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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 $\mathcal{O}(\frac{1}{\sqrt{N}})$, 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.

A recent tractable approach is a mean-field approach by considering MARL in the regime
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 9 MARL. The first one is called mean-field MARL (MF-MARL), which refers to the empirical 10 average of the states or actions of a *finite* population. For example, [52] proposes to approx-11 imate interactions within the population of agents by averaging the actions of the overall 12 population or neighboring agents. [35] proposes a mean-field proximal policy optimization 13 algorithm for a class of MARL with permutation invariance. The second one is called mean-14 field game (MFG), which describes the asymptotic limit of non-cooperative stochastic games 15 as the number of agents goes to infinity [30, 27, 8]. Recently, a rapidly growing literature 16 studies MFG for noncooperative MARL either in a model-based way [53, 6, 26] or by a 17 model-free approach [25, 48, 18, 14, 44]. The third one is called mean-field control (MFC), 18 which is closely related to MFG yet different from MFG in terms of learning goals. For 19 cooperative MFC, the Bellman equation for the value function is defined on an enlarged 20 space of probability measures, and MFC is always reformulated as a new Markov decision 21 process (MDP) with continuous state-action space. [9] shows the existence of optimal poli-22 cies for MFC in the form of mean-field MDP and adapts classical reinforcement learning 23 (RL) methods to the mean-field setups. [23] approximates MARL by a MFC approach, and 24 proposes a model-free kernel-based Q-learning algorithm (MFC-K-Q) that enjoys a linear 25 convergence rate and is independent of the number of agents. [44] presents a model-based 26 RL algorithm M3-UCRL for MFC with a general regret bound. [2] proposes a unified two-27 timescale learning framework for MFG and MFC by tuning the ratio of learning rates of Q28 function and the population state distribution. Under the framework of MFC, [41] proposes 29 locally executable policies such that the resulting discounted sum of average rewards well 30 approximates the optimal value function over all policies with theoretical guarantee. 31

One restriction of the mean-field theory is that it eliminates the difference among agents 32 and interactions between agents are assumed to be uniform. However, in many real world 33 scenarios, strategic interactions between agents are not always uniform and rely on the 34 relative positions of agents. To develop scalable learning algorithms for multi-agent systems 35 with heterogeneous agents, one approach is to exploit the local network structure of agents 36 [45, 37]. Another approach is to consider mean-field systems on large graphs and their 37 asymptotic limits, which leads to graphon mean-field theory [39]. So far, most existing 38 works on graphon mean-field theory consider either diffusion processes without learning in 39 continuous time or non-cooperative graphon mean-field game (GMFG) in discrete time. [3] 40 considers uncontrolled graphon mean-field systems in continuous time. [17] studies MFG 41 on an Erdös-Rényi graph. [19] studies the convergence of weighted empirical measures 42 described by stochastic differential equations. [4] studies propagation of chaos of weakly 43 interacting particles on general graph sequences. [5] considers general GMFG and studies 44 ε -Nash equilibria of the multi-agent system by a PDE approach in continuous time. [29] 45 studies stochastic games on large graphs and their graphon limits. It shows that GMFG 46 is viewed as a special case of MFG by viewing the label of agents as a component of the 47 state process. [21, 22] study continuous-time cooperative graphon mean-field systems with 48 linear dynamics. On the other hand, [7] studies static finite-agent network games and their 49 associated graphon games. [49] provides a sequential decomposition algorithm to find Nash 50 equilibria of discrete-time GMFG. [15] constructs a discrete-time learning GMFG framework 51

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to analyze approximate Nash equilibria for MARL with nonuniform interactions. However, 52 little is focused on learning cooperative graphon mean-field systems in discrete time, except 53 for [42, 43] on particular forms of nonuniform interactions among agents. [43] proves that 54 when the reward is affine in the state distribution and action distribution, MARL with 55 nonuniform interactions can still be approximated by classic MFC. [42] considers multi-56 class MARL, where agents belonging to the same class are homogeneous. In contrast, we 57 consider a general discrete-time GMFC framework under which agents are allowed to be 58 fully heterogeneous and interact non-uniformly on any network captured by a graphon. 59

Our Work. In this work, we propose a general discrete-time GMFC framework to approx-60 imate cooperative heterogeneous MARL on large graphs by combining classical MFC and 61 network games. Theoretically, we first show that GMFC can be reformulated as a new 62 MDP with deterministic dynamics and infinite-dimensional state-action space, hence the 63 Bellman equation for Q function is established on the space of probability measure ensem-64 bles. It shows that GMFC approximates cooperative MARL well in terms of both value 65 function and optimal policies. The approximation error is at order $\mathcal{O}(1/\sqrt{N})$, where N is 66 the number of agents. Furthermore, instead of learning infinite dimensional GMFC directly, 67 we introduce a smaller class called block GMFC by discretizing the graphon index, which 68 can be recast as a new MDP with deterministic dynamic and finite-dimensional continuous 69 state-action space. We show that the optimal policy ensemble learned from block GMFC 70 is near optimal for cooperative MARL. Using the approach in [38], we develop a proximal 71 policy optimization (PPO) based algorithm for block GMFC, which, together with approxi-72 mation result between block GMFC and cooperative MARL, shows that the proposed PPO 73 algorithm converges to the optimal policy of MARL with the sample complexity guarantee. 74 Empirically, our experiments in Section 5 demonstrate that when the number of agents be-75 comes large, the mean episode reward of MARL becomes increasingly close to that of block 76 GMFC, which verifies our theoretical findings. Furthermore, our block GMFC approach 77 achieves comparable performances with other popular existing MARL algorithms in the 78 finite-agent setting. 79

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 cooperative MARL. The main theoretical proofs are presented in Section 4. Section 5 tests the performance of block GMFC experimentally.

86 2. Mean-Field MARL on Dense Graphs

87 2.1. Preliminary: Graphon Theory

In the following, we consider a cooperative multi-agent system and its associated meanfield limit. In this system, each agent is affected by all others, with different agents exerting different effects on her. This multi-agent system with N agents can be described by a 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 ⁹³ of G_N is represented as $\{\xi_{i,j}^N\}_{1 \le i,j \le N}$. To study the limit of the multi-agent system as N⁹⁴ 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.

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

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

For each weighted graph $G_N = (\mathcal{V}_N, \mathcal{E}_N)$, we consider the correspondence between the 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 $\begin{pmatrix} i-1\\N\\N \end{pmatrix} \times (\frac{j-1}{N}, \frac{j}{N}] \times (\frac{j-1}{N}, \frac{j}{N}]$. We make the following condition on the strength of interaction $\xi_{i,j}^N$ between agents *i* and *j* and the associated W_N .

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

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

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

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

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

or

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

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

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

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

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:

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

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

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

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

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

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

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

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

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

$$r^{i}\left(s_{t}^{i}, \ \mu_{t}^{i,W_{N}}, \ a_{t}^{i}\right), \quad i \in [N],$$

$$(2.3)$$

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 a transition probability such that

$$s_{t+1}^{i} \sim P^{i}\left(\cdot \mid s_{t}^{i}, \mu_{t}^{i,W_{N}}, a_{t}^{i}\right), \quad i \in [N], \ s_{0}^{i} \sim \mu \in \mathcal{P}(\mathcal{S}),$$

$$(2.4)$$

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 t depend on both her individual information (s_t^i, a_t^i) and neighborhood empirical measure μ_t^{i,W_N} .

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

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

which maps agent *i*'s state to a randomized action. (2.5) is called global policy since the policy of agent *i* depends on both her own state and the aggregate information of the whole 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 aggregation 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:

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

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

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 meanfield theory with uniform interactions [9, 23]. Furthermore, our framework is flexible enough to include the nonuniform interactions of actions via $\nu_t^{i,W_N} = \frac{1}{N} \sum_{j \in \mathcal{V}_N} \xi_{i,j}^N \delta_{a_t^j}(\cdot)$.

The expected discounted accumulated reward of agent i is

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

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

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

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

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

To study Pareto optimality, we introduce the expected discounted accumulated rewardaveraged over all agents, i.e.,

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

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

is shown to be a Pareto optimality in Definition 2.4. Therefore, searching for Pareto optimality 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 weak notion of ε -Pareto optimality. **Definition 2.5 (\varepsilon-Pareto Optimality)** $(\pi_{\varepsilon}^{1,*}, \ldots, \pi_{\varepsilon}^{N,*}) \in \Pi^{N}$ is called ε -Pareto optimality for the multi-agent system (2.2)-(2.5) if there does not exist $(\pi^{1}, \ldots, \pi^{N}) \in \Pi^{N}$ such that

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

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

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

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

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

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

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 the *neighborhood mean-field measure* of agent α :

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

with the graphon W given in Assumption 2.1.

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

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

$$V(\boldsymbol{\mu}) := \sup_{\boldsymbol{\pi} \in \boldsymbol{\Pi}} J(\boldsymbol{\mu}, \boldsymbol{\pi})$$

$$= \sup_{\boldsymbol{\pi} \in \boldsymbol{\Pi}} \int_{\mathcal{I}} \mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^{t} r^{\alpha} (s_{t}^{\alpha}, \ \mu_{t}^{\alpha, W}, \ a_{t}^{\alpha}) \ \middle| \ s_{0}^{\alpha} \sim \mu^{\alpha}, a_{t}^{\alpha} \sim \pi^{\alpha} (\cdot | s_{t}^{\alpha}, \mu_{t}^{\alpha, W}) \right] d\alpha.$$

$$(2.11)$$

184 3. Main Results

185 3.1. Reformulation of GMFC

In this section, we show that GMFC (2.9)-(2.11) can be reformulated as a MDP with deterministic dynamics and continuous state-action space $\mathcal{M} \times \Pi$. **Theorem 3.1** *GMFC* (2.9)-(2.11) can be reformulated as

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

189 subject to

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

where the aggregated reward $R: \mathcal{M} \times \Pi \to \mathbb{R}$ and the aggregated transition dynamics Φ : $\mathcal{M} \times \Pi \to \mathcal{M}$ 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)

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

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

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

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

201 Hence its Bellman equation is given by

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

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

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

with the initial condition $\tilde{s}_0 \sim \mu_0$, $\tilde{\alpha}_0 \sim Unif(0,1)$. It is worth pointing out such a labelstate formulation has also been studied in GMFG [29, 15]. 208 3.2. Approximation

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

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

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

Assumption 3.3 is common in graphon mean-field theory [21, 15, 29]. Indeed, the Lipschitz continuity assumption on W in Assumption 3.3 can be relaxed to piecewise Lipschitz continuity on W.

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

$$\|P^{\alpha}(\cdot|s,\mu_{1},a) - P^{\beta}(\cdot|s,\mu_{2},a)\|_{1} \le L_{P} \cdot \|\mu_{1} - \mu_{2}\|_{1} + L_{P} \cdot |\alpha - \beta|,$$

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

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

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

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

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

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

To show approximation properties of GMFC in the large-scale multi-agent system, we need to relate policy ensembles of GMFC to policies of the multi-agent system. On one hand, one can see that any $\boldsymbol{\pi} \in \boldsymbol{\Pi}$ 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)

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

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

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

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

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

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

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

This section will show that discretizing the graphon index $\alpha \in \mathcal{I}$ of GMFC enables to approximate Q function in (3.6) by an approximated Q function in (3.11) below defined on 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 approximate each agent $\alpha \in \mathcal{I}$ by the nearest $\alpha_m \in \mathcal{I}_M$ close to it. Introduce $\widetilde{\mathcal{M}}_M :=$ $\mathcal{P}(\mathcal{S})^{\mathcal{I}_M}, \widetilde{\mathbf{\Pi}}_M := \mathcal{P}(\mathcal{A})^{\mathcal{S} \times \mathcal{I}_M}$. Meanwhile, $\widetilde{\boldsymbol{\mu}} := (\widetilde{\mu}^{\alpha_m})_{m \in [M]} \in \widetilde{\mathcal{M}}_M$ and $\widetilde{\boldsymbol{\pi}} := (\widetilde{\pi}^{\alpha_m})_{m \in [M]} \in$ $\widetilde{\mathbf{\Pi}}_M$ can be viewed as a piecewise constant state distribution ensemble in \mathcal{M} and a piecewise constant policy ensemble in $\mathbf{\Pi}$, respectively. Our arguments can be easily generalized to nonuniform grids.

Consequently, instead of performing algorithms according to (3.6) with a continuum of 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

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

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

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

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

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

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

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

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

Theorem 3.9 Assume $\gamma \cdot (1 + L_P + L_{\Pi}) < \infty$ and Assumptions 2.1, 3.3, 3.4, 3.5 and 3.6. Under either (C1) or (C2), for any $\varepsilon > 0$, there exists N_{ε} , M_{ε} such that for $N \ge N_{\varepsilon}$, the optimal policy ensemble $\tilde{\pi}^*$ of block GMFC (3.11) with M_{ε} blocks provides an ε -Pareto 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.

When model parameters P^{α}, r^{α} and W are known, one can easily extract the optimal 284 policy based on Bellman equation. If any of these model parameters P^{α}, r^{α} and W is 285 unknown, we take a model-free approach. The key issue is to handle population state 286 distribution ensemble $\tilde{\mu}$, which is an input of Q function in (3.11). We assume that we 287 have a block GMFC simulator $\mathcal{G}(\tilde{\boldsymbol{\mu}}, \tilde{\boldsymbol{\pi}}) = (\tilde{\boldsymbol{\mu}}', R)$. That is, for any pair of population state 288 distribution ensemble and policy ensemble $(\tilde{\boldsymbol{\mu}}, \tilde{\boldsymbol{\pi}})$, we can sample the aggregated reward R 289 and the next population state distribution ensemble $\tilde{\mu}'$. To learn the optimal policy of block 290 GMFC, one can adopt any existing techniques for standard MFC, such as a kernel-based Q 291 learning method in [23] and a uniform discretization method in [9]. 292

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

Algorithm 1 Neural PPO for block GMFC

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 $(\tilde{\boldsymbol{\mu}}_t, \tilde{\boldsymbol{\pi}}_t, \tilde{\boldsymbol{R}}_t, \tilde{\boldsymbol{\mu}}'_t, \tilde{\boldsymbol{\pi}}'_t)_{t=1}^T$ 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 $M \ge M_{\varepsilon}$ and $N \ge N_{\varepsilon}$, and the policy attained by Algorithm 1 denoted as π_{PPO}

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

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

By setting $K = \frac{C}{\varepsilon^2}$, the optimal empirical value function of MARL is approximated by the 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 $\mathcal{O}(\frac{1}{\varepsilon^2})$, Algorithm 1 generates a $\mathcal{O}(\varepsilon)$ -Pareto optimality of cooperative MARL.

To evaluate the performance of Algorithm 1 and to validate our theoretical findings, we describe the deployment of block GMFC in the multi-agent system in Algorithm 2, which 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 $\tilde{\pi} \in \widetilde{\Pi}_M$ 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 $m(i) = \underset{m \in [M]}{\arg \min} |\frac{i}{N} - \frac{m}{M}|$ 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

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

313 4.1. Proof of Theorem 3.7

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

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

Lemma 4.1 shows the convergence of the neighborhood empirical measure to the neighborhood mean-field measure.

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

$$\sum_{i=1}^{N} \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \mathbb{E}\left[\|\mu_{t}^{i, W_{N}} - \mu_{t}^{\alpha, W}\|_{1} \right] d\alpha \to 0, \quad as \ N \to \infty,$$
(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 $\mathcal{O}(\frac{1}{\sqrt{N}})$, then

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

Proof of Lemma 4.1 We first prove (4.2) under the condition (C1) and then show (4.2) also holds under the condition (C2). **Case 1:** $\xi_{i,j}^N = W_N(\frac{i}{N}, \frac{j}{N})$. Note that under the condition (C1), $\mu_t^{i,W_N} = \int_{\mathcal{I}} W_N(\frac{i}{N}, \beta) \mu_t^{N,\beta} d\beta$ by the definition of $\mu_t^{N,\alpha}$ in (4.1). Then

$$\begin{split} &\sum_{i=1}^{N} \int_{(\frac{i-1}{N},\frac{i}{N}]} \mathbb{E} \big[\| \mu_{t}^{i,W_{N}} - \mu_{t}^{\alpha,W} \|_{1} \big] d\alpha \\ &= \sum_{i=1}^{N} \int_{(\frac{i-1}{N},\frac{i}{N}]} \mathbb{E} \big[\Big\| \int_{\mathcal{I}} W_{N}(\frac{i}{N},\beta) \mu_{t}^{N,\beta} d\beta - \int_{\mathcal{I}} W(\alpha,\beta) \mu_{t}^{\beta} d\beta \Big\|_{1} \big] d\alpha \\ &\leq \sum_{i=1}^{N} \int_{(\frac{i-1}{N},\frac{i}{N}]} \mathbb{E} \big[\Big\| \int_{\mathcal{I}} W_{N}(\frac{i}{N},\beta) \mu_{t}^{N,\beta} d\beta - \int_{\mathcal{I}} W_{N}(\frac{i}{N},\beta) \mu_{t}^{\beta} d\beta \Big\|_{1} \big] d\alpha \\ &+ \sum_{i=1}^{N} \int_{(\frac{i-1}{N},\frac{i}{N}]} \mathbb{E} \big[\Big\| \int_{\mathcal{I}} W_{N}(\frac{i}{N},\beta) \mu_{t}^{\beta} d\beta - \int_{\mathcal{I}} W(\alpha,\beta) \mu_{t}^{\beta} d\beta \Big\|_{1} \big] d\alpha \\ &= : I_{1} + I_{2}. \end{split}$$

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

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

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 $\mathcal{O}(\frac{1}{\sqrt{N}})$.

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

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$$I_{2} = \sum_{i=1}^{N} \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right)} \left\| \int_{\mathcal{I}} W_{N}\left(\frac{\lceil N\alpha \rceil}{N}, \beta\right) \mu_{t}^{\beta} d\beta - \int_{\mathcal{I}} W(\alpha, \beta) \mu_{t}^{\beta} d\beta \right\|_{1} d\alpha$$

$$= \sum_{i=1}^{N} \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right)} \left\| \int_{\mathcal{I}} W_{N}(\alpha, \beta) \mu_{t}^{\beta} d\beta - \int_{\mathcal{I}} W(\alpha, \beta) \mu_{t}^{\beta} d\beta \right\|_{1} d\alpha$$

$$= \int_{\mathcal{I}} \left\| \int_{\mathcal{I}} W_{N}(\alpha, \beta) \mu_{t}^{\beta} d\beta - \int_{\mathcal{I}} W(\alpha, \beta) \mu_{t}^{\beta} d\beta \right\|_{1} d\alpha$$

$$= \sum_{s \in \mathcal{S}} \int_{\mathcal{I}} \left| \int_{\mathcal{I}} W_{N}(\alpha, \beta) \mu_{t}^{\beta}(s) d\beta - \int_{\mathcal{I}} W(\alpha, \beta) \mu_{t}^{\beta}(s) d\beta \right| d\alpha$$

$$\to 0,$$

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

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

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

³³² Case 2: $\xi_{i,j}^N$ are random variables with Bernoulli $(W_N(\frac{i}{N},\frac{j}{N}))$.

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

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 $\mathcal{O}(\frac{1}{\sqrt{N}})$. Therefore, it is enough to estimate I_1 .

$$I_{1} = \mathbb{E} \left\| \frac{1}{N} \sum_{j=1}^{N} \xi_{ij}^{N} \delta_{s_{t}^{j}} - \int_{\mathcal{I}} W_{N}(\frac{i}{N}, \beta) \mu_{t}^{N, \beta} d\beta \right\|_{1}$$

$$\leq \mathbb{E} \left[\mathbb{E} \left[\sup_{f: \mathcal{S} \to \{-1, 1\}} \left\{ \frac{1}{N} \sum_{j=1}^{N} \xi_{ij}^{N} f(s_{t}^{j}) - \frac{1}{N} \sum_{j=1}^{N} W_{N}(\frac{i}{N}, \frac{j}{N}) f(s_{t}^{j}) \right\} \middle| s_{t}^{1}, \dots, s_{t}^{N} \right] \right].$$

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 , $\left\{\xi_{ij}^N f(s_t^j) - W_N(\frac{i}{N}, \frac{j}{N}) f(s_t^j)\right\}_{j=1}^N$ is a sequence of independent mean-zero random variables bounded in [-1, 1] due to $\mathbb{E}[\xi_{i,j}^N] = W_N(\frac{i}{N}, \frac{j}{N})$. This implies that each $\xi_{ij}^N f(s_t^j) - W_N(\frac{i}{N}, \frac{j}{N}) f(s_t^j)$ is a sub-Gaussian with variance bounded by 4. As a result, conditioned on s_t^1, \ldots, s_t^N , $\left\{\frac{1}{N}\sum_{j=1}^N \xi_{ij}^N f(s_t^j) - \frac{1}{N}\sum_{j=1}^N W_N(\frac{i}{N}, \frac{j}{N}) f(s_t^j)\right\}_{i=1}^N$ is a mean-zero sub-Gaussian random variable with variance $\frac{4}{N}$. By the equation (2.66) in [51], we have

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

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

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

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

$$\sup_{\{g^{\alpha}\}_{\alpha\in\mathcal{I}}\in\mathcal{G}}\sum_{i=1}^{N}\int_{(\frac{i-1}{N},\frac{i}{N}]}\left|\mathbb{E}[g^{\alpha}(s_{t}^{i})-g^{\alpha}(s_{t}^{\alpha})]\right|d\alpha\to0,\tag{4.3}$$

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 $\mathcal{O}(\frac{1}{\sqrt{N}})$, then

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

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

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

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

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

$$(4.4)$$

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

First term of (4.4).

$$\begin{split} I &= \sum_{i=1}^{N} \int_{(\frac{i-1}{N}, \frac{i}{N}]} \left| \mathbb{E} \left[l_{g^{\alpha}}^{\frac{i}{N}}(s_{t}^{i}, \mu_{t}^{i, W_{N}}, \pi^{i}) \right] - \mathbb{E} \left[l_{g^{\alpha}}^{\alpha}(s_{t}^{i}, \mu_{t}^{\alpha, W}, \pi^{i}) \right] \right| d\alpha \\ &\leq M_{g} \Big(L_{P} \sum_{i=1}^{N} \int_{(\frac{i-1}{N}, \frac{i}{N}]} \mathbb{E} \left[\| \mu_{t}^{i, W_{N}} - \mu_{t}^{\alpha, W} \|_{1} \right] d\alpha + \tilde{L}_{P} \sum_{i=1}^{N} \int_{(\frac{i-1}{N}, \frac{i}{N}]} |\alpha - \frac{i}{N}| d\alpha \Big) \\ &\to 0, \quad \text{as } N \to \infty \end{split}$$

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

Second term of (4.4). One can view $l_{g^{\alpha}}^{\alpha}(s, \mu_{t}^{\alpha,W}, \pi^{i})$ as a function of $s \in \mathcal{S}$ for any fixed $\mu_{t}^{\alpha,W}$ 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 independent of $\mu_{t}^{\alpha,W}, \pi^{i}$. Since (4.3) holds at t, then

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

$$\to 0, \text{ as } N \to \infty.$$

Third term of (4.4).

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

$$\leq M_{g} \sum_{i=1}^{N} \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \mathbb{E} \left[\|\pi^{i}(s_{t}^{\alpha}) - \pi^{\alpha}(s_{t}^{\alpha})\|_{1} \right] d\alpha$$

$$\leq M_{g} L_{\Pi} \sum_{i=1}^{N} \int_{\left(\frac{i-1}{N}, \frac{i}{N}\right]} \max_{\alpha \in \left(\frac{i-1}{N}, \frac{i}{N}\right]} \left| \frac{i}{N} - \alpha \right| d\alpha$$

$$= \mathcal{O}(\frac{1}{N}),$$

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

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

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

Proof of Theorem 3.7

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

$$(4.5)$$

where we use (3.8) in the second inequality.

First term of (4.5).

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

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

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

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

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

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

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

Third term of (4.5).

$$III \leq \sup_{\boldsymbol{\pi}} L_r \sum_{t=0}^{\infty} \gamma^t \sum_{i=1}^{N} \int_{(\frac{i-1}{N}, \frac{i}{N}]} \max_{s \in \mathcal{S}} \|\pi^i(s) - \pi^\alpha(s)\|_1 d\alpha$$
$$\leq L_r \tilde{L}_{\Pi} \sup_{\boldsymbol{\pi}} \sum_{t=0}^{\infty} \gamma^t \sum_{i=1}^{N} \int_{(\frac{i-1}{N}, \frac{i}{N}]} |\frac{i}{N} - \alpha| d\alpha$$
$$= \mathcal{O}(\frac{1}{N}).$$

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

365 4.2. Proof of Theorem 3.8

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

$$\widetilde{V}^{M}(\widetilde{\boldsymbol{\mu}}) := \sup_{\widetilde{\boldsymbol{\pi}} \in \widetilde{\mathbf{\Pi}}_{M}} \widetilde{J}^{M}(\widetilde{\boldsymbol{\mu}}, \widetilde{\boldsymbol{\pi}})$$

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

The associated Q function of (4.7) is defined as

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

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

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

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

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

Proof of Lemma 4.3 First, define $\frac{M_r}{1-\gamma}$ -bounded function space $\mathcal{Q} := \{f : \widetilde{\mathcal{M}}_M \times \widetilde{\Pi}_M \rightarrow [-\frac{M_r}{1-\gamma}, \frac{M_r}{1-\gamma}]\}$. Then we define a Bellman operator $B : \mathcal{Q} \to \mathcal{Q}$

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

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

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

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

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

$$\begin{split} \tilde{Q}^{\tilde{\pi}^{*}}(\tilde{\mu},\tilde{\pi}) &= \tilde{R}(\tilde{\mu},\tilde{\pi}) + \gamma \tilde{Q}^{\tilde{\pi}^{*}}(\tilde{\Phi}(\tilde{\mu},\tilde{\pi}),\tilde{\pi}^{*}) \\ &= \tilde{R}(\tilde{\mu},\tilde{\pi}) + \gamma \sup_{\tilde{\pi}' \in \widehat{\Pi}_{M}} \tilde{Q}(\tilde{\Phi}(\tilde{\mu},\tilde{\pi}),\tilde{\pi}') = \tilde{Q}(\tilde{\mu},\tilde{\pi}), \end{split}$$

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

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

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

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

389 From (4.8) and (3.13),

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

390 By induction, we obtain

$$\frac{1}{M} \sum_{m=0}^{M-1} \|\tilde{\mu}_{t}^{\alpha_{m}} - \tilde{\mu}_{n,t}^{\alpha_{m}}\|_{1}$$

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

$$- \sum_{s \in S} \sum_{a \in A} P^{\alpha_{m}}(s'|s, a, \tilde{\mu}_{n,t-1}^{\alpha_{m}, W}) \tilde{\mu}_{n,t-1}^{\alpha_{m}}(s) \tilde{\pi}(\alpha|s, \tilde{\mu}_{n,t-1}^{\alpha_{m}, W}) \|$$

$$\leq (L_{P} + L_{\Pi} + 1) \cdot \frac{1}{M} \sum_{m=0}^{M-1} \|\tilde{\mu}_{t-1}^{\alpha} - \tilde{\mu}_{n,t-1}^{\alpha}\|_{1}$$

$$\leq \dots \leq (L_{P} + L_{\Pi} + 1)^{(t-1)} \frac{1}{M} \sum_{m=0}^{M-1} \|\tilde{\mu}_{1}^{\alpha} - \tilde{\mu}_{n,1}^{\alpha}\|_{1}$$

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

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

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

Now we prove Theorem 3.8.

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

see ensemble
$$\tilde{\pi}^* \in \Pi_M$$
.

397 4.3. Proof of Theorem 3.9

We first prove the following Lemma, which shows that GMFC and block GMFC become 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

$$\sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right]} \|\mu_{t}^{\alpha, W} - \tilde{\mu}_{t}^{\alpha_{m}, W}\|_{1} d\alpha \leq \left[(1 + L_{P} + L_{\Pi})^{t} - 1 \right] \frac{\tilde{L}_{\Pi} + \tilde{L}_{P} + 2(L_{P} + L_{\Pi})L_{W}}{M} + \frac{2L_{W}}{M},$$
$$\sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right]} \|\mu_{t}^{\alpha} - \tilde{\mu}_{t}^{\alpha_{m}}\|_{1} d\alpha \leq \left[(1 + L_{P} + L_{\Pi})^{t} - 1 \right] \frac{\tilde{L}_{\Pi} + \tilde{L}_{P} + 2(L_{P} + L_{\Pi})L_{W}}{M}.$$

Proof of Lemma 4.5

$$\sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right]} \|\mu_{t}^{\alpha, W} - \tilde{\mu}_{t}^{\alpha_{m}, W}\|_{1} d\alpha \qquad (4.9)$$

$$\leq \sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right]} \|\mu_{t}^{\alpha, W} - \mu_{t}^{\alpha_{m}, W}\|_{1} d\alpha + \frac{1}{M} \sum_{m=1}^{M} \|\mu_{t}^{\alpha_{m}, W} - \bar{\mu}_{t}^{\alpha_{m}, W}\|_{1}$$

$$+ \frac{1}{M} \sum_{m=1}^{M} \|\bar{\mu}_{t}^{\alpha_{m}, W} - \tilde{\mu}_{t}^{\alpha_{m}, W}\|_{1},$$

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where $\bar{\mu}^{\alpha_m,W} := \frac{1}{M} \sum_{m'=1}^{M} W(\alpha_m, \alpha_{m'}) \mu^{\alpha_{m'}}$. 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 Lipschitz continuity of W in Assumption 3.3, 402 403

$$\sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right]} \|\mu_{t}^{\alpha, W} - \mu_{t}^{\alpha_{m}, W}\|_{1} d\alpha \leq \sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right]} \|\mu_{t}^{\alpha} - \mu_{t}^{\alpha_{m}}\|_{1} d\alpha + \frac{L_{W}}{M}, \quad (4.10)$$

$$\frac{1}{M} \sum_{m=1}^{M} \|\mu_{m}^{\alpha, W} - \mu_{m}^{\alpha_{m}, W}\|_{1} \leq L_{W}$$

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

$$\frac{1}{M}\sum_{m=1}^{M} \|\bar{\mu}_{t}^{\alpha_{m},W} - \tilde{\mu}_{t}^{\alpha_{m},W}\|_{1} = \frac{1}{M}\sum_{m=1}^{M} \|\mu_{t}^{\alpha_{m}} - \tilde{\mu}_{t}^{\alpha_{m}}\|_{1}.$$
(4.12)

404 Plugging these into (4.9),

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

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

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

$$\sum_{m=1}^{M} \int_{\left(\frac{m-1}{M}, \frac{m}{M}\right]} \|\mu_{t}^{\alpha} - \mu_{t}^{\alpha_{m}}\|_{1} d\alpha + \frac{1}{M} \sum_{m=1}^{M} \|\mu_{t}^{\alpha_{m}} - \tilde{\mu}_{t}^{\alpha_{m}}\|_{1} = A_{t}.$$
 (4.15)

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

408 that $A_0 = 0$.

$$\begin{aligned} & = \sum_{m=1}^{M} \int_{(\frac{m-1}{M}, \frac{m}{M}]} \|\mu_{t+1}^{\alpha} - \mu_{t+1}^{\alpha_{m}}\|_{1} d\alpha + \frac{1}{M} \sum_{m=1}^{M} \|\mu_{t+1}^{\alpha_{m}} - \tilde{\mu}_{t+1}^{\alpha_{m}}\|_{1} \\ & = \sum_{m=1}^{M} \int_{(\frac{m-1}{M}, \frac{m}{M}]} \left\|\sum_{s \in \mathcal{S}} \sum_{a \in \mathcal{A}} \left(P^{\alpha}(\cdot | s, \mu_{t}^{\alpha, W}, a) \pi^{\alpha}(a | s, \mu_{t}^{\alpha, W}) \mu_{t}^{\alpha}(s) \right. \\ & \left. -P^{\alpha_{m}}(\cdot | s, a, \mu_{t}^{\alpha_{m}, W}) \mu_{t}^{\alpha_{m}}(s) \pi^{\alpha_{m}}(a | s, \mu_{t}^{\alpha_{m}, W}) \right) \right\|_{1} d\alpha \\ & \left. + \frac{1}{M} \sum_{m=1}^{M} \left\|\sum_{s \in \mathcal{S}} \sum_{a \in \mathcal{A}} \left(P^{\alpha_{m}}(\cdot | s, \mu_{t}^{\alpha_{m}, W}, a) \pi^{\alpha_{m}}(a | s, \mu_{t}^{\alpha_{m}, W}) \mu_{t}^{\alpha_{m}}(s) \right. \\ & \left. -P^{\alpha_{m}}(\cdot | s, a, \tilde{\mu}_{t}^{\alpha_{m}, W}) \tilde{\mu}_{t}^{\alpha_{m}}(s) \tilde{\pi}^{\alpha_{m}}(a | s, \tilde{\mu}_{t}^{\alpha_{m}, W}) \right) \right\|_{1} \\ & \leq \sum_{m=1}^{M} \int_{(\frac{m-1}{M}, \frac{m}{M}]} \left((L_{P} + L_{\Pi}) \cdot \|\mu_{t}^{\alpha, W} - \mu^{\alpha_{m}, W}\|_{1} + \frac{\tilde{L}_{H}}{M} + \|\mu_{t}^{\alpha} - \mu_{t}^{\alpha_{m}}\|_{1} \right) d\alpha \\ & \left. + \frac{1}{M} \sum_{m=1}^{M} \left((L_{P} + L_{\Pi}) \cdot \|\mu_{t}^{\alpha_{m}, W} - \tilde{\mu}^{\alpha_{m}, W}\|_{1} + \frac{\tilde{L}_{P}}{M} + \|\mu_{t}^{\alpha_{m}} - \tilde{\mu}_{t}^{\alpha_{m}}\|_{1} \right) \right. \\ & \leq (1 + L_{P} + L_{\Pi}) A_{t} + (\tilde{L}_{\Pi} + \tilde{L}_{P} + 2(L_{P} + L_{\Pi}) L_{W}) \frac{1}{M}, \end{aligned}$$

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

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

412

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

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

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

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

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

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

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

$$\begin{aligned} \sup_{\boldsymbol{\pi}\in\boldsymbol{\Pi}} \left| \tilde{J}^{M}(\boldsymbol{\mu},\boldsymbol{\pi}) - J(\boldsymbol{\mu},\boldsymbol{\pi}) \right| \\ &\leq \sup_{\boldsymbol{\pi}\in\boldsymbol{\Pi}} \sum_{t=0}^{\infty} \gamma^{t} \left| \tilde{R}(\tilde{\boldsymbol{\mu}}_{t},\tilde{\boldsymbol{\pi}}(\tilde{\boldsymbol{\mu}}_{t})) - R(\boldsymbol{\mu}_{t},\boldsymbol{\pi}(\boldsymbol{\mu}_{t})) \right| \\ &\leq \sup_{\boldsymbol{\pi}\in\boldsymbol{\Pi}} \sum_{t=0}^{\infty} \gamma^{t} \left| \tilde{R}(\tilde{\boldsymbol{\mu}}_{t},\tilde{\boldsymbol{\pi}}(\tilde{\boldsymbol{\mu}}_{t})) - R(\boldsymbol{\mu}_{t},\tilde{\boldsymbol{\pi}}(\boldsymbol{\mu}_{t})) \right| + \sup_{\boldsymbol{\pi}\in\boldsymbol{\Pi}} \sum_{t=0}^{\infty} \gamma^{t} \left| R(\boldsymbol{\mu}_{t},\tilde{\boldsymbol{\pi}}(\boldsymbol{\mu}_{t})) - R(\boldsymbol{\mu}_{t},\boldsymbol{\pi}(\boldsymbol{\mu}_{t})) \right| \\ &\coloneqq I + II. \end{aligned}$$

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

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

423 By Lemma 4.5,

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

For the term II, 424

$$\begin{split} \sup_{\boldsymbol{\pi}\in\boldsymbol{\Pi}} \sum_{t=0}^{\infty} \gamma^t \Big| R(\boldsymbol{\mu}_t, \tilde{\boldsymbol{\pi}}(\boldsymbol{\mu}_t)) - R(\boldsymbol{\mu}_t, \boldsymbol{\pi}(\boldsymbol{\mu}_t)) \Big| \\ &\leq \sup_{\boldsymbol{\pi}\in\boldsymbol{\Pi}} \sum_{t=0}^{\infty} \gamma^t M_r \sum_{m=1}^{M} \int_{(\frac{m-1}{M}, \frac{m}{M}]} \max_{s\in\mathcal{S}} \|\pi^{\alpha} - \pi^{\alpha^{m}}\|_1 d\alpha \\ &+ \sup_{\boldsymbol{\pi}\in\boldsymbol{\Pi}} \sum_{t=0}^{\infty} \gamma^t M_r \sum_{m=1}^{M} \int_{(\frac{m-1}{M}, \frac{m}{M}]} \|\boldsymbol{\mu}_t^{\alpha, W} - \tilde{\boldsymbol{\mu}}_t^{\alpha_{m}, W}\|_1 d\alpha \\ &\leq \frac{C(\gamma, L_{\Pi}, L_P, L_W, L_r, M_r)}{M}. \end{split}$$

425

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

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

where by (3.8), $\boldsymbol{\pi}^{N,*} := \sum_{i=1}^{N} \pi^{i,*} \mathbf{1}_{\alpha \in (\frac{i-1}{N}, \frac{i}{N}]}$ From Theorem 3.7, for any $\varepsilon > 0$, there exists N_{ε} such that for all $N \ge N_{\varepsilon}$ 429

430

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

Then we have 431

$$\geq \underbrace{\begin{array}{l} J_{N}(\mu,\tilde{\pi}^{1,*},\ldots,\tilde{\pi}^{N,*}) - J_{N}(\mu,\pi^{1,*},\ldots,\pi^{N,*}) \\ \geq \underbrace{J_{N}(\mu,\tilde{\pi}^{1,*},\ldots,\tilde{\pi}^{N,*}) - J(\mu,\tilde{\pi}^{*})}_{I_{1}} + \underbrace{J(\mu,\tilde{\pi}^{*}) - \tilde{J}_{M_{\varepsilon}}(\mu,\tilde{\pi}^{*})}_{I_{2}} \\ + \underbrace{\tilde{J}^{M_{\varepsilon}}(\mu,\tilde{\pi}^{*}) - \tilde{J}^{M_{\varepsilon}}(\mu,\pi^{N,*})}_{I_{3}} + \underbrace{\tilde{J}^{M_{\varepsilon}}(\mu,\pi^{N,*}) - J_{N}(\mu,\pi^{1,*},\ldots,\pi^{N,*})}_{I_{4}} \\ \geq \underbrace{\frac{\varepsilon}{3} - \frac{\varepsilon}{3} - \frac{\varepsilon}{3}}_{3} - \varepsilon.$$

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

5. Experiments 435

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

438 5.1. SIS Graphon Model

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

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

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

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

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

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

where c_1 represents the cost of being infected such as the cost of medical treatment, c_2 represents the cost of keeping social distance, and c_3 represents the penalty of going out if the agent is infected.

In our experiment, we set $\beta_1=0.8$, $\beta_2=0$, $\delta=0.3$ for the transition dynamics and $c_1=2$, $c_2=0.3$, $c_3=0.5$ for the reward function. The initial mean field μ_0 is taken as the uniform 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 $S = \{0, 1, ..., K - 1\}, K \in \mathbb{N}$, 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

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

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

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

Here considering the heterogeneity of agents, we use $W(\alpha, \beta)$ to denote the *importance* effect 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 by other agents and c_2 is the cost of taking action a_t .

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

462 5.3. Performance of N-agent GMFC on Multi-Agent System

For both models, we use PPO [47] to train the block GMFC agent in the infinite-agent 463 environment and obtain the policy ensembles and further use Algorithm 2 to deploy them 464 in the finite-agent environment. We test the performance of N-agent GMFC with 10 blocks 465 to different numbers of agents, i.e., from 10 to 100. For each case, we run 1000 times of 466 simulations and show the mean and standard variation (Green shadows in Figure 1 and 467 Figure 2) of the mean episode reward. We can see that in both scenarios and for different 468 types of graphons, the mean episode rewards of the N-agent GMFC become increasingly 469 close to that of block GMFC as the number of agents grows. (See Figure 1 and Figure 2). 470 This verifies our theoretical findings empirically. 471



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



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

472 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-decentralizedexecution(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 comparable 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 performance 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.

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			
Graphon Type	111	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
2 Stochastic Block 5 10	-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	М	7	Algorithm		
Graphon Type		N-agent GMFC I-DQN I-PPO		QMIX	
	2	-5.21	-5.11	-5.31	-6.05
Erdős Rényi	5	-5.21	-5.30	-5.26	-6.13
	10	-5.21	-5.14	-5.27	-5.21
	2	-5.16	-5.21	-5.37	-5.88
Stochastic Block	5	-5.10	-5.19	-5.31	-5.70
	10	-5.09	-5.05	-5.28	-5.27
	2	-5.02	-5.21	-5.27	-5.35
Random Geometric	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

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

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.

Algorithms	GMFC PPO	I-DQN	I-PPO	QMIX
Learning rate	0.0005	0.0005	0.0001	0.00005
Learning rate decay	True	True	True	False
Discount factor	0.95	0.95	0.95	0.95
Batch size	128	128	128	128
KL coefficient	0.2		0.2	-
KL target	0.01	-	0.01	-
Buffer size	-	2000	-	2000
Target network update frequency	-/~	2000	-	1000

Table	3:	RL	Algorithm	Setting
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506 6. Conclusion

In this work, we have proposed a discrete-time GMFC framework for MARL with nonuni-507 form interactions and heterogeneous reward functions and transition functions across the 508 agents on dense graphs. Theoretically, we have shown that under suitable assumptions, 509 GMFC approximates MARL well with approximation error of order $\mathcal{O}(\frac{1}{\sqrt{N}})$. To reduce the 510 dimension of GMFC, we have introduced block GMFC by discretizing the graphon index 511 and shown that it also approximates MARL well. Empirical studies on several examples 512 have verified the plausibility of the GMFC framework. For future research, we wish to ex-513 plore more on how to extract the optimal policy of cooperative MARL without the simulator 514 for population state distribution ensemble and to extend our framework to heterogeneous 515 MARL on sparse graphs. 516

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641 Declaration of Competing Interest

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

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