alpha_m, W} - \bar{\mu}_t^{\alpha_m, W}\|_1 \le \frac{L_W}{M},\tag{4.11}
$$

$$
\frac{1}{M} \sum_{m=1}^{M} \|\bar{\mu}_t^{\alpha_m, W} - \tilde{\mu}_t^{\alpha_m, W}\|_1 \leq \sum_{M} \sum_{m=1}^{M} \|\mu_t^{\alpha_m} - \tilde{\mu}_t^{\alpha_m}\|_1. \tag{4.12}
$$

⁴⁰⁴ Plugging these into (4.9),

$$
\sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right]} \|\mu_t^{\alpha, W} - \tilde{\mu}_t^{\alpha_m, W}\|_1 d\alpha \le A_t + \frac{2L_W}{M},\tag{4.13}
$$

405 where $A_t := \sum_{m=1}^M \int_{(\frac{m-1}{M}, \frac{m}{M}]} \|\mu_t^{\alpha} - \mu_t^{\alpha_m}\|_1 d\alpha + \frac{1}{M} \sum_{m=1}^M \|\mu_t^{\alpha_m} - \tilde{\mu}_t^{\alpha_m}\|_1.$ ⁴⁰⁶ On the other hand, M

$$
\sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right]} \|\mu_t^{\alpha} - \tilde{\mu}_t^{\alpha_m}\|_1 d\alpha \tag{4.14}
$$

$$
\leq \sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right]} \|\mu_t^{\alpha} - \mu_t^{\alpha_m}\|_1 d\alpha + \frac{1}{M} \sum_{m=1}^{M} \|\mu_t^{\alpha_m} - \tilde{\mu}_t^{\alpha_m}\|_1 = A_t.
$$
 (4.15)

407 Therefore, it is enough to estimate A_t . We next estimate A_{t+1} by an inductive way. Note

l

408 that $A_0 = 0$.

$$
A_{t+1} = \sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right]} |\mu_{t+1}^{\alpha} - \mu_{t+1}^{\alpha_m}||_1 d\alpha + \frac{1}{M} \sum_{m=1}^{M} ||\mu_{t+1}^{\alpha_m} - \tilde{\mu}_{t+1}^{\alpha_m}||_1
$$

\n
$$
= \sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right]} \left\| \sum_{s \in S} \sum_{a \in \mathcal{A}} \left(P^{\alpha}(\cdot | s, \mu_t^{\alpha, W}, a) \pi^{\alpha} (a | s, \mu_t^{\alpha, W}) \mu_t^{\alpha} (s) - P^{\alpha_m}(\cdot | s, a, \mu_t^{\alpha_m, W}) \mu_t^{\alpha_m} (s) \pi^{\alpha_m} (a | s, \mu_t^{\alpha_m, W}) \right) \right\|_1 d\alpha
$$

\n
$$
+ \frac{1}{M} \sum_{m=1}^{M} \left\| \sum_{s \in S} \sum_{a \in \mathcal{A}} \left(P^{\alpha_m}(\cdot | s, \mu_t^{\alpha_m, W}, a) \pi^{\alpha_m} (a | s, \mu_t^{\alpha_m, W}) \mu_t^{\alpha_m} (s) - P^{\alpha_m}(\cdot | s, a, \tilde{\mu}_t^{\alpha_m, W}) \tilde{\mu}_t^{\alpha_m} (s) \tilde{\pi}^{\alpha_m} (a | s, \tilde{\mu}_t^{\alpha_m, W}) \right) \right\|_1
$$

\n
$$
\leq \sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right]} \left((L_P + L_{\Pi}) \cdot \|\mu_t^{\alpha, W} - \mu_{\alpha_m, W}\|_1 + \frac{\tilde{L}_{\Pi}}{M} + \|\mu_t^{\alpha} - \mu_t^{\alpha_m}\|_1 \right) d\alpha
$$

\n
$$
+ \frac{1}{M} \sum_{m=1}^{M} \left((L_P + L_{\Pi}) \cdot \|\mu_t^{\alpha_m, W} - \tilde{\mu}_{\alpha_m, W}\|_1 + \frac{\tilde{L}_P}{M} + \|\mu_t^{\alpha_m} - \tilde{\mu}_t^{\alpha_m}\|_1 \right)
$$

\n
$$
\le
$$

409 where the second equality is from (3.4) and (3.14) , and we use Assumptions 3.3, 3.4 and 3.6 410 in the third inequality, and we use $(4.10)-(4.12)$ in the last inequality. ⁴¹¹ By induction, we have

$$
A_{t+1} \leq \left[(1 + L_P + L_{\Pi})^t - 1 \right] \frac{\tilde{L}_{\Pi} + \tilde{L}_P + 2(L_P + L_{\Pi}) L_W}{M}.
$$

⁴¹³ Based on Lemma 4.5, we have the following Proposition.

414 Proposition 4.6 Assume Assumptions 3.3, 3.4, 3.5, 3.6, and $\gamma \cdot (L_P + L_{\Pi} + 1) < 1$. Then
415 we have for any $\mu \in \mathcal{P}(\mathcal{S})$ we have for any $\mu \in \mathcal{P}(\mathcal{S})$

$$
\sup_{\pi \in \Pi} \left| \tilde{J}^M(\mu, \pi) - J(\mu, \pi) \right| \to 0, \quad \text{as } M \to +\infty,
$$
\n(4.16)

416 where \tilde{J}^M and J are given in (4.7) and (2.11), respectively.

417 Proof of Proposition 4.6 Recall from (3.12) that

$$
\widetilde{J}^M(\mu, \widetilde{\boldsymbol{\pi}}) = \sum_{t=0}^{\infty} \gamma^t \widetilde{R}(\widetilde{\boldsymbol{\mu}}_t, \widetilde{\boldsymbol{\pi}}(\widetilde{\boldsymbol{\mu}}_t)),
$$

⁴¹⁸ subject to $\tilde{\mu}_{t+1}^{\alpha_m} = \tilde{\Phi}^{\alpha_m}(\tilde{\mu}_t^{\alpha_m}, \tilde{\pi}^{\alpha_m}), t \in \mathbb{N}_+, \tilde{\mu}_0^{\alpha} \equiv \mu$, and $\tilde{\mu}_t^{\alpha_m, W}$ given in (3.12).

l

$$
J(\mu, \boldsymbol{\pi}) = \sum_{t=0}^{\infty} \gamma^t R(\boldsymbol{\mu}_t, \boldsymbol{\pi}(\boldsymbol{\mu}_t)),
$$

419 subject to $\mu_{t+1}^{\alpha} = \Phi^{\alpha}(\mu_t^{\alpha}, \pi^{\alpha}), t \in \mathbb{N}_+, \mu_0^{\alpha} \equiv \mu$, and $\mu_t^{\alpha, W}$ given in (2.10). Since $\tilde{\pi} :=$ 420 $(\tilde{\pi}^{\alpha_m})_{m \in [M]} \in \tilde{\Pi}_M$ can be viewed as a piecewise-constant projection of $\pi \in \Pi$ onto $\tilde{\Pi}_M$. ⁴²¹ Then,

$$
\sup_{\pi \in \Pi} \left| \tilde{J}^{M}(\mu, \pi) - J(\mu, \pi) \right|
$$
\n
$$
\leq \sup_{\pi \in \Pi} \sum_{t=0}^{\infty} \gamma^{t} \left| \tilde{R}(\tilde{\mu}_{t}, \tilde{\pi}(\tilde{\mu}_{t})) - R(\mu_{t}, \pi(\mu_{t})) \right|
$$
\n
$$
\leq \sup_{\pi \in \Pi} \sum_{t=0}^{\infty} \gamma^{t} \left| \tilde{R}(\tilde{\mu}_{t}, \tilde{\pi}(\tilde{\mu}_{t})) - R(\mu_{t}, \tilde{\pi}(\mu_{t})) \right| + \sup_{\pi \in \Pi} \sum_{t=0}^{\infty} \gamma^{t} \left| R(\mu_{t}, \tilde{\pi}(\mu_{t})) - R(\mu_{t}, \pi(\mu_{t})) \right|
$$
\n
$$
:= I + II.
$$

422 In terms of the term I, we first estimate $\left| \tilde{R}(\tilde{\boldsymbol{\mu}}_t, \tilde{\boldsymbol{\pi}}) - R(\boldsymbol{\mu}_t, \tilde{\boldsymbol{\pi}}) \right|$:

$$
\begin{split} &\left| \tilde{R}(\tilde{\pmb{\mu}}_{t}, \tilde{\pmb{\pi}}(\tilde{\pmb{\mu}}_{t})) - R(\pmb{\mu}_{t}, \tilde{\pmb{\pi}}(\pmb{\mu}_{t})) \right| \\ & = \left| \sum_{m=1}^{M} \int_{(\frac{m-1}{M}, \frac{m}{M})} \sum_{s \in S} \sum_{a \in \mathcal{A}} r^{\alpha_{m}}(s, a, \tilde{\mu}_{t}^{\alpha_{m}, V}) \hat{\mu}_{t}^{\alpha_{m}}(s) \tilde{\pi}^{\alpha_{m}}(a|s, \tilde{\mu}_{t}^{\alpha_{m}, W}) d\alpha \right| \\ & \leq \left| \sum_{m=1}^{M} \int_{(\frac{m-1}{M}, \frac{m}{M})} \sum_{s \in S} \sum_{a \in \mathcal{A}} r^{\alpha}(s, a, \mu_{t}^{\alpha, W}) \mu_{t}^{\alpha}(s) \tilde{\pi}^{\alpha_{m}}(a|s, \mu_{t}^{\alpha, W}) d\alpha \right| \\ & \leq \left| \sum_{m=1}^{M} \int_{(\frac{m-1}{M}, \frac{m}{M})} \sum_{s \in S} \sum_{a \in \mathcal{A}} \left(r^{\alpha_{m}}(s, a, \tilde{\mu}_{t}^{\alpha_{m}, W}) - r^{\alpha}(s, a, \mu_{t}^{\alpha, W}) \right) \tilde{\mu}_{t}^{\alpha_{m}}(s) \tilde{\pi}^{\alpha_{m}}(a|s, \tilde{\mu}_{t}^{\alpha_{m}, W}) d\alpha \right| \\ & + \left| \sum_{m=1}^{M} \int_{(\frac{m-1}{M}, \frac{m}{M})} \sum_{s \in S} \sum_{a \in \mathcal{A}} r^{\alpha}(s, a, \mu_{t}^{\alpha, W}) (\tilde{\mu}_{t}^{\alpha_{m}}(s) - \mu_{t}^{\alpha}(s)) \tilde{\pi}^{\alpha_{m}}(a|s, \tilde{\mu}_{t}^{\alpha_{m}, W}) d\alpha \right| \\ & \leq L_{r} \cdot \sum_{m=1}^{M} \int_{(\frac{m-1}{M}, \frac{m}{M})} \left| \mu_{t}^{\alpha, W} - \tilde{\mu}_{t}^{\alpha_{m}, W} \right| \left| d\alpha + \frac{\tilde{L}_{r}}{M} \right| \\ & + M_{r} \cdot
$$

⁴²³ By Lemma 4.5,

$$
I \leq \frac{C(\gamma, L_{\Pi}, L_P, L_W, L_r, M_r)}{M}.
$$

l

 424 For the term II ,

$$
\sup_{\pi \in \Pi} \sum_{t=0}^{\infty} \gamma^{t} \left| R(\boldsymbol{\mu}_{t}, \tilde{\pi}(\boldsymbol{\mu}_{t})) - R(\boldsymbol{\mu}_{t}, \pi(\boldsymbol{\mu}_{t})) \right|
$$
\n
$$
\leq \sup_{\pi \in \Pi} \sum_{t=0}^{\infty} \gamma^{t} M_{r} \sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right]} \max_{s \in S} \|\pi^{\alpha} - \pi^{\alpha^{m}}\|_{1} d\alpha
$$
\n
$$
+ \sup_{\pi \in \Pi} \sum_{t=0}^{\infty} \gamma^{t} M_{r} \sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right]} \|\mu_{t}^{\alpha, W} - \tilde{\mu}_{t}^{\alpha_{m}, W}\|_{1} d\alpha
$$
\n
$$
\leq \frac{C(\gamma, L_{\Pi}, L_{P}, L_{W}, L_{r}, M_{r})}{M}.
$$
\n425

426 Proof of Theorem 3.9 Suppose that $\tilde{\pi}^* \in \tilde{\Pi}_M \subset \Pi$ and $(\pi^{1,*}, \ldots, \pi^{N,*}) \in \Pi^N$ are optimal 427 policies of the problems (4.7) and (2.7), respectively. From Proposition 4.6, for any $\varepsilon > 0$, 428 there exists sufficiently large $M_{\varepsilon} > 0$

$$
|\tilde{J}^{M_{\varepsilon}}(\mu,\tilde{\boldsymbol{\pi}}^*)-J(\mu,\tilde{\boldsymbol{\pi}}^*)|\leq \frac{\varepsilon}{3},
$$

429 where by (3.8) , $\bm{\pi}^{N,*} := \sum_{i=1}^N \pi^{i,*} \bm{1}_{\alpha \in (\frac{i-1}{N}, \frac{i}{N})^*}$

430 From Theorem 3.7, for any $\varepsilon > 0$, there exists N_{ε} such that for all $N \ge N_{\varepsilon}$

$$
|J_N(\mu, \tilde{\pi}^{1,*}, \dots, \tilde{\pi}^{N,*}) - J(\mu, \tilde{\pi}^*)| \leq \frac{\varepsilon}{3}, \ \ |J_N(\mu, \pi^{1,*}, \dots, \pi^{N,*}) - J(\mu, \pi^{N,*})| \leq \frac{\varepsilon}{3}.
$$

⁴³¹ Then we have

$$
\geq \frac{J_N(\mu, \tilde{\pi}^{1,*}, \dots, \tilde{\pi}^{N,*}) - J_N(\mu, \pi^{1,*}, \dots, \pi^{N,*})}{J_N(\mu, \tilde{\pi}^{1,*}, \dots, \tilde{\pi}^{N,*}) - J(\mu, \tilde{\pi}^{*}) + \underbrace{J(\mu, \tilde{\pi}^{*}) - \tilde{J}_{M_{\varepsilon}}(\mu, \tilde{\pi}^{*})}_{I_2} + \underbrace{\tilde{J}^{M_{\varepsilon}}(\mu, \tilde{\pi}^{*}) - \tilde{J}^{M_{\varepsilon}}(\mu, \pi^{N,*})}_{I_3} + \underbrace{\tilde{J}^{M_{\varepsilon}}(\mu, \pi^{N,*}) - J_N(\mu, \pi^{1,*}, \dots, \pi^{N,*})}_{I_4}
$$
\n
$$
\geq \frac{\varepsilon}{3} - \frac{\varepsilon}{3} - \frac{\varepsilon}{3} = -\varepsilon.
$$

432 where $I_3 \geq 0$ due to the optimality of $\tilde{\pi}^*$ for $\tilde{V}^{M_{\varepsilon}}$. This means that the optimal policy of 433 block GMFC provides an ε -optimal policy for the multi-agent system with $(\tilde{\pi}_1^*, \ldots, \tilde{\pi}_N^*) :=$ $\Gamma_N(\tilde{\pi}^*$ 434 $\Gamma_N(\tilde{\bm{\pi}}^*).$

⁴³⁵ 5. Experiments

⁴³⁶ In this section, we provide an empirical verification of our theoretical results, with two ⁴³⁷ examples adapted from existing works on learning MFGs [16, 10] and learning GMFGs [15].

⁴³⁸ 5.1. SIS Graphon Model

We consider a SIS graphon model in [16] under a cooperative setting. In this model, 440 each agent $\alpha \in \mathcal{I}$ shares a state space $\mathcal{S} = \{S, I\}$ and an action space $\mathcal{A} = \{C, NC\}$, where 441 S is susceptible, I is infected, C represents keeping contact with others, and NC means 442 keeping social distance. The transition probability of each agent α is represented as follows

l

$$
P^{\alpha}(s_{t+1} = I | s_t = S, a_t = C, \mu_t^{\alpha, W}) = \beta_1 \mu_t^{\alpha, W}(I),
$$

\n
$$
P^{\alpha}(s_{t+1} = I | s_t = S, a_t = NC, \mu_t^{\alpha, W}) = \beta_2 \mu_t^{\alpha, W}(I),
$$

\n
$$
P^{\alpha}(s_{t+1} = S | s_t = I, \mu_t^{\alpha, W}) = \delta,
$$

443 where β_1 is the infection rate with keeping contact with others, β_2 is the infection rate 444 under social distance, and δ is the fixed recovery rate. We assume $0 < \beta_2 < \beta_1$, meaning ⁴⁴⁵ that keeping social distance can reduce the risk of being infected. The individual reward ⁴⁴⁶ function is defined as

$$
r^{\alpha}(s,\mu_t^{\alpha,W},a) = -c_1 \mathbf{1}_{\{I\}}(s) - c_2 \mathbf{1}_{\{NC\}}(a) - c_3 \mathbf{1}_{\{I\}}(s) \mathbf{1}_{\{C\}}(a),
$$

447 where c_1 represents the cost of being infected such as the cost of medical treatment, c_2 $\frac{448}{448}$ represents the cost of keeping social distance, and c_3 represents the penalty of going out if ⁴⁴⁹ the agent is infected.

450 In our experiment, we set $\beta_1=0.8$, $\beta_2=0$, $\delta=0.3$ for the transition dynamics and $c_1=2$, 451 c₂=0.3, c₃ = 0.5 for the reward function. The initial mean field μ_0 is taken as the uniform ⁴⁵² distribution. We set the episode length to 50.

⁴⁵³ 5.2. Malware Spread Graphon Model

We consider a malware spread model in [10] under a cooperative setting. In this model, let $S = \{0, 1, \ldots, K - 1\}, K \in \mathbb{N}$, denote the health level of the agent, where $s_t = 0$ and $s_t = K - 1$ represents the best level and the worst level, respectively. All agents can take two actions: $a_t = 0$ means doing nothing, and $a_t = 1$ means repairing. The state transition is given by

$$
s_{t+1} = \begin{cases} s_t + \lfloor (K - s_t) \chi_t \rfloor, & \text{if } a_t = 0, \\ 0, & \text{if } a_t = 1, \end{cases}
$$

454 where $\chi_t, t \in \mathbb{N}$ are i.i.d. random variables with a certain probability distribution. Then 455 after taking action a_t , agent α will receive an individual reward

$$
r^{\alpha}(s_t, \mu_t^{\alpha, W}, a_t) = -(c_1 + \langle \mu_t^{\alpha, W} \rangle) s_t / K - c_2 a_t.
$$

456 Here considering the heterogeneity of agents, we use $W(\alpha, \beta)$ to denote the *importance* effect 457 of agent β on agent α . $\langle \mu_t^{\alpha,W} \rangle := \int_{\beta \in \mathcal{I}} \sum_{s \in \mathcal{S}} sW(\alpha,\beta) \mu_t^{\beta}(s) d\beta$ is the risk of being infected 458 by other agents and c_2 is the cost of taking action a_t .

459 In our experiment, we set $K=3$, $c_1=0.3$, and $c_2=0.5$. In addition, to stabilize the training 460 of the RL agent, we fix χ_t to a static value, i.e., 0.7. In this model, we set the episode length ⁴⁶¹ to 10.

5.3. Performance of N-agent GMFC on Multi-Agent System

l

 For both models, we use PPO [47] to train the block GMFC agent in the infinite-agent environment and obtain the policy ensembles and further use Algorithm 2 to deploy them in the finite-agent environment. We test the performance of N-agent GMFC with 10 blocks to different numbers of agents, i.e., from 10 to 100. For each case, we run 1000 times of simulations and show the mean and standard variation (Green shadows in Figure 1 and Figure 2) of the mean episode reward. We can see that in both scenarios and for different types of graphons, the mean episode rewards of the N-agent GMFC become increasingly close to that of block GMFC as the number of agents grows. (See Figure 1 and Figure 2). This verifies our theoretical findings empirically.

Figure 1: Experiments for different graphons in SIS finite-agent environment

Figure 2: Experiments for different graphons in Malware Spread finite-agent environment

5.4. Comparison with Other Algorithms

 For different types of graphons, we compare our algorithm N-agent GMFC with three existing MARL algorithms, including two independent learning algorithms, i.e., independent DQN [40], independent PPO [47] and a powerful centralized-training-and-decentralized- execution(CTDE)-based algorithm QMIX [46]. We test the performance of those algorithms with different numbers of blocks, i.e., 2, 5, 10, to the multi-agent systems with 40 agents. The results are reported in Table 1 and Table 2.

 In the SIS graphon model, N-agent GMFC shows dominating performance in most cases and outperforms independent algorithms by a large margin. Only QMIX can reach compa- rable results. And in the malware spread graphon model, N-agent GMFC outperforms other algorithms in more than half of the cases. Only independent DQN has comparable perfor-mance in this environment. And we can see that in both environments, the performance gap between N-agent GMFC and other MARL algorithms is shrinking as the number of blocks goes larger. This is mainly because the action space of block GMFC increases more quickly than MARL algorithms as the block number increases. And it is hard to train RL agents when the action space is too large.

l

 \mathcal{A}_{488} Beyond the visible results shown in Tables 1 and 2, when the number of agents N grows larger, classic MARL methods become infeasible because of the curse of dimensionality and the restriction of memory storage, while N-agent GMFC is trained only once and independent of the number of agents N, hence is easier to scale up in a large-scale regime and enjoys a more stable performance. We can see that N-agent GMFC shows more stable results when N increases as shown in Figure 1 and Figure 2.

Graphon Type	М	Algorithm			
		N-agent GMFC	I-DQN	I-PPO	QMIX
Erdős Rényi	2	-15.37	-17.58	-20.63	-20.51
	5	-15.74	-16.17	-20.42	16.94
	10	-15.67	-17.55	-21.38	-14.45
Stochastic Block	$\overline{2}$	-13.58	-16.05	-18.38	-17.69
	5	-13.67	-15.91	-20.13	-13.79
	10	-13.57	-15.52	-14.87	-13.86
Random Geometric	2	-12.45	-17.93	-14.82	-14.52
	5	-9.82	-12.81	-12.99	-10.84
	10	-10.52	-11.68	-12.66	-12.60

Table 1: Mean Episode Reward for SIS with 40 agents

Graphon Type		Algorithm				
		N-agent GMFC	I-DQN	I-PPO	QMIX	
Erdős Rényi	\mathfrak{D}	-5.21	-5.11	-5.31	-6.05	
	5	-5.21	-5.30	-5.26	-6.13	
Stochastic Block	10	-5.21	-5.14	-5.27	-5.21	
	2	-5.16	-5.21	-5.37	-5.88	
	5	-5.10	-5.19	-5.31	-5.70	
	10	-5.09	-5.05	-5.28	-5.27	
Random Geometric	2	-5.02	-5.21	-5.27	-5.35	
	5	-4.85	-5.03	-5.04	-5.05	
	10	-4.82	-4.83	-5.14	-4.83	

Table 2: Mean Episode Reward for Malware Spread with 40 agents

⁴⁹⁴ 5.5. Implementation Details

495 We use three graphons in our experiments: (1) Erdős Rényi: $W(\alpha, \beta) = 0.8$; (2) Stochas-496 tic block model: $W(\alpha, \beta) = 0.9$, if $0 \le \alpha, \beta \le 0.5$ or $0.5 \le \alpha, \beta \le 1$, $W(\alpha, \beta) = 0.4$, 497 otherwise; (3) Random geometric graphon: $W(\alpha, \beta) = f(\min(|\beta - \alpha|, 1 - |\beta - \alpha|))$, where 498 $f(x) = e^{-\frac{x^2}{0.5-x}}$.

l

For the RL algorithms, we use the implementation of RLlib $[36]$ (version 1.11.0, Apache- 2.0 license). For PPO used to learn an optimal policy ensemble in block GFMC, we use a 64-dimensional linear layer to encode the observation and 2-layer MLPs with 256 hidden units per layer for both value network and actor network. For independent DQN and independent PPO, we use the default weight-sharing model with 64-dimensional embedding layers. We train the GMFC PPO agent for 1000 iterations, and other three MARL agents for 200 iterations. The specific hyper-parameters are listed in Table 3.

⁵⁰⁶ 6. Conclusion

 In this work, we have proposed a discrete-time GMFC framework for MARL with nonuni- form interactions and heterogeneous reward functions and transition functions across the agents on dense graphs. Theoretically, we have shown that under suitable assumptions, GMFC approximates MARL well with approximation error of order $\mathcal{O}(\frac{1}{\sqrt{l}})$ 510 GMFC approximates MARL well with approximation error of order $\mathcal{O}(\frac{1}{\sqrt{N}})$. To reduce the dimension of GMFC, we have introduced block GMFC by discretizing the graphon index and shown that it also approximates MARL well. Empirical studies on several examples have verified the plausibility of the GMFC framework. For future research, we wish to ex- plore more on how to extract the optimal policy of cooperative MARL without the simulator for population state distribution ensemble and to extend our framework to heterogeneous MARL on sparse graphs.

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⁶⁴¹ Declaration of Competing Interest

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⁶⁴² The authors declare that they have no known competing financial interests or personal ⁶⁴³ relationships that could have appeared to influence the work reported in this paper.

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