Agent-Level Maximum Entropy Inverse Reinforcement Learning for Mean Field Games

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Abstract

Mean field games (MFG) facilitate the application of reinforcement learning (RL) in large-scale multi-agent systems, through reducing interplays among agents to those between an individual agent and the average effect from the population. However, RL agents are notoriously prone to unexpected behaviours due to the reward mis-specification. Although inverse RL (IRL) holds promise for automatically acquiring suitable rewards from demonstrations, its extension to MFG is challenging due to the complicated notion of mean-field-type equilibria and the coupling between agent-level and population-level dynamics. To this end, we propose a novel IRL framework for MFG, called Mean Field IRL (MFIRL), where we build upon a new equilibrium concept and the maximum entropy IRL framework. Crucially, MFIRL is brought forward as the first IRL method that can recover the agent-level (ground-truth) reward functions for MFG. Experiments show the superior performance of MFIRL on sample efficiency, reward recovery and robustness against varying environment dynamics, compared to the state-of-the-art method.

1 Introduction

Although reinforcement learning (RL) has achieved significant success in many multi-agent tasks, its application is often hindered by a large number of agents. As the population of agents grows, the computational complexity of a (Nash) equilibrium grows exponentially due to the explosion of joint state-action spaces. For anonymous and homogeneous agents, though, a natural way to simplify the model is to consider the asymptotical limit, i.e., assuming the number of agents approaches infinity. This assumption warrants the formulation of mean field games (MFG) that analyse system behaviours in the asymptotic limit. Through mean field approximation, MFG leverages an empirical distribution, termed mean field, to represent aggregated behaviours of the population at large. The interactions among agents are thus reduced to those between a single representative agent and the population seen as a whole. This reduction to a dual-view interplay motivates the solution concept of mean field Nash equilibrium (MFNE), where an agent’s policy is a best response to the mean field, which is in turn consistent with the policy. Importantly, MFNE is shown to constitute an approximate Nash equilibrium in the corresponding finite-agent game. In this sense, MFG facilitates RL in large-scale multi-agent systems, which inspires the recent emergence of many RL methods for computing MFNE and its variants.

However, as an inherited issue from RL, these burgeoning RL methods for MFG can result in unexpected behaviours if the reward function does not capture all important aspects of a task. Hand-tuning rewards for RL agents is challenging as it requires human domain knowledge. In MFG, since the reward of an agent is coupled with the population via the mean field, manually designing reward functions becomes more difficult. Inverse reinforcement learning (IRL) provides a framework to automatically acquire reward functions from expert demonstrations. IRL assumes that...
We test MFIRL on five simulated MFG tasks. Experimental results demonstrate the outperformance which resolves the policy ambiguity by extending MaxEnt IRL to MFG: (1) We build MFIRL upon would prevent us from directly maximising the likelihood of expert demonstrations. Second, the reward ambiguity can be mitigated by supplying a potential-based reward shaping function \[ \text{potential-based reward shaping function} \] – a reward transformation that ensures the policy invariance – as the reward regularisation \[ [33] \]. Combining the two techniques gives IRL methods that can learn robust reward functions \[ [18, 46] \]. Unfortunately, this paradigm is not suitable for MFG due to the following issues. First and foremost, extending MaxEnt IRL to MFG is challenging due to two reasons: (1) the equilibrium solution concept of MFNE is incompatible with MaxEnt IRL as it assumes that agents never take sub-optimal actions. As a result, it cannot provide a tractable trajectory distribution which we can use to maximise the likelihood of expert demonstrations. (2) Since the agent-level and population-level dynamics are coupled (the policy and mean field are interdependent), the mean field (under an equilibrium) is analytically intractable to express in terms of rewards. Consequently, even if we have a compatible solution concept, the presence of the mean field in the reward function would prevent us from directly maximising the likelihood of expert demonstrations. Second, the reward ambiguity presents the requirement of a reward shaping function for MFG that can ensure the invariance of the set of mean-field-type equilibria, which has yet to be explored in the literature.

Notably, studying IRL for MFG is new in the literature albeit a recent attempt relies on reformulating MFNE as an optimal solution to a Markov decision processes (MDP) \[ [44] \], where the mean field and policy in a MFG serve as the state and action in the MDP. Accordingly, performing IRL on this MDP infers the population’s aggregated societal reward. Although this “centralised” setting can sidestep the above two problems in extending MaxEnt IRL to MFG, several implicit flaws are brought. First, the reformulation holds only for the MFNE that is socially optimal, as it presupposes that agents are cooperative to optimise a common societal reward. Thus, the inference would be biased if expert demonstrations are sampled from an ordinary MFNE as multiple MFNE might coexist \[ [40, 3] \]. Second, sampling mean fields and policies at the population level requires the access to each agent’s state-action configuration at the agent level, which might result in sample inefficiency.

In this paper, considering the insufficient investigation of IRL for MFG and flaws of population-level inference \[ [44] \], we study IRL for MFG from the agent level, i.e., inferring ground-truth reward functions. Our primary contribution is a novel IRL framework for MFG, called mean field IRL (MFIRL), which resolves the policy ambiguity by extending MaxEnt IRL to MFG: (1) We build MFIRL upon a new solution concept, termed entropy regularised MFNE (ERMFNE), which incorporates the causal entropy regularisation into rewards, has a good property of uniqueness, and can characterise the trajectory distribution induced by a reward function in a principle way (see Proposition \[ 1 \]). (2) MFIRL is capable to decouple agent’s and population’s dynamics without sacrificing the asymptotic consistency guarantee of the maximum likelihood estimation (see Theorem \[ 1 \]). To alleviate the reward ambiguity, we further give a mean-field-type potential-based reward shaping function \[ [33] \] that can preserve the invariance of ERMFNE (see Theorem \[ 2 \]). Meanwhile, thanks to the agent-level inference, MFIRL avoids the issues of biased inference and sample inefficient of population-level inference. We test MFIRL on five simulated MFG tasks. Experimental results demonstrate the outperformance of MFIRL over the population-level-inference method in sample efficiency, reward recovery and robustness against changing environment dynamics.

## 2 Preliminaries

### 2.1 Mean Field Games

To simplify the exposition, we restrict ourself to MFG with a large but finite number of agents \[ [36] \], finite state and action spaces and a finite time horizon \[ [16] \]. We will later show that our method requires no extra efforts to be applied to more general cases. First, consider an \( N \)-player game with state space \( \mathcal{S} \) and action space \( \mathcal{A} \). A joint state of \( N \) agents is a tuple \( (s^1, \ldots, s^N) \) \( \in \mathcal{S}^N \) where \( s^i \in \mathcal{S} \) is the state of the \( i \)th agent. As \( N \) goes large, instead of modelling each agent individually, MFG models a representative agent and collapses the joint state into an empirical distribution, called a mean field, given by \( \mu(s) \equiv \frac{1}{N} \sum_{i=1}^{N} 1_{\{s^i = s\}} \), where \( 1 \) denotes the indicator function. To describe
the game dynamics, write \( \mathcal{P}(\mathcal{X}) \) for the set of probability distributions over set \( \mathcal{X} \). The transition function \( \mathcal{P}(\mathcal{X}) \) specifies how states evolve at the agent-level, i.e., an agent’s next state depends on its current state, action, and the current mean field. This function also induces a transition of the mean field at the population level which maps a current mean field to the next mean field based on all agents’ current states and actions. Let \( T - 1 \geq 0 \) denote a finite time horizon. A mean field flow (MF flow) thus consists of a sequence of \( T \) mean fields \( \mu \triangleq \{ \mu_t \}_{t=0}^{T-1} \), where the initial value \( \mu_0 \) is given, and each \( \mu_t (0 < t < T) \) is the empirical distribution obtained by applying the transition above to \( \mu_{t-1} \). The running reward of an agent at each step is specified by the reward function \( r : \mathcal{S} \times \mathcal{A} \times \mathcal{P}(\mathcal{S}) \rightarrow \mathbb{R} \). The agent’s long-term reward is thus the sum \( \sum_{t=0}^{T-1} \gamma^t r(s_t, a_t, \mu_t) \), where \( \gamma \in (0, 1) \) is the discounted factor. Summarising the above, MFG is defined as the tuple \((\mathcal{S}, \mathcal{A}, p, \mu_0, r, \gamma)\). A time-varying stochastic policy in a MFG is \( \pi \triangleq \{ \pi_t \}_{t=0}^{T-1} \) where \( \pi_t : \mathcal{S} \rightarrow \mathcal{P}(\mathcal{A}) \) is the per-step policy at step \( t \), i.e., \( \pi_t \) directs the agent to choose action \( a_t \sim \pi_t(\cdot|s_t) \). Given MF flow \( \mu \) and policy \( \pi \), the agent’s expected return during the whole course of the game is written as \( J(\mu, \pi) \triangleq \mathbb{E}_{\mu, \pi} \left[ \sum_{t=0}^{T-1} \gamma^t r(s_t, a_t, \mu_t) \right] \), where \( s_0 \sim \mu_0, a_t \sim \pi_t(\cdot|s_t), s_{t+1} \sim p(\cdot|s_t, a_t, \mu_t) \).

2.2 The Solution Concept for MFG

An agent seeks an optimal policy so as to maximise the expected return. If a MF flow \( \mu \) is fixed, we will derive an induced MDP with a non-stationary transition function. An optimal policy of the induced MDP is called a best response to the corresponding fixed MF flow. We denote the set of all best-response policies to a fixed MF flow \( \mu \) by \( \Psi(\mu) \triangleq \arg \max_\pi J(\mu, \pi) \). However, since all agents optimise their policies simultaneously, the MF flow would shift. The solution thus needs to consider how the policy at the agent level affects MF flow at the population level. Since all agents are identical and rational, at optimality everyone would follow the same policy. Under this assumption, the dynamics of MF flow is governed by the (discrete-time) McKean-Vlasov (MKV) equation [9]:

\[
\mu_{t+1}(s') = \sum_{s \in \mathcal{S}} \mu_t(s) \sum_{a \in \mathcal{A}} \pi_t(a|s) p(s'|s, a, \mu_t).
\]

Denote \( \mu = \Phi(\pi) \) as the MF flow induced by a policy that fulfils MKV equation. The conventional solution concept for MFG is the mean field Nash equilibrium (MFNE), where agents adopt the same policy that is a best response to the MF flow, and in turn, the MF flow is consistent with the policy.

**Definition 1** (Mean Field Nash Equilibrium). A pair of MF flow and policy \((\mu^*, \pi^*)\) constitutes a mean field Nash equilibrium if \( \pi^* \in \Psi(\mu^*) \) and \( \mu^* = \Phi(\pi^*) \).

Shown in [36][11], a MFNE is guaranteed to exist under the standard assumptions that both the reward function and the transition function are continuous and bounded. Through defining any mapping \( \Psi : \mu \mapsto \pi \) that identifies a policy in \( \Psi(\mu) \), we get a composition \( \Gamma = \Phi \circ \Psi \), the so-called MFNE operator. Repeating the MFNE operator, we derive the fixed point iteration for the MF flow. The standard assumption for the uniqueness of MFNE is the contractivity of \( \Gamma \) [10][20]. However, the contractivity does not hold in general [11], which results in the coexistence of multiple MFNE.

2.3 Maximum Entropy Inverse Reinforcement Learning

We next give an overview of the maximum entropy inverse reinforcement learning (MaxEnt IRL) [48] under an MDP defined by \((\mathcal{S}, \mathcal{A}, p, \rho_0, r, \gamma)\), where \( r(s, a) \) is the reward function and the environment dynamics is determined by the transition function \( p(s'|s, a) \) and initial state distribution \( \rho_0(s) \). In (forward) RL, an optimal policy might not exist uniquely. The maximum entropy RL (MaxEnt RL) can solve this policy ambiguity by augmenting the expected return with a causal entropy [47] regularisation \( H(\pi) \triangleq \mathbb{E}_{\pi}[-\log \pi(\cdot|s)] \), i.e., the objective is to find a policy \( \pi^* \) such that \( \pi^* = \arg \max_\pi \mathbb{E}_{\tau \sim \pi} \left[ \sum_{t=0}^{T-1} \gamma^t r(s_t, a_t) + \beta H(\pi(\cdot|s_t)) \right] \), where \( \tau = \{(s_t, a_t)\}_{t=0}^{T-1} \) is a state-action trajectory sampled via \( s_0 \sim \rho_0, a_t \sim \pi(\cdot|s_t) \) and \( \beta > 0 \) controls relative importance of reward and entropy. Now, suppose we do not know the reward function \( \tau \) but have a set of demonstrated trajectories sampled from an unknown expert policy \( \pi^E \) obtained by the above MaxEnt RL procedure. MaxEnt IRL aims to infer the reward function \( \tau \) by rationalising expert demonstrations. Let \( r_{\omega}(s, a) \) denote an \( \omega \)-parameterised reward function. Shown in [47], with \( \beta = 1 \), a trajectory induced by the optimal policy found by MaxEnt RL can be characterised with an energy-based model:

\[
\Pr_\omega(\tau) \propto \rho_0(s_0) \exp \left( \sum_{t=0}^{T-1} \gamma^t r_{\omega}(s_t, a_t) \right) \prod_{t=0}^{T-1} p(s_{t+1}|s_t, a_t).
\]
MaxEnt IRL thus tunes the reward parameter $\omega$ by maximising the likelihood of demonstrations, which can be reduced to the following maximum likelihood estimation (MLE) problem:

$$\max_{\omega} \mathbb{E}_{\tau \sim \pi^E} [\log \Pr_{\omega}(\tau)] = \mathbb{E}_{\tau \sim \pi^E} \left[ \sum_{t=0}^{T-1} \gamma^t r_\omega(s_t, a_t) \right] - \log Z_\omega.$$ 

Here, $Z_\omega \triangleq \int_{\tau \sim \pi^E} \exp(\sum_{t=0}^{T-1} \gamma^t r_\omega(s_t, a_t))$ is the partition function of Eq. (2), i.e., an integral over all feasible trajectories. Computing $Z_\omega$ is intractable if state-action spaces are large or continuous.

To mitigate the reward ambiguity, where a class of reward functions can induce the same optimal policy, the works [13,14] further restricts the parameterised reward function to a specific structure by supplying a potential-based reward shaping function $f_\phi(s)$ as a regularisation term:

$$r_\omega,\phi(s_t, a_t, s_{t+1}) = r_\omega(s_t, a_t) + \gamma f_\phi(s_{t+1}) - f_\phi(s_t).$$

Shown in [13], under certain conditions, $r_\omega$ in the above reward structure will recover the ground-truth reward function up to a constant.

### 3 Method

#### 3.1 Problem Statement

The agent-level IRL for MFG aims to infer its ground-truth reward function from expert demonstrations. Formally, suppose we have no access to the reward function $r(s, a, \mu)$ but have a set of expert trajectories $D_E = \{(\tau_1, \ldots, \tau_M) \}_{j=1}^M$ sampled from a total number of $M$ game plays under an unknown equilibrium $(\mu^E, \pi^E)$. Each $\tau_j = ((s_{t_j}, a_{t_j})_{t=0}^{T-1}$ is the state-action trajectory of the $i$th agent in the $j$th game play. Also assume that $D_E$ provides the entire supervision signals, i.e., we cannot further communicate with experts for additional information [22]. Agent-level IRL for MFG asks for a reward function under which $(\mu^E, \pi^E)$ achieves an equilibrium. Note that at this stage, agent-level IRL for MFG is still ill-defined due to the aforementioned policy ambiguity and reward ambiguity. We address both issues in this section and derive a novel IRL framework for MFG.

#### 3.2 Entropy-Regularised Mean Field Nash Equilibrium

To address the policy ambiguity, we need to generalise MaxEnt IRL to MFG. However, the solution concept of MFNE cannot provide a tractable trajectory distribution which we can use in maximising the likelihood of demonstrated trajectories, as it requires the policy to be a strictly best response to the MF flow, whereas in MaxEnt IRL an expert takes sub-optimal actions with low probabilities due to the entropy regularisation. To resolve this issue, a natural way is to incorporate entropy regularisation into the objective of MFG. This inspires a new solution concept – entropy-regularised mean field Nash equilibrium (ERMFNE) – where an agent aims to maximise the entropy-regularised rewards:

$$\tilde{J}(\mu, \pi) \triangleq \mathbb{E}_{\mu, \pi} \left[ \sum_{t=0}^{T-1} \gamma^t (r(s_t, a_t, \mu_t) + \beta H(\pi_t(s_t)) \right].$$

**Definition 2** (Entropy-Regularised MFNE). A pair of MF flow and policy $(\mu^*, \pi^*)$ is called an entropy-regularised mean field Nash equilibrium if $\tilde{J}(\mu^*, \pi^*) = \max_{\mu, \pi} \tilde{J}(\mu, \pi)$ and $\mu^* = \Phi(\pi^*)$.

Note that a similar solution concept is independently proposed in [11] but is motivated from forward RL for MFG, in order to achieve more reliable convergence. Shown in Appendix [A.1] with entropy regularisation, the optimal policy $\tilde{\pi}$ to a MF flow $\mu$ exists uniquely and fulfils an energy based model

$$\tilde{\pi}(a_t|s_t) \propto \exp \left( \frac{1}{\beta} Q_{\text{soft}}^{\mu,\tilde{\pi}}(s_t, a_t, \mu_t) \right),$$

where $Q_{\text{soft}}^{\mu,\tilde{\pi}}(s_t, a_t, \mu) \triangleq r(s_t, a_t, \mu_t) + \mathbb{E}_{\tilde{\pi}} \left[ \sum_{\ell=t+1}^{T-1} \gamma^{t-\ell} (r(s_\ell, a_\ell, \mu_\ell) + H(\tilde{\pi}_\ell(s_\ell))) \right]$ denotes the soft $Q$-functions for MFG. Analogous to MFNE, ERMFNE exists for any temperatures $\beta > 0$ if the reward function and transition function are continuous and bounded [11]. Using $\hat{\Psi}(\mu) = \tilde{\pi}$ to denote the policy specified by Eq. (3), we obtain the ERMFNE operator $\hat{\Gamma} = \Phi \circ \hat{\Psi}$. It is shown in [11, Theorem 3] that $\hat{\Gamma}$ achieves a contraction under suitably large $\beta$, and thereby implies a unique ERMFNE. Since we can always adjust the relative importance of reward and entropy by scaling reward functions, without loss of generality, we assume $\beta = 1$ in the remainder of analysis.
Besides uniqueness, another good property of ERMFNE is that its induced trajectory distribution can be characterised with an energy-based formulation. Intuitively, fixing MF flow $\mu^*$, we can show that the induced MDP (with non-stationary dynamics) persists the property of the maximum entropy trajectory distribution, under the best-response policy $\pi^*$. The proof is deferred until Appendix A.1.

**Proposition 1.** Let $(\mu^*, \pi^*)$ be a ERMFNE with $\beta = 1$ for a MFG $(S, A, p, \mu_0, r, \gamma)$. A representative agent’s trajectory $\tau = \{(s_t, a_t)\}_{t=0}^{T-1}$ induced by $(\mu^*, \pi^*)$ fulfils the following generative process

$$\Pr(\tau) \propto \mu_0(s_0) \exp \left( \sum_{t=0}^{T-1} \gamma^t r(s_t, a_t, \mu^*_t) \right) \prod_{t=0}^{T-1} p(s_{t+1}|s_t, a_t, \mu^*_t).$$  \hspace{1cm} (4)

### 3.3 Mean Field Inverse Reinforcement Learning

From now on, we assume that expert trajectories are sampled from a unique ERMFNE $(\mu^E, \pi^E)$. Let $r_\omega(s, a, \mu)$ be an $\omega$-parameterised reward function and $(\mu^{\omega^*}, \pi^{\omega^*})$ denote the ERMFNE induced by $\omega$. Also assume $(\mu^E, \pi^E)$ is induced by some unknown true parameter $\omega^*$, i.e., $(\mu^E, \pi^E) = (\mu^{\omega^*}, \pi^{\omega^*})$.

According to Proposition 1, taking ERMFNE as the optimal notion allows us to rationalise the expert behaviours by maximising the likelihood of demonstrated trajectories with respect to the distribution defined by Eq. (4). Due to the homogeneity of agents, trajectories of all $N$ expert agents are drawn from the same maximum entropy distribution. Hence, we can tune $\omega$ by maximising the likelihood over trajectories of all $N$ expert agents, which can be reduced to the following MLE problem:

$$\max_{\omega} L(\omega) \triangleq \mathbb{E}_{\tau \sim \tau^E} \left[ \log \Pr(\tau(\omega)) \right]$$

$$= \frac{1}{M} \sum_{j=1}^{M} \frac{1}{N} \sum_{i=1}^{N} \sum_{t=0}^{T-1} \left( \gamma^t r_\omega(s^j_{s,t}, a^j_{s,t}, \mu^*_t) + \log p(s^j_{s,t+1}|s^j_{s,t}, a^j_{s,t}, \mu^*_t) \right) - \log Z_\omega,$$

where $Z_\omega$ is the partition function of the distribution defined in Eq. (4) such that

$$Z_\omega = \frac{M}{\sum_{j=1}^{M} \sum_{i=1}^{N} \exp \left( \sum_{t=0}^{T-1} \gamma^t r_\omega \left( s^i_{s,t}, a^i_{s,t}, \mu^*_t \right) \right) \prod_{t=0}^{T-1} p(s^i_{s,t+1}|s^i_{s,t}, a^i_{s,t}, \mu^*_t).}$$

The initial mean field $\mu_0$ is omitted in Eq. (5) and Eq. (6) since it does not depend on $\omega$.

However, directly optimising the MLE objective in Eq. (5) is intractable since we cannot analytically derive the induced MF flow $\mu^{\omega^*}$. In fact, this problem has its origin in the nature of MFG that the policy and MF flow are coupled with each other [23], as $\pi^* = \Psi(\mu^*)$ and in turn $\mu^* = \Phi(\pi^*)$. As a result, computing a ERMFNE is analytically intractable. Worse yet, the transition function $p(s, a, \mu)$ also depends on reward parameter $\omega$ due to the presence of $\mu^{\omega^*}$. This poses an extra layer of complexity since the environment dynamics is generally unknown in the real world.

While, notice that if we have access to an oracle MF flow, then the agent would be decoupled from the population. Inspired by this fact, we sidestep this problem by substituting $\mu^{\omega^*}$ with the empirical value of the expert MF flow estimated from expert demonstrations: For each sample of game play, we derive an empirical value of $\mu^E$, denoted by $\hat{\mu}^E$, by averaging the frequencies of occurrences of states, i.e., $\hat{\mu}^E(s) \triangleq \frac{1}{N} \sum_{i=1}^{N} \mathbb{I}_{\{s^i_{s,t} = s\}}$. By calculating the expectation over all $M$ game plays, we obtain an empirical estimation of the expert MF flow $\hat{\mu}^E = \frac{1}{M} \sum_{j=1}^{M} \hat{\mu}^E_j \approx \mu^E$. Meanwhile, by substituting $\hat{\mu}^E$ for $\mu^{\omega^*}$, the transition function $p(s_t, a_t, \mu^E_t)$ is decoupled from the reward parameter $\omega$ as $\mu^E$ does not depend on $\omega$, and henceforth being omitted in the likelihood function. Finally, with this substitution, we obtain a tractable version of the original MLE objective in Eq. (5):

$$\max_{\omega} \hat{L}(\omega; \mu^E) \triangleq \frac{1}{M} \sum_{j=1}^{M} \frac{1}{N} \sum_{i=1}^{N} \sum_{t=0}^{T-1} \gamma^t r_\omega \left( s^i_{s,t}, a^i_{s,t}, \hat{\mu}^E_t \right) - \log \hat{Z}_\omega,$$$$

where the partition function is simplified as $\hat{Z}_\omega \triangleq \frac{1}{M} \sum_{j=1}^{M} \sum_{i=1}^{N} \exp \left( \sum_{t=0}^{T-1} \gamma^t r_\omega \left( s^i_{s,t}, a^i_{s,t}, \hat{\mu}^E_t \right) \right)$.

Intuitively, one can interpret Eq. (7) in such a way that we maximise the likelihood of expert trajectories with respect to the trajectory distribution induced by the best-response policy to $\mu^E$.

Statistically, we use a likelihood function of a “mis-specified” model that treats the policy and MF flow as being independent, and replaces MF flow with its empirical value. With this manner, we construct an estimate of the true parameter $\omega^*$ by maximising a simplified form of the actual log-likelihood.
As mentioned earlier, IRL also faces the reward ambiguity. This issue is often referred as the effect of reward shaping [17, 18], which is a policy gradient method dedicated to maximising the entropy-regularised expected return. We implement soft Q-learning with adaptive samplers \( q^0 \) to sample a set of trajectories \( \mathcal{D}_{\text{samp}} \) and estimate \( Z_\omega \) as follows:

\[
\hat{Z}_\omega \approx \frac{1}{|\mathcal{D}_{\text{samp}}|} \sum_{\tau \sim \mathcal{D}_{\text{samp}}} \frac{\exp \left( \sum_{t=0}^{T-1} \gamma^t r_\omega(s_t, a_t, \hat{\mu}^E) \right)}{\prod_{t=0}^{T-1} q^{\theta_t}(a_t|s_t)}. \tag{8}
\]

The update of policy parameters \( \theta \) is interleaved with the update of the reward parameter \( \omega \). Intuitively, tuning \( q^0 \) can be considered as a policy optimisation procedure, which is to find the optimal policy induced by the current reward parameter, in order to minimise the variance of importance sampling. In the context of MFG, given the estimated expert MF flow \( \hat{\mu}^E \) and fixing the reward parameter \( \omega \), we obtain an induced finite-horizon MDP with the reward function \( r_\omega(s_t, a_t, \hat{\mu}^E) \) a non-stationary transition function \( p(s_{t+1}, a_t, \hat{\mu}^E) \). We design a forward RL solver for MFG that tunes \( q^0 \) using soft Q-learning [21], which is a policy gradient method dedicated to maximising the entropy-regularised expected return. We implement soft Q-learning with backward induction, i.e., tuning \( q^0 \) based on \( q^{\theta_{t+1}}, \ldots, q^{\theta_{T-1}} \) that are already well tuned. See Appendix B for detailed training procedures of \( q^0 \).

### 3.4 Mean-Field Potential-Based Reward Shaping

As mentioned earlier, IRL also faces the reward ambiguity. This issue is often referred as the effect of reward shaping [33], i.e., there is a class of reward transformations that induce the same set of optimal policies (equilibria for games), where IRL cannot identify the ground-truth one without prior knowledge on environments. It is shown that for any state-only potential function \( f : S \rightarrow \mathbb{R} \), the reward transformation \( r'(s_t, a_t, s_{t+1}) = r(s_t, a_t) + \gamma f(s_{t+1}) - f(s_t) \) (potential-based reward shaping) is the sufficient and necessary condition to ensure policy (equilibrium) invariance for both MDP [33] and stochastic games [14]. In the context of MFG, we show that for any potential function \( g : S \times \mathcal{P}(S) \rightarrow \mathbb{R} \), the potential-based reward shaping is the sufficient and necessary condition to ensure the invariance of both MFNE and ERMFNE.

**Theorem 2.** Let any \( S, A, \gamma \) be given. We say \( F : S \times A \times \mathcal{P}(S) \times S \times \mathcal{P}(S) \rightarrow \mathbb{R} \) is a potential-based reward shaping for MFG if there exists a real-valued function \( g : S \times \mathcal{P}(S) \rightarrow \mathbb{R} \) such that \( F(s_t, a_t, \mu_t, s_{t+1}, \mu_{t+1}) = g(s_{t+1}, \mu_{t+1}) - g(s_t, \mu_t) \). Then, \( F \) is sufficient and necessary to guarantee the invariance of the set of MFNE and ERMFNE in the sense that: **Sufficiency:** Every MFNE or ERMFNE in the MFG \( M' = (S, A, p, \mu_0, r + F, \gamma) \) is also a MFNE or ERMFNE in
$\mathcal{M} = (S, A, p, \mu_0, r, \gamma)$; \textbf{Necessity:} If $F$ is not a potential-based reward shaping, then there exist a initial mean field $\mu_0$, transition function $p$, horizon $T$, temperature $\beta$ (for ERMFNE only) and reward function $r$ such that no MFNE or ERMFNE in $\mathcal{M}'$ is an equilibrium in $\mathcal{M}$.

The proof is given in Appendix A.4. Intuitively, we prove the sufficiency using the same technique as in [33, 13] to show the invariance of the set of best-response policies to a MF flow. We then argue the necessity by finding a counter-example where an action-based reward transformation can change MFNE and ERMFNE. To mitigate the effecting of reward shaping, similar to the setting in IRL methods for MDP [13] and stochastic games [46], we assume that the parameterised reward function is in the following structure where a potential-based reward shaping serves as a regularisation term:

$$r_{\omega, \phi}^t(s_t, a_t, \mu_t, s_{t+1}, \mu_{t+1}) = r_\omega(s_t, a_t, \mu_t) + \gamma g_\phi(s_{t+1}, \mu_{t+1}) - g_\phi(s_t, \mu_t).$$

Here, $g_\phi$ is the $\phi$-parameterised potential function for MFG. We tune $\phi$ together with $\omega$, in order to recover a reward function with higher linear correlation to the ground truth one [18, 46]. As a summary, we name our algorithm the \textit{mean field IRL (MFIRL)} and present the pseudocode in Alg. 1.

\begin{algorithm}
\caption{Mean Field Inverse Reinforcement Learning (MFIRL)}
1: Input: MFG with parameters $(S, A, p, \mu_0, \gamma)$ and demonstrations $D_E = \{ (\tau^j_1, \ldots, \tau^j_{T^j}) \}^M_{j=1}$.
2: Initialization: reward parameter $\omega$ and potential function parameter $\phi$.
3: Estimate the empirical expert MF flow $\hat{\mu}_E$ from $D_E$.
4: for each epoch do
5: Train adaptive samplers $q^\theta$ with respect to $r_\omega$ using soft Q learning (Alg. 2 in Appendix B).
6: Sample a set of trajectories $D_{samp}$ using adaptive samplers $q^\theta$.
7: Estimate the partition function $Z_\omega$ from $D_{samp}$ according to Eq. (8).
8: Sample a minibatch of trajectories $D$ from $D_E$.
9: Update $\omega$ and $\phi$ according to the empirical gradients $\nabla_\omega \hat{L}$ and $\nabla_\phi \hat{L}$ of Eq. (7) on $D$.
10: end for
11: Output: Learned reward function $r_\omega$.
\end{algorithm}

4 Related Works and Discussions

RL for MFG. MFG were pioneered by [28] in the continuous setting. Mathematically, the dynamics of the system is governed by two stochastic differential equations: the Hamilton-Jacobi-Bellman equation models the backward dynamics of a representative agent’s value functions and the Fokker-Planck equation models the forward dynamics of mean fields. Discrete MFG models were then proposed in [19]. Learning in MFG has attracted great attention and most methods are based on RL. Yang et al. use mean field theory to approximate joint actions in large-population stochastic games to approximate Nash equilibria [45]. Guo et al. present a Q-learning-based algorithm for computing stationary MFNE [20]. Subramanian et al. use RL to compute local MFNE (a relaxed version) [40]. While, all these works rely on the presence of reward functions. Our work takes a complementary view where the reward function is not given, and hence the need for IRL for MFG.

IRL for MAS. Recently, IRL has been extended to the multi-agent setting. Most works assume specific reward structures, including fully cooperative games [6, 4], fully competitive games [31], or either of the two [42, 35]. For general stochastic games, Yu et al. present MA-AIRL [46], a multi-agent IRL method using adversarial learning. However, all these prior methods are not scalable to games with a large population of agents. Notably, Šošić et al. propose SwarmIRL [39] that views an MAS as an swarm system consisting of homogeneous agents, sharing the same idea of mean field approximation. But it cannot handle non-stationary (time-varying) policies and non-linear reward functions. Our MFIRL makes no modelling assumptions on policies and reward functions.

IRL for MFG. As discussed earlier, the most related work is [44] that proposes an IRL method for MFG, which we call MFG-MDP IRL. It focuses on population’s behaviours by reformulating MFNE as an optimal solution to a MDP, and applies MaxEnt IRL on this MDP. This “centralised view” implies that it assumes the policy-mean field trajectories at the population level fulfill the maximum entropy distribution rather than state-action trajectories at the agent level. We technically reiterate two issues associated with this setting: (1) \textit{Biased inference}. Reformulating MFG as MDP implies that a MFNE optimises population’s societal rewards, but a MFNE (or ERMFNE) is not necessarily socially optimal if multiple equilibria exist [40, 3, 13]; (2) \textit{Sample inefficiency}. It can only obtain
a single policy-mean field sample from one sample of game play, whereas each game play contributes $N$ samples in our MFIRL. We present detailed explanations and discussions about MFG-MDP IRL in Appendix C. In contrast, from a “decentralised view”, the expert policy must be a best response to the expert MF flow. Therefore, our MFIRL can recover the ground-truth reward functions without bias.

**Generality of MFIRL.** To simplify notations, we present MFIRL on finite-horizon discrete MFG. The results of MFIRL continue to hold for the following generalisations.  
- Continuous state-action spaces. The arguments hold under standard conditions on continuous of the rewards and dynamics, and compactness of the state-action spaces, to ensure the existence and uniqueness of ERMFNE. Technically, one exception is that we might need to discretise the mean field because it turns to a probability density function if states are continuous.  
- Infinite time horizon. When the time horizon tends to infinity, the mean field is shown to converge almost surely to a constant limit, resulting in the stationary MFNE [20, 40]. MFIRL is clearly compatible with infinite time horizons, since non-stationary equilibria recover stationary ones as special cases.  
- Generalised mean fields. Some works [20] generalise the mean field $\mu \in \mathcal{P}(S)$ to $(\mu, \alpha) \in \mathcal{P}(S \times A)$ by additionally considering population’s average action $\alpha \in \mathcal{P}(A)$. MFIRL is adaptive to generalised mean fields by simply incorporating the marginal distribution $\alpha$ in all arguments.

5 Experiments

**Tasks and Baseline.** We evaluate MFIRL on five simulated MFG tasks: investment in product quality [38, 40] (INVEST for short), malware spread [24, 25, 40] (MALWARE), virus infection [11] (VIRUS), Rock-Paper-Scissors [11] (RPS) and Left-Right [11] (LR), ordered in decreasing complexity. Detailed descriptions and settings can be found in Appendix E. We test MFIRL against MFG-MDP IRL [44], as it is the only IRL method for MFG in the literature, as of the present.

**Performance Metrics.** A learned reward function is considered of good quality if its induced ERMFNE is close to that induced by the ground-truth reward function. Thus, we evaluate a learned reward function using the following three indicators that measure the gap between the two ERMFNE:

- Expected return. The expected return of the ERMFNE induced by a learned reward function.
- Deviation from expert MF flow (Dev. MF). We use the cumulative KL-divergence, $\sum_{t=0}^{T-1} D_{KL}(\mu^E_t \parallel \mu^\mu_t)$, to measure the distance over the MF flow.
- Deviation from expert policy (Dev. Policy). We measure the distance over the policy by $\sum_{t=0}^{T-1} \sum_{s \in S} \mu^E_t(s) D_{KL}(\pi^E_t(\cdot | s) \parallel \pi^\mu_t(\cdot | s))$, where the KL-divergence over policies with respect to state $s$ is weighted by the proportion of $s$ specified by the expert ERMFNE.

**Training Procedures.** In simulated tasks, we have access to ground-truth reward functions and environment dynamics, which enables us to numerically compute ground-truth equilibria. We take 100 agents and sample expert trajectories with 50 time steps, which is same as the number of time steps used in [38, 46, 11]. We use one-hot encoding to represent states and actions. For both MFIRL and MFG-MDP IRL, we adopt the same neural network architecture as the reward model: two hidden layers of 64 leaky rectified linear units (ReLU) each. Implementation details are in Appendix E.

**Verification of the Bias in Population-Level Inference.** We verify our claim on the bias in MFG-MDP IRL on MALWARE, as it is known to have at least one non-socially-optimal MFNE [40]. We train two experts: following [10], the socially optimal MFNE is computed by using DDPG [30] to solve the MDP reduced from MFG (see Appendix C for details); the ordinary one is obtained by repeating the MFNE operator. To indicate the bias, we calculate expected returns of the socially optimal MFNE induced by the learned function and the ground truth, respectively. Results are presented in Fig. 1. MFG-MDP IRL shows expert-like performance if trajectories are sampled from a socially optimal MFNE but shows large deviations under an ordinary MFNE. This verifies the implicit bias of population-level inference.

**Reward Recovery under Original Dynamics.** We first carry out tests with unchanged dynamics. For fairness, we use a small temperature $\beta = 0.1$ for all tasks. Results are depicted in Fig. 2. On
all tasks, MFIRL is more sample efficient than MFG-MDP IRL, verifying our arguments on the sample inefficiency of MFG-MDP IRL. Meanwhile, MFIRL achieves near-expert performance, while MFG-MDP IRL shows larger deviations on INVEST and MALWARE even though with a large number of samples, since they might have multiple ERMFNE as we use a weak entropy regularisation.

Figure 2: Results for original environments. The solid line shows the median and the shaded area represents the standard deviation over 10 independent runs.

Table 1: Results for new environments. Mean and variance are taken across 10 independent runs.

| Metric          | Algorithm  | Task       | INVEST | MALWARE | VIRUS | RPS    | LR    |
|-----------------|------------|------------|--------|---------|-------|--------|-------|
| Expected Return | EXPERT     | 93.156     | -35.192 ± 0.511 | -18.409 ± 0.141 | -1.240 | 0.523 ± 0.011 | 1.763 ± 0.181 | 0.459 ± 0.366 | 0.366 ± 0.035 |
|                 | MFIRL      | -35.192 ± 0.511 | 93.156 ± 0.442 | -18.409 ± 0.141 | -1.240 | 0.523 ± 0.011 | 1.763 ± 0.181 | 0.459 ± 0.366 | 0.366 ± 0.035 |
|                 | MFG-MDP IRL | -34.947 ± 2.410 | -16.131 ± 0.402 | -2.638 ± 0.145 | -0.402 | 1.802 ± 0.435 | 1.481 ± 0.006 | 6.106 ± 0.459 | 0.574 ± 0.039 |

Re-optimisation under New Dynamics. To investigate the robustness against changing environment dynamics, we then change the transition function (see Appendix [D] for details), recompute ERMFNE induced by the ground truth and the learned reward functions (trained with 10 game plays), and calculate three metrics again. Results are summarised in Tab. 1. Consistently, MFIRL outperforms MFG-MDP IRL on all tasks. We owe the high robustness of reward functions learned by MFIRL to two reasons: (1) MFIRL uses a potential function to mitigate the effect of reward shaping while MFG-MDP does not; (2) the issue of biased inference in MFG-MDP IRL can be exacerbated by the changing dynamics. To summarise, MFIRL recovers ground-truth reward functions with high sample efficiency and high robustness, in line with our theoretical analysis.

6 Conclusion and Future Work

This paper amounts to an effort towards agent-level IRL for MFG. We propose MFIRL, the first IRL method that can recover the ground-truth reward function for MFG, based on a new solution concept termed ERMFNE. ERMFNE incorporates the entropy regularisation into rewards, and allows us to characterise the expert demonstrated trajectories with an energy-based model. Most critically, MFIRL decouples the agent-level and population-level dynamics by substituting the mean field with its empirical estimation. With this manner, MFIRL constructs an asymptotically consistent estimation of the ground-truth reward function. We also come up with the mean-field-type potential-based reward shaping in order to reduce the reward ambiguity. Experimental results show that MFIRL can learn robust ground-truth reward functions with high sample efficiency. A direction for future work is to combine MFIRL with generative learning or adversarial learning as in [38, 46], in order to make MFIRL more efficient on high dimensional and continuous tasks.
References

[1] Yong-Yeol Ahn, Seungyeop Han, Haewoon Kwak, Sue Moon, and Hawoong Jeong. Analysis of topological characteristics of huge online social networking services. In Proceedings of the 16th International Conference on World Wide Web, pages 835–844, 2007.

[2] Dario Amodei and Jack Clark. Faulty reward functions in the wild. URL: https://blog.openai.com/faulty-reward-functions, 2016.

[3] Martino Bardi and Markus Fischer. On non-uniqueness and uniqueness of solutions in finite-horizon mean field games. ESAIM: Control, Optimisation and Calculus of Variations, 25:44, 2019.

[4] Samuel Barrett, Avi Rosenfeld, Sarit Kraus, and Peter Stone. Making friends on the fly: Cooperating with new teammates. Artificial Intelligence, 242:132–171, 2017.

[5] Ana LC Bazzan. Opportunities for multiagent systems and multiagent reinforcement learning in traffic control. Autonomous Agents and Multi-Agent Systems, 18(3):342, 2009.

[6] Kenneth Bogert and Prashant Doshi. Multi-robot inverse reinforcement learning under occlusion with interactions. In Proceedings of the 13th International Conference on Autonomous Agents and Multi-agent Systems, pages 173–180. Citeseer, 2014.

[7] Michael Bowling and Manuela Veloso. Multiagent learning using a variable learning rate. Artificial Intelligence, 136(2):215–250, 2002.

[8] René Carmona, François Delarue, et al. Probabilistic Theory of Mean Field Games with Applications I-II. Springer, 2018.

[9] René Carmona, François Delarue, and Aimé Lachapelle. Control of mckean–vlasov dynamics versus mean field games. Mathematics and Financial Economics, 7(2):131–166, 2013.

[10] René Carmona, Mathieu Laurière, and Zongjun Tan. Model-free mean-field reinforcement learning: mean-field mdp and mean-field q-learning. arXiv preprint [arXiv:1910.12802], 2019.

[11] Kai Cui and Heinz Koeppl. Approximately solving mean field games via entropy-regularized deep reinforcement learning. In International Conference on Artificial Intelligence and Statistics, pages 1909–1917. PMLR, 2021.

[12] Constantinos Daskalakis, Paul W Goldberg, and Christos H Papadimitriou. The complexity of computing a nash equilibrium. SIAM Journal on Computing, 39(1):195–259, 2009.

[13] François Delarue and Rinel Foguen Tchuendom. Selection of equilibria in a linear quadratic mean-field game. Stochastic Processes and their Applications, 130(2):1000–1040, 2020.

[14] Sam Devlin and Daniel Kudenko. Theoretical considerations of potential-based reward shaping for multi-agent systems. In The 10th International Conference on Autonomous Agents and Multiagent Systems, pages 225–232. ACM, 2011.

[15] Jodi Dianetti, Giorgio Ferrari, Markus Fischer, and Max Nendel. Submodular mean field games: Existence and approximation of solutions. arXiv preprint [arXiv:1907.10968], 2019.

[16] Romuald Elie, Julien Pérolat, Mathieu Laurière, Matthieu Geist, and Olivier Pietquin. On the convergence of model free learning in mean field games. In Thirty-Fourth AAAI Conference on Artificial Intelligence, pages 7143–7150, 2020.

[17] Chelsea Finn, Sergey Levine, and Pieter Abbeel. Guided cost learning: deep inverse optimal control via policy optimization. In Proceedings of the 33rd International Conference on International Conference on Machine Learning, pages 49–58, 2016.

[18] Justin Fu, Katie Luo, and Sergey Levine. Learning robust rewards with adversarial inverse reinforcement learning. In International Conference on Learning Representations, 2018.

[19] Diogo A Gomes, Joana Mohr, and Rafael Rigao Souza. Discrete time, finite state space mean field games. Journal de Mathématiques Pures et Appliquées, 93(3):308–328, 2010.

[20] Xin Guo, Anran Hu, Renyuan Xu, and Junzi Zhang. Learning mean-field games. In Advances in Neural Information Processing Systems, pages 4967–4977, 2019.

[21] Tuomas Haarnoja, Haoran Tang, Pieter Abbeel, and Sergey Levine. Reinforcement learning with deep energy-based policies. In International Conference on Machine Learning, pages 1352–1361. PMLR, 2017.
[22] Jonathan Ho and Stefano Ermon. Generative adversarial imitation learning. In Advances in Neural Information Processing Systems, pages 4565–4573, 2016.

[23] Junling Hu and Michael P Wellman. Nash q-learning for general-sum stochastic games. Journal of Machine Learning Research, 4(Nov):1039–1069, 2003.

[24] Minyi Huang and Yan Ma. Mean field stochastic games: Monotone costs and threshold policies. In 2016 IEEE 55th Conference on Decision and Control (CDC), pages 7105–7110. IEEE, 2016.

[25] Minyi Huang and Yan Ma. Mean field stochastic games with binary actions: Stationary threshold policies. In 2017 IEEE 56th Annual Conference on Decision and Control (CDC), pages 27–32. IEEE, 2017.

[26] Minyi Huang, Roland P Malhamé, Peter E Caines, et al. Large population stochastic dynamic games: closed-loop mckean-vlasov systems and the nash certainty equivalence principle. Communications in Information & Systems, 6(3):221–252, 2006.

[27] Seong Hoon Jeong, Ah Reum Kang, and Huy Kang Kim. Analysis of game bot’s behavioral characteristics in social interaction networks of mmorpg. ACM SIGCOMM Computer Communication Review, 45(4):99–100, 2015.

[28] Jean-Michel Lasry and Pierre-Louis Lions. Mean field games. Japanese journal of mathematics, 2(1):229–260, 2007.

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

[30] Timothy P Lillicrap, Jonathan J Hunt, Alexander Pritzel, Nicolas Heess, Tom Erez, Yuval Tassa, David Silver, and Daan Wierstra. Continuous control with deep reinforcement learning. arXiv preprint arXiv:1509.02971, 2015.

[31] Xiaomin Lin, Peter A Beling, and Randy Cogill. Multi-agent inverse reinforcement learning for zero-sum games. arXiv preprint arXiv:1403.6508, 2014.

[32] Pinxin Long, Tingxiang Fanl, Xinyi Liao, Wenxi Liu, Hao Zhang, and Jia Pan. Towards optimally decentralized multi-robot collision avoidance via deep reinforcement learning. In 2018 IEEE International Conference on Robotics and Automation (ICRA), pages 6252–6259. IEEE, 2018.

[33] Andrew Y Ng, Daishi Harada, and Stuart Russell. Policy invariance under reward transformations: Theory and application to reward shaping. In ICML, volume 99, pages 278–287, 1999.

[34] Andrew Y Ng and Stuart J Russell. Algorithms for inverse reinforcement learning. In Proceedings of the Seventeenth International Conference on Machine Learning, pages 663–670, 2000.

[35] Tummalapalli Sudhamsh Reddy, Vamsikrishna Gopikrishna, Gergely Zaruba, and Manfred Huber. Inverse reinforcement learning for decentralized non-cooperative multiagent systems. In 2012 IEEE International Conference on Systems, Man, and Cybernetics (SMC), pages 1930–1935. IEEE, 2012.

[36] Naci Saldi, Tamer Basar, and Maxim Raginsky. Markov–nash equilibria in mean-field games with discounted cost. SIAM Journal on Control and Optimization, 56(6):4256–4287, 2018.

[37] Lloyd Shapley. Some topics in two-person games. Advances in game theory, 52:1–29, 1964.

[38] Jiaming Song, Hongyu Ren, Dorsa Sadigh, and Stefano Ermon. Multi-agent generative adversarial imitation learning. In Advances in Neural Information Processing Systems, pages 7461–7472, 2018.

[39] Adrian Šošić, Wasiur R KhudaBukhsh, Abdelhak M Zoubir, and Heinz Koeppl. Inverse reinforcement learning in swarm systems. In Proceedings of the 16th International Conference on Autonomous Agents and MultiAgent Systems, pages 1413–1421, 2017.

[40] Jayakumar Subramanian and Aditya Mahajan. Reinforcement learning in stationary mean-field games. In Proceedings of the 18th International Conference on Autonomous Agents and MultiAgent Systems, pages 251–259, 2019.
[41] Oriol Vinyals, Igor Babuschkin, Wojciech M Czarnecki, Michaël Mathieu, Andrew Dudzik, Jun-young Chung, David H Choi, Richard Powell, Timo Ewalds, Petko Georgiev, et al. Grandmaster level in starcraft ii using multi-agent reinforcement learning. Nature, 575(7782):350–354, 2019.

[42] Kevin Waugh, Brian D Ziebart, and J Andrew Bagnell. Computational rationalization: the inverse equilibrium problem. In Proceedings of the 28th International Conference on Machine Learning, pages 1169–1176, 2011.

[43] Gabriel Y Weintraub, C Lanier Benkard, and Benjamin Van Roy. Computational methods for oblivious equilibrium. Operations research, 58(4-part-2):1247–1265, 2010.

[44] Jiachen Yang, Xiaojing Ye, Rakshit Trivedi, Huan Xu, and Hongyuan Zha. Learning deep mean field games for modeling large population behavior. In International Conference on Learning Representations, 2018.

[45] Y Yang, R Luo, M Li, M Zhou, W Zhang, and J Wang. Mean field multi-agent reinforcement learning. In 35th International Conference on Machine Learning, volume 80, pages 5571–5580. PMLR, 2018.

[46] Lantao Yu, Jiaming Song, and Stefano Ermon. Multi-agent adversarial inverse reinforcement learning. In International Conference on Machine Learning, pages 7194–7201, 2019.

[47] Brian D Ziebart, J Andrew Bagnell, and Anind K Dey. Modeling interaction via the principle of maximum causal entropy. In Proceedings of the 27th International Conference on Machine Learning, pages 1255–1262, 2010.

[48] Brian D Ziebart, Andrew Maas, J Andrew Bagnell, and Anind K Dey. Maximum entropy inverse reinforcement learning. In Proceedings of the 23rd AAAI Conference on Artificial Intelligence, pages 1433–1438, 2008.
Appendix

A Proofs

A.1 Proof of Proposition\[1\]

**Proposition**\[1\] Let \((\mu^*, \pi^*)\) be a ERMFNE with \(\beta = 1\) for a MFG \((S, A, p, \mu_0, r, \gamma)\). A representative agent’s trajectory \(\tau = \{(s_t, a_t)\}_{t=0}^{T-1}\) induced by \((\mu^*, \pi^*)\) fulfils the following generative process

\[
\Pr(\tau) \propto \mu_0(s_0) \exp \left( \sum_{t=0}^{T-1} \gamma^t r(s_t, a_t, \mu^*_t) \right) \prod_{t=0}^{T-1} p(s_{t+1} | s_t, a_t, \mu^*_t). \tag{A1}
\]

**Proof.** For an arbitrary policy \(\pi\), the probability of a trajectory \(\tau = \{(s_t, a_t)\}_{t=0}^{T-1}\) induced by \((\mu^*, \pi)\) satisfies the distribution defined as follows:

\[
\Pr'(\tau) = \mu_0(s_0) \prod_{t=0}^{T-1} \pi_t(s_t | a_t) \prod_{t=0}^{T-1} p(s_{t+1} | s_t, a_t, \mu^*_t). \tag{A2}
\]

Let \(D_{KL}\) denote the Kullback–Leibler (KL) divergence. To show Proposition\[1\] it suffices to show that the policy \(\pi^*\) in ERMFNE is the optimal solution to the following optimisation problem:

\[
\min_{\pi} D_{KL} \left( \Pr'(\tau) \parallel \Pr(\tau) \right). \tag{A3}
\]

Our proof is in a manner of dynamic programming. We construct the basic case for step \(T - 1\), where Eq. \(A3\) obviously holds according to the definition of the policy in ERMFNE (see Eq. \(5\)). Then, for each \(t < T - 1\), we construct the optimal policy for steps from \(t\) to \(T - 1\) based on the optimal policy that is already constructed from \(t + 1\) to \(T - 1\). We show that the constructed optimal policy that minimises the above KL divergence is consistent with \(\pi^*\) in ERMFNE. For simplicity, we omit the partition function for \(\Pr\) since it is a constant. Substituting \(\Pr'(\tau)\) and \(\Pr(\tau)\) in Eq. \(A3\) with their definitions and roll out the KL-divergence, we obtain that maximising the KL-divergence between \(\Pr'\) and \(\Pr\) is equivalent to the following optimisation problem

\[
\max_{\pi} \mathbb{E}_{\tau \sim \Pr'} \left[ \log \frac{\Pr(\tau)}{\Pr'(\tau)} \right] = \mathbb{E}_{\tau \sim \Pr'} \left[ \log \mu_0^*(s_0) + \sum_{t=0}^{T-1} \left( \gamma^t r(s_t, a_t, \mu^*_t) + \log p(s_{t+1} | s_t, a_t, \mu^*_t) \right) - \log \mu_0^*(s_0) - \sum_{t=0}^{T-1} \left( \log \pi_t(s_t | a_t) + \log p(s_{t+1} | s_t, a_t, \mu^*_t) \right) \right] \nonumber
\]

\[
= \mathbb{E}_{\tau \sim \Pr'} \left[ \sum_{t=0}^{T-1} \left( \gamma^t r(s_t, a_t, \mu^*_t) - \log \pi_t(s_t) \right) \right] \tag{A4}
\]

We maximise the objective in Eq. \(A4\) using a dynamic programming method. We construct the base case that maximises \(\pi_{T-1}\):

\[
\max_{\pi_{T-1}} \mathbb{E}_{(s_{T-1}, a_{T-1}) \sim \Pr'} \left[ r(s_{T-1}, a_{T-1}, \mu^*_T) - \log \pi_{T-1}(a_{T-1} | s_{T-1}) \right] \nonumber
\]

\[
= \mathbb{E}_{(s_{T-1}, a_{T-1}) \sim \Pr'} \left[ -D_{KL} \left( \pi_{T-1}(a_{T-1} | s_{T-1}) \parallel \exp \left( \frac{r(s_{T-1}, a_{T-1}, \mu^*_T)}{\exp(V(s_{T-1}, \mu^*_T))} \right) \right) \right] + V(s_{T-1}, \mu^*_T), \tag{A5}
\]

where we define

\[
V(s_{T-1}, \mu^*_T) \triangleq \log \sum_{a' \in A} \exp \left( r(s_{T-1}, a', \mu^*_T) \right).
\]
The optimal $\pi_{T-1}$ for Eq. (A5) is

$$\pi_{T-1}^{\ast}(a_{T-1}|s_{T-1}) = \frac{\exp \left( r(s_{T-1}, a_{T-1}, \mu_{T-1}^{\ast}) \right)}{\exp(V(s_{T-1}, \mu_{T-1}^{\ast}))} = \frac{\exp \left( r(s_{T-1}, a_{T-1}, \mu_{T-1}^{\ast}) \right)}{\sum_{a' \in A} \exp \left( r(s_{T-1}, a', \mu_{T-1}^{\ast}) \right)},$$

(A6)

which coincides with the policy in ERMFNE (see Eq. (3)).

With the optimal policy given in Eq. (A6), the KL-divergence in Eq. (A5) attains 0 and Eq. (A5) attains the minimum $V(s_{T-1}, \mu_{T-1}^{\ast})$.

Then recursively we can show that for any step $t < T - 1$, $\pi_{t}$ is the maximiser of the following optimisation problem:

$$\max_{\pi_{t}} \mathbb{E}_{(s_{t}, a_{t}) \sim P_{t}} \left[ -D_{KL} \left( \pi_{t}(a_{t}|s_{t}) \middle| \frac{\exp \left( Q_{\pi_{t+1:T-1}}^{\mu_{t+1:T-1}}(s_{t}, a_{t}, \mu_{t}) \right)}{\exp \left( V_{\pi_{t+1:T-1}}^{\mu_{t+1:T-1}}(s_{t}, \mu_{t}) \right)} \right) \right],$$

where

$$V_{\pi_{t+1:T-1}}^{\mu_{t+1:T-1}}(s_{t}, \mu_{t}) \triangleq \log \sum_{a' \in A} \exp \left( Q_{\pi_{t+1:T-1}}^{\mu_{t+1:T-1}}(s_{t}, a_{t}, \mu_{t}) \right).$$

(A7)

In fact, $V_{\pi_{t+1:T-1}}^{\mu_{t+1:T-1}}$ denotes the MFG counterpart of the soft value function in soft Q-learning [21]. The optimal policy for Eq. (A7) is given by

$$\pi_{t}(a_{t}|s_{t}) = \frac{\exp \left( Q_{\pi_{t+1:T-1}}^{\mu_{t+1:T-1}}(s_{t}, a_{t}, \mu_{t}) \right)}{\sum_{\sigma \in A} \exp \left( Q_{\pi_{t+1:T-1}}^{\mu_{t+1:T-1}}(s_{t}, a_{t}, \mu_{t}) \right)},$$

which coincides with the policy defined in ERMFNE.

A.2 Proof of Theorem

Theorem 1 Let the demonstrated trajectories in $D_{E} = \{(\tau_{1}^{j}, \ldots, \tau_{N}^{j})\}_{j=1}^{M}$ be independent and identically distributed (i.i.d.) and sampled from a unique ERMFNE induced by an unknown parameterised reward function $r_{\omega}(s, a, \mu)$. Suppose for all $s \in S$, $a \in A$ and $\mu \in \mathcal{P}(S)$, $r_{\omega}(s, a, \mu)$ is differentiable with respect to $\omega$. Then, with probability 1 as the number of samples $M \to \infty$, the equation $\frac{\partial}{\partial \omega} \nabla_{\omega} \hat{L}(\omega; \hat{\mu}^{E}) = 0$ has a root $\hat{\omega}$ such that $\hat{\omega} = \omega^{\ast}$.

Proof The derivative of $\hat{L}$ with respect to $\omega$ is given by:

$$\frac{\partial}{\partial \omega} \hat{L}(\omega; \hat{\mu}^{E}) = \frac{1}{M} \sum_{j=1}^{M} \frac{1}{N} \sum_{i=1}^{N} \sum_{t=0}^{T-1} \gamma^{t} \frac{\partial}{\partial \omega} r_{\omega}(s_{j,t}^{i}, a_{j,t}^{i}, \hat{\mu}_{t}^{E}) - \frac{\partial}{\partial \omega} \log \hat{Z}_{\omega}$$

$$= \frac{1}{M} \sum_{j=1}^{M} \frac{1}{N} \sum_{i=1}^{N} \sum_{t=0}^{T-1} \gamma^{t} \frac{\partial}{\partial \omega} r_{\omega}(s_{j,t}^{i}, a_{j,t}^{i}, \hat{\mu}_{t}^{E}) - \frac{1}{\hat{Z}_{\omega}} \frac{\partial}{\partial \omega} \hat{Z}_{\omega}$$

$$= \frac{1}{M} \sum_{j=1}^{M} \frac{1}{N} \sum_{i=1}^{N} \sum_{t=0}^{T-1} \gamma^{t} \frac{\partial}{\partial \omega} r_{\omega}(s_{j,t}^{i}, a_{j,t}^{i}, \hat{\mu}_{t}^{E})$$

$$- \sum_{j=1}^{M} \sum_{i=1}^{N} \frac{\exp \left( \sum_{t=0}^{T-1} \gamma^{t} r_{\omega}(s_{j,t}^{i}, a_{j,t}^{i}, \hat{\mu}_{t}^{E}) \right)}{\hat{Z}_{\omega}} \sum_{t=0}^{T-1} \gamma^{t} \frac{\partial}{\partial \omega} r_{\omega}(s_{j,t}^{i}, a_{j,t}^{i}, \hat{\mu}_{t}^{E})$$

(A8)
Let \( \Pr_D(\tau) \triangleq \frac{1}{M} \sum_{j=1}^{M} \frac{1}{N} \sum_{i=1}^{N} 1_{\{\tau_j^i = \tau\}} \) denote the empirical trajectory distribution, then Eq. (A8) is equivalent to

\[
\frac{\partial}{\partial \omega} \hat{L}(\omega; \mu_E) = \sum_{i=1}^{N} \sum_{j=1}^{M} \Pr_D(\tau_j^i) \sum_{t=0}^{T-1} \gamma_t \frac{\partial}{\partial \omega} r_\omega(s_{j,t}, a_{j,t}, \hat{\mu}_t^E) \\
- \sum_{j=1}^{M} \sum_{i=1}^{N} \exp \left( \sum_{t=0}^{T-1} \gamma_t r_\omega(s_{j,t}, a_{j,t}, \hat{\mu}_t^E) \right) \sum_{t=0}^{T-1} \gamma_t \frac{\partial}{\partial \omega} r_\omega(s_{j,t}, a_{j,t}, \hat{\mu}_t^E) \\
= \sum_{i=1}^{N} \sum_{j=1}^{M} \left( \Pr_D(\tau_j^i) - \exp \left( \sum_{t=0}^{T-1} \gamma_t r_\omega(s_{j,t}, a_{j,t}, \hat{\mu}_t^E) \right) \right) \sum_{t=0}^{T-1} \gamma_t \frac{\partial}{\partial \omega} r_\omega(s_{j,t}, a_{j,t}, \hat{\mu}_t^E). \\
(A9)
\]

When the number of samples \( M \to \infty \), \( \Pr_D(\tau) \) tends to the true trajectory distribution \( \Pr(\tau) \) induced by ERMFNE (see Eq. (4)). Meanwhile, according to the law of large numbers, \( \hat{\mu} \to \mu_E = \mu^* \) with probability 1 as the number of samples \( M \to \infty \). Thus, taking the limit \( M \to \infty \) and the optimality \( \omega = \omega^* \), we have:

\[
\frac{\exp \left( \sum_{t=0}^{T-1} \gamma_t r_\omega^*(s_{j,t}, a_{j,t}, \tilde{\mu}_t) \right)}{\hat{Z}_{\omega^*}} = \frac{\exp \left( \sum_{t=0}^{T-1} \gamma_t r_\omega^*(s_{j,t}, a_{j,t}, \tilde{\mu}_t) \right)}{\sum_{j=1}^{M} \sum_{i=1}^{N} \exp \left( \sum_{t=0}^{T-1} \gamma_t r_\omega^*(s_{j,t}, a_{j,t}, \tilde{\mu}_t) \right)} = \Pr_D(\tau_j^i) = \Pr_D(\tau_j^i)
\]

Therefore, the gradient in Eq. (A9) will be zero, and hence the proof is complete. \( \square \)

### A.3 Proof of Proposition 2

**Proposition 2** Define a norm on \( \prod_{t=0}^{T-1} \mathcal{P}(S) \) by \( \| \mu \| = \max_{1 \leq t \leq T-1} \max_{s \in S} \mu_t(s) \). Let any \( \epsilon, \delta \in (0, 1) \) be given. Under the i.i.d. assumption, to ensure \( \| \hat{\mu}^E - \mu_E \| \leq \epsilon \) with probability at least \( 1 - \delta \), it suffices that \( M \geq \frac{1}{\delta^2} \log \frac{2|S|(T-1)}{\epsilon} \).

**Proof.** Since a mean field \( \mu \) is a probability simplex over the finite state space \( S \), each component of \( \mu \) is bounded between \([0, 1]\). By applying the Hoeffding inequality, we have

\[
\Pr \left( \| \mu_t^E(s) - \hat{\mu}_t^E(s) \| > \epsilon \right) \leq 2 \exp \left( -2\epsilon^2 M \right), \forall s \in S, 1 \leq t \leq T - 1. \tag{10}
\]

Applying a union bound for all \( s \in S \) and \( t = 1, \ldots, T - 1 \) gives

\[
\Pr \left( \exists s \in S, 1 \leq t \leq T - 1, \ | \mu_t^E(s) - \hat{\mu}_t^E(s) | \geq \epsilon \right) \leq 2|S|(T-1) \exp \left( -2\epsilon^2 M \right), \tag{11}
\]

which is equivalent to

\[
\Pr \left( \max_{1 \leq t \leq T-1 \ s \in S} | \mu_t^E - \hat{\mu}_t^E | \leq \epsilon \right) \geq 1 - 2|S|(T-1) \exp \left( -2\epsilon^2 M \right), \forall t = 1, \ldots, T - 1. \tag{12}
\]

Substituting \( 2|S|(T-1) \exp \left( -2\epsilon^2 M \right) = \delta \) gives the final result. \( \square \)

### A.4 Proof of Theorem 2

**Theorem 2** Let any \( S, A, \gamma \) be given. We say \( F : S \times A \times \mathcal{P}(S) \times S \times \mathcal{P}(S) \to \mathbb{R} \) is a potential-based reward shaping for MFG if there exists a real-valued function \( q : S \times \mathcal{P}(S) \to \mathbb{R} \) such that \( F(s_t, a_t, \mu_t, s_{t+1}, \mu_{t+1}) = \gamma q(s_{t+1}, \mu_{t+1}) - q(s_t, \mu_t) \). Then, \( F \) is sufficient and necessary to guarantee the invariance of the set of MFNE and ERMFNE in the sense that: **Sufficiency:** Every MFNE or ERMFNE in the MFG \( \mathcal{M}' = (S, A, p, r + F, \gamma) \) is also a MFNE or ERMFNE in \( \mathcal{M} = (S, A, p, \mu_0, r, \gamma) \); **Necessity:** If \( F \) is not a potential-based reward shaping, then there exist a initial mean field \( \mu_0 \), transition function \( p \), horizon \( T \), temperature \( \beta \) (for ERMFNE only) and reward function \( r \) such that no MFNE or ERMFNE in \( \mathcal{M}' \) is an equilibrium in \( \mathcal{M} \).
We next show the necessity by constructing a counter-example where a non-potential-based reward shaping $F$. Let $\mu$ be an arbitrary MF flow. The optimal Q value functions for the MDP induced by $\mu$, denoted by $Q^*$, fulfill the Bellman equation:

$$Q^*(s_t, a_t) = r(s_t, a_t, \mu_t) + \gamma \mathbb{E}_{s_{t+1} \sim p} \left[ \max_{a_{t+1} \in A} Q^*(s_{t+1}, a_{t+1}) \right].$$

Applying some simple algebraic manipulation gives:

$$Q^*(s_t, a_t) - g(s_t, \mu_t) = r(s_t, a_t, \mu_t) - g(s_t, \mu_t) + \gamma g(s_{t+1}, \mu_{t+1}) + \gamma \mathbb{E}_{s_{t+1} \sim p} \left[ \max_{a_{t+1} \in A} (Q^*(s_{t+1}, a_{t+1}) - g(s_{t+1}, \mu_{t+1})) \right]$$

$$= r(s_t, a_t, \mu_t) + F(s_t, a_t, \mu_t, s_{t+1}, \mu_{t+1}) + \gamma \mathbb{E}_{s_{t+1} \sim p} \left[ \max_{a_{t+1} \in A} (Q^*(s_{t+1}, a_{t+1}) - g(s_{t+1}, \mu_{t+1})) \right]$$

From here, we know that the above equation is exactly the Bellman equation for the MDP induced by $\mu$ with the reward function $r + F$, and $Q^*(s_t, a_t) - g(s_t, \mu_t)$ is the unique set of optimal Q values for this MDP. Since $\arg \max_{a \in A} Q^*(s_t, a) - g(s_t, \mu_t) = \arg \max_{a \in A} Q^*(s_t, a)$, we have that for any fix a MF flow, any optimal policy for the induced MDP of $\mathcal{M}$ is also an optimal policy for the induced MDP of $\mathcal{M}$. Hence, we finish the proof of the sufficiency for MFNE.

Next, we will show the sufficiency for ERMFNE. We write $Q^*_{soft}$ for the optimal soft Q functions for the induced MDP such that

$$Q^*_{soft}(s_t, a_t) = r(s_t, a_t, \mu_t) + \gamma \mathbb{E}_{s_{t+1} \sim p} \left[ \sum_{a_{t+1} \in A} \frac{\exp(\frac{1}{\beta} Q^*_{soft}(s_{t+1}, a_{t+1}))}{\sum_{a' \in A} \exp(\frac{1}{\beta} Q^*_{soft}(s_t, a'))} Q^*_{soft}(s_{t+1}, a_{t+1}) \right].$$

Using the same manner as we show the invariance of MFNE, we have:

$$Q^*_{soft}(s_t, a_t) - g(s_t, \mu_t) = r(s_t, a_t, \mu_t) - g(s_t, \mu_t) + g(s_{t+1}, \mu_{t+1})$$

$$+ \gamma \mathbb{E}_{s_{t+1} \sim p} \left[ \frac{\exp(\frac{1}{\beta} (Q^*_{soft}(s_{t+1}, a_{t+1}) - g(s_{t+1}, \mu_{t+1})))}{\sum_{a' \in A} \exp(\frac{1}{\beta} Q^*_{soft}(s_t, a') - g(s_{t+1}, \mu_{t+1}))} \right] (Q^*_{soft}(s_{t+1}, a_{t+1}) - g(s_{t+1}, \mu_{t+1}))$$

$$= r(s_t, a_t, \mu_t) - g(s_t, \mu_t) + \gamma g(s_{t+1}, \mu_{t+1})$$

$$+ \gamma \mathbb{E}_{s_{t+1} \sim p} \left[ \frac{\exp(\frac{1}{\beta} Q^*_{soft}(s_{t+1}, a_{t+1}))}{\sum_{a' \in A} \exp(\frac{1}{\beta} Q^*_{soft}(s_t, a'))} \right] (Q^*_{soft}(s_{t+1}, a_{t+1}) - g(s_{t+1}, \mu_{t+1}))$$

Hence, we know that $Q^*_{soft}(s_t, a_t) - g(s_t, \mu_t)$ is the set of optimal soft Q values for the MDP induced by $\mu$ with reward function $r + F$. Thus, any optimal policy for the induced MDP of $\mathcal{M}$ is also an optimal policy for the induced MDP of $\mathcal{M}$. Hence, we finish the proof of sufficiency for MFNE.

We next show the necessity by constructing a counter-example where a non-potential-based reward shaping $F$. Let $\mu$ be an arbitrary MF flow. Consider the Left-Right problem [11], which is also used as a task in experiments. At each step, each agent is at a position (state) of either “left”, “right” or “center”, and can choose to move either “left” or “right”, receives a reward according the current population density (mean field) at each position, and with probability one (dynamics) reaches “left” or “right”. Once an agent leaves “center”, she can never head back and can only be in either left or right thereafter. Formally, we configure the MFG as follows: $S = \{C, L, R\}$, $A = S \setminus \{C\}$, initial mean field $\mu_0(C) = 1$ (i.e., all agents are at “center” initially), $\gamma = 1$ and the reward function $r(s, a, \mu_t) = -\mathbb{1}_{\{s=L\}} \cdot \mu_t(L) - \mathbb{1}_{\{s=R\}} \cdot \mu_t(R)$. This reward setting means that each agent will incur a negative reward determined by the population density at her current position. The transition function is deterministic that directs an agent to the next state with probability one:

$$p(s_{t+1}|s_t, a_t, \mu_t) = \mathbb{1}_{\{s_{t+1}=a_t\}}.$$
This configuration is illustrated below.

Now, we consider the case that the time horizon \( \beta = 1 \) (for ERMFNE only).

Since all agents are at “center” initially, we have that \( \mu_1^*(L) = \pi_0^*(L|C) \) and \( \mu_1^*(R) = \pi_0^*(R|C) \).

Therefore, we have that the expected return of each agent under MFNE is 
\[
-1 \cdot \pi_0^*(L|C) \cdot \mu_1^*(L) - 1 \cdot \pi_0^*(R|C) \cdot \mu_1^*(R)
= - (\pi_0^*(L|C))^2 - (1 - \pi_0^*(L|C))^2
= - (2\pi_0^*(L|C))^2 - 2\pi_0^*(L|C) + 1.
\]

Clearly, the expected return attains the maximum when \( \pi_0^*(L|C) = 1/2 \). Therefore, any MFNE \((\mu^*, \pi^*)\) under the configuration above must fulfil \( \pi_0^*(R|C) = \pi_0^*(L|C) = 1/2 \) and \( \mu_1^* \) can be arbitrary. And clearly, there exist a unique ERMFNE \((\mu^*, \pi^*)\) such that any action at any state and any time step is chosen with probability 1/2. This result is also shown in [11] as a case study.

Next, we change the reward function by adding an additional reward based on actions to the original reward function. We penalise the action “left” by a negative value \(-1\), i.e.,
\[
r'(s, a, \mu_t) = r(s, a, \mu_t) - \mathbb{1}_{\{a=L\}} = -\mathbb{1}_{\{s=L\}} \cdot \mu_t(L) - \mathbb{1}_{\{s=R\}} \cdot \mu_t(R) - \mathbb{1}_{\{a=L\}}.
\]

This equivalent to that an action-based reward shaping function \( F(s_t, a_t, \mu_t, s_{t+1}, \mu_{t+1}) = \gamma g(s_{t+1}, a_{t+1}, \mu_{t+1}) - g(s_t, a_t, \mu_t) \) is added to the original reward function where
\[
g(s_t, a_t, \mu_t) = -\mathbb{1}_{\{a_t=L\}}.
\]

The following diagram shows this new reward configuration.

Now, let us investigate the form of MFNE and ERMFNE under this new reward configuration. We first show the set of MFNE induced by the new reward function is no longer same as that induced by the original reward function. Consider the step \( t = 1 \) (the last step), since the reward of moving right is always higher than moving left by 1 and MFNE aims to maximise cumulative rewards, all agent will move right, i.e., \( \pi_1^*(R|L) = \pi_1^*(R|R) = 1 \). Hence, each agent earns a reward \(-\mu_1^*(L)\) if she is at “left” and \(-\mu_1^*(R)\) otherwise. Using the fact that \( \mu_1^*(L) = \pi_0^*(L|C) \) and \( \mu_1^*(R) = \pi_0^*(R|C) \), we have that the expected return of each agent under MFNE is 
\[
-1 \cdot \pi_0^*(L|C) + 0 \cdot \pi_0^*(R|C) - \mu_1^*(L) \cdot \pi_0^*(L|C) - \mu_1^*(R) \cdot \pi_0^*(R|C)
= - \pi_0^*(L|C) - (\pi_0^*(L|C))^2 - (\pi_0^*(R|C))^2
= - \pi_0^*(L|C) - (\pi_0^*(L|C))^2 - (1 - \pi_0^*(L|C))^2
= - (2\pi_0^*(L|C))^2 - \pi_0^*(L|C) + 1).
\]

From here, we have that the expected return attains the maximum when \( \pi_0^*(L|C) = 1/4 \), contradicting the MFNE induced by the original reward function.
Next, we show that the ERMFNE induced by the new reward function also changes. Again, consider the last step. According to the definition of ERMFNE, we have

\[ \pi^*_t(L|L) = \frac{\exp(-\mu^*_t(L))}{\exp(-\mu^*_t(L)) + \exp(-\mu^*_t(L) - 1)}. \]

Therefore, \( \pi^*_t(L|L) = 1/2 \) if and only if \( \mu^*_t(L) = \mu^*_t(L) + 1 \). A contradiction occurs. \( \square \)

**B Training Adaptive Samplers Using Soft Q Learning**

The update of adaptive sampler (policy) parameters is interleaved with the update of the reward parameter \( \omega \). Fixing the current reward parameter \( \omega \) and the estimated expert MF flow \( \mu^E \), we obtain an induced MDP with a reward function \( r^E(s_t, a_t, \mu^E) \) a non-stationary transition function \( p(s_{t+1}, a_t, \mu^E) \). We use notions \( Q^\text{soft}_{\mu^E,\pi^E+1:T-1} \) in the main text and \( V^\text{soft}_{\mu^E,\pi^E+1:T-1} \) in the proof of Proposition 1 to denote the soft Q value functions and soft value functions, respectively. As mentioned before, similar to the standard soft Q learning defined on infinite-horizon MDP with stationary transition functions, in MFG we have that \( Q^\text{soft}_{\mu^E,\pi^E+1:T-1} \) and \( V^\text{soft}_{\mu^E,\pi^E+1:T-1} \) fulfil

\[
Q^\text{soft}_{\mu^E,\pi^E+1:T-1}(s_t, a_t, \mu_t) = r(s_t, a_t, \mu_t) + \sum_{s_{t+1} \in S} p(s_{t+1}|s_t, a_t, \mu_t) V^\text{soft}_{\mu^E,\pi^E+1:T-1}(s_{t+1}, \mu_{t+1})
\]

and

\[
V^\text{soft}_{\mu^E,\pi^E+1:T-1}(s_t, \mu_t) = \log \sum_{a_t \in A} \exp \left( Q^\text{soft}_{\mu^E,\pi^E+1:T-1}(s_t, a_t, \mu_t) \right).
\]

For a fixed MF flow \( \mu \), to simplify notations, we omit \( \mu \) and adopt \( Q^\text{soft}(s_t, a_t) \) and \( V^\text{soft}(s_t) \) to denote the soft Q function and value functions. For the finite-horizon MDP induce by some MF flow \( \mu \), we can perform Eq. 13 and Eq. 14 from \( t = T - 1 \) to 0, i.e., the backward induction. And the obtained optimal policy fulfils Eq. 3, which we rewrite here using simplified notations for convenience for reference:

\[
\hat{\pi}(a_t|s_t) = \frac{\exp \left( Q^\text{soft}(s_t, a_t) \right)}{\sum_{a_t \in A} \exp \left( Q^\text{soft}(s_t, a_t) \right)} = \exp \left( Q^\text{soft}(s_t, a_t) - V^\text{soft}(s_t) \right).
\]

However, it is difficult to execute the backward induction in practice. First, the dynamics \( P(s, a, \mu) \) is unknown in general. Second, when the state-action space is large or continuous, computing the integral over all states in Eq. 13 and all actions in Eq. 14 is intractable. To this end, we adopt soft Q learning, an actor-critic-like policy gradient method to approximately compute a policy that maximises entropy regularised cumulative rewards. We perform soft Q learning alongside with the integral over all states in Eq. 13 and all actions in Eq. 14. For step \( t = T - 1 \), derivation of \( q^{\beta T-1} \) is trivial since \( Q^\text{soft}(s_{T-1}, a_{T-1}) = r(s_{T-1}, a_{T-1}, \mu_{T-1}) \):

\[
q^{\beta T-1}(a|s) = \frac{\exp \left( r(s, a, \mu_{T-1}) \right)}{\sum_{a' \in A} \exp \left( r(s, a', \mu_{T-1}) \right)}
\]

Then for each \( 0 \leq t \leq T - 2 \), we model the soft Q values with a function approximator with parameter \( \alpha^t \) and denote it as \( Q^\alpha_{\text{soft}}(s_t, a_t) \). And hence we obtain a parameterised soft value function

\[
V^\alpha_{\text{soft}}(s_t) = \log \sum_{a_t \in A} \exp \left( Q^\alpha_{\text{soft}}(s_t, a_t) \right)
\]

We update \( \alpha_t \) by minimising the expectation of difference between \( Q^\alpha_{\text{soft}}(s_t, a_t) \) and its “true value”

\[
Q^\alpha_{\text{soft}}(s_t, a_t) \triangleq r(s_t, a_t, \mu_t) + \gamma E_{s_{t+1} \sim p(\cdot|s_t, a_t, \mu_t)} \left[ V^\alpha_{\text{soft}}(s_{t+1}) \right].
\]
We present a detailed explanation for the reduction from MFG to MDP. Since a MFG is the limiting case of the corresponding stochastic game as the number of agents $N$ tends to infinity, MFG inherits the Markovian nature. In spirit of this, [44] converts a special type of MFG (finite-horizon and without actions) to an MDP. Also, [10] reformulates MFG with deterministic policies as MDP, based on which authors use DDPG to compute an MFNE. Note that the reductions hold under the assumption that all agents are rational, i.e., they always use an identical policy.

Here, we give a general description of these reduction methods through reformulating an discrete-time and stochastic-policy MFG as an MDP. Formally, let $(S, A, p, \mu_0, r, \gamma)$ be an MFG, we construct a MDP as follows:

\[ Q^{\alpha_{t+1}}(s_t, a_t) = \frac{1}{2} \left( Q^{\alpha_{t+1}}_{\text{soft}}(s_t, a_t) - Q^{\alpha_t}_{\text{soft}}(s_t, a_t) \right)^2. \]

In soft Q learning, we calculate the expectation using real samples from rollouts of the optimal policy induced by $Q^{\alpha_t}$, which is exactly the adaptive sampler $q^{\theta_t}$ we aim to seek, i.e.,

\[ q^{\theta_t}(a_t|s_t) \propto \exp \left( Q^{\alpha_t}_{\text{soft}}(s_t, a_t) \right). \]

When $\alpha_t$ achieves optimality, our adaptive sampler $q^{\theta_t}$ will approximate the optimal policy. In soft Q learning, we tune policy parameter $\theta_t$, so that the induced distribution by $q^{\theta_t}$ approximates the that induced by $Q^{\alpha_t}_{\text{soft}}$ in terms of KL divergence:

\[ J(q; s_t) = D_{KL} (q^{\theta_t}(s_t)\| \exp(\alpha^{\alpha_{t+1}}_{\text{soft}}(s_t, \cdot) - V^{\alpha_{t}}_{\text{soft}}(s_t))). \]

In fact, soft Q learning uses a parameterised policy $q^{\theta_t}(a_t|s_t)$ to approximate the optimal policy induced by $\alpha_t$ due to that sampling from an energy-based distributions is generally intractable. As a summary, we present the pseudocode for training adaptive samplers in Alg. [2]

**Algorithm 2 Soft Q learning for training the adaptive sampler at step $t$ ($0 \leq t \leq T - 2$)**

1: **Input:** Reward parameter $\omega$; Estimated expert MF flow $\tilde{\mu}^E$; Already learned soft Q value parameter $\alpha_{t+1}$ for the next step.

2: **Initialisation:** Initialise soft Q value parameter $\alpha_t$, adaptive sampler parameter $\theta_t$; Replay memory $D_{\text{replay}} \leftarrow \emptyset$.

3: for each epoch do

4: Collect experience

5: Sample an action for $s_t$: $a_t \leftarrow q^{\theta_t}(a_t|s_t)$.

6: Sample next state from the environment: $s_{t+1} \sim p(s_{t+1}|s_t, a_t, \tilde{\mu}^E_t)$.

7: Save the experience in the replay memory: $D_{\text{replay}} \leftarrow D_{\text{replay}} \cup \{(s_t, a_t, r_w(s_t, a_t, \tilde{\mu}^E_t), s_{t+1})\}$

8: Sample a minibatch of size $X$ from the replay memory

9: $(\{(s_t^{(x)}, a_t^{(x)}, r_w(s_t^{(x)}, a_t^{(x)}, \tilde{\mu}^E_t), s_{t+1}^{(x)})\}_{x=1}^X) \sim D_{\text{replay}}$.

10: Update the soft Q value parameter

11: Compute empirical evaluation of $\nabla_{\alpha_t} J_Q$ on the sampled minibatch.

12: Update $\alpha_t$ according to empirical $\nabla_{\alpha_t} J_Q$.

13: Update policy

14: Sample a set of $Y$ actions $\{(a^{(x, y)}(s_t^{(x)})\}_{y=1}^Y \sim q^{\theta_t}$ for each $s_t^{(x)}$.

15: Compute empirical evaluation of gradient $\nabla_{\theta_t} J_q$ using sampled actions.

16: Update $\theta_t$ according to empirical $\nabla_{\theta_t} J_q$.

17: **Output:** Q value parameter $\alpha_t$ and adaptive sampler parameter $\theta_t$.

18: end for

## C Reducing MFG to MDP

We present a detailed explanation for the reduction from MFG to MDP. Since a MFG is the limiting case of the corresponding stochastic game as the number of agents $N$ tends to infinity, MFG inherits the Markovian nature. In spirit of this, [44] converts a special type of MFG (finite-horizon and without actions) to an MDP. Also, [10] reformulates MFG with deterministic policies as MDP, based on which authors use DDPG to compute an MFNE. Note that the reductions hold under the assumption that all agents are rational, i.e., they always use an identical policy.

Here, we give a general description of these reduction methods through reformulating an discrete-time and stochastic-policy MFG as an MDP. Formally, let $(S, A, p, \mu_0, r, \gamma)$ be an MFG, we construct a MDP as follows:
The definitions of consistency and optimality are different. Consistency is defined with respect to the mean field flow corresponding to \( \pi \), which we rephrase using notations in our work:

Authors in [40] presents a detailed explanation about the difference between MFNE and MF-SO, another issue caused by the reduction to MDP is that there will be a bias in the estimation of the cumulative rewards. Hence, reduction from MFG to MDP implicitly assumes that an MFG is fully constructed MDP can always induce an MFNE which attains a ground-truth reward functions. We explain the reason for this issue as follows. The optimal policy of the constructed MDP cannot induce an MFNE that maximises the population’s societal reward. However, a MFNE is unique in general, and does not necessarily always maximises the population’s societal reward. Therefore, IRL on this MDP rationalises expert behaviours by finding reward function constellations an MFNE for the original MFG.

Let \( \bar{\pi} \) be an optimal policy for the constructed MDP, then the action trajectory generated by \( \bar{\pi} \) constitutes an MFNE for the original MFG.

Authors in [44] proposes an IRL method for MFG by directly applying standard MaxEnt IRL (as introduced in Sec. 2.3) to the constructed MDP. Intuitively, MFG-MDP IRL takes a centralised view and runs at the population level. More formally, MFG-MDP IRL assumes the expert trajectories are in the form of \{ \{ \pi_{j,t}, \mu_{j,t} \}_{t=0}^{T-1} \}_{j=1}^M \} sample from a total number of \( M \) game plays, where each \( \pi_{j,t} \) and \( \mu_{j,t} \) is estimated by:

\[
\pi_{j,t} = \frac{\sum_{i=1}^N \mathbb{1}\{s_{j,t} = s, a_{j,t} = a\}}{\sum_{i=1}^N \mathbb{1}\{s_{j,t} = s\}},
\]

\[
\mu_{j,t}(s) = \frac{1}{N} \sum_{i=1}^N \mathbb{1}\{s_{j,t} = s\}.
\]

Clearly, MFG-MDP IRL obtains only one expert trajectory from a sample of game play over \( N \) players. While, due to running at the agent level, a sample of game play over \( N \) players contributes \( N \) expert trajectories in our MFIRL. This means our MFIRL has a higher sample efficiency.

Another issue caused by the reduction to MDP is that there will be a bias in the estimation of the ground-truth reward functions. We explain the reason for this issue as follows. The optimal policy of the constructed MDP can always induce an MFNE which attains a maximum of the average expected cumulative rewards. Hence, reduction from MFG to MDP implicitly assumes that an MFG is fully cooperative in the sense that all agents aim to maximise the average reward (the societal reward) of the population. Therefore, IRL on this MDP rationalises expert behaviours by finding reward function under which the expert policy maximises the population’s societal reward. However, a MFNE is not unique in general, and does not necessarily always maximises the population’s societal reward [3, 15, 13, 11]. In particular, Subramanian and Mahajan [40] analyses the MFNE that maximises societal reward, where authors call such MFNE the mean-field social-welfare optimal (MF-SO).

Definition 3 (Mean-Field Social-Welfare Optimal [40]). A policy \( \pi \) is mean-field social welfare optimal (MF-SO) if for any other policy \( \pi' \), \( J(\mu, \pi) \geq J(\mu', \pi') \), where \( \mu = \Phi(\pi) \) and \( \mu' = \Phi(\pi') \).

Authors in [40] presents a detailed explanation about the difference between MFNE and MF-SO, which we rephrase using notations in our work:

The definitions of consistency and optimality are different. Consistency is defined with respect to the mean-field; while considering the performance of an alternative policy \( \pi' \), it is assumed that the mean-field does not change. In contrast, optimality is a property of a policy; while considering the performance of an alternative policy \( \pi' \), the mean-field approximation of the performance is with respect to the mean field flow corresponding to \( \pi \). Thus, in general, MFNE and MF-SO are different.

\[1\text{Here, we abuse the notation } \Phi \text{ to denote the next mean field induced by the current mean field and current per-policy, according to the MKV equation.} \]
As a result, if expert trajectories are sampled from an equilibrium that is not a MF-SO, a bias in the estimation of the reward parameter will occur. In contrast, from a decentralised view, the expert policy must be optimal with respect to the expert MF flow. Therefore, our MFIRL can recover the ground-truth with no bias.

D Task Description

D.1 Investment in Product Quality

Model. This model is adapted from [43] and [40] that captures the investment decisions in a fragmented market with a large number of firms. Each firm produces a same kind of product. The state of a firm \( s \in S = \{0, 1, \ldots, 9\} \) denotes the product quality. At each step, each firm decides whether or not to invest in improving the quality of the product. Thus the action space is \( A = \{0, 1\} \).

When a firm decides to invest, the quality of product manufactured by it increases uniformly at a rate \( \chi_t \), where \( \chi_t \) is a cost due to its investment and earns a positive reward due to its own product quality. Thus the action space is \( A = \{0, 1\} \).

As a result, if expert trajectories are sampled from an equilibrium that is not a MF-SO, a bias in the estimation of the reward parameter will occur. In contrast, from a decentralised view, the expert policy must be optimal with respect to the expert MF flow. Therefore, our MFIRL can recover the ground-truth with no bias.

The final reward is given as:

\[
r(s_t, a_t, \mu_t) = d \cdot s_t / 10 - c \cdot \langle \mu_t \rangle - \alpha \cdot a_t
\]

Settings. We set \( d = 0.3, c = 0.2, \alpha = 0.2 \) and probability density \( f \) for \( \chi_t \) as \( U(0, 1) \). We set the threshold \( q \) to 4 and 5 for the original and new environments, respectively. The initial mean field \( \mu_0 \) is set as a uniform distribution, i.e., \( \mu_0(s) = 1/|S| \) for all \( s \in S \).

D.2 Malware Spread

Model. The malware spread model is presented in [24, 25] and used as a numerical study for MFG in [40]. This model is representative of several problems with positive externalities, such as flu vaccination and economic models involving entry and exit of firms. Here, we present a discrete version of this problem: Let \( S = \{0, 1, \ldots, 9\} \) denote the state space (level of infection), where \( s = 0 \) is the most healthy state and \( s = 9 \) is the least healthy state. The action space \( A = \{0, 1\} \), where \( a = 0 \) means DoNothing and \( a = 1 \) means Intervene. The dynamics is given by

\[
s_{t+1} = \begin{cases} s_t + [\chi_t(10 - s_t)], & \text{if } \langle \mu_t \rangle < q \text{ and } a_t = 1 \\ s_t + [\chi_t(10 - s_t)/2], & \text{if } \langle \mu_t \rangle \geq q \text{ and } a_t = 1 \\ s_t, & \text{if } a_t = 0 \end{cases}
\]

An agent incurs a cost due to its investment and earns a positive reward due to its own product quality and a negative reward due to the average product quality, which we denote by \( \langle \mu_t \rangle \). The final reward is given as:

\[
r(s_t, a_t, \mu_t) = \frac{d}{10} \cdot s_t - a \cdot \langle \mu_t \rangle - \alpha \cdot a_t
\]

Settings. We set \( d = 0.3, c = 0.2, \alpha = 0.2 \) and probability density \( f \) for \( \chi_t \) as \( U(0, 1) \). We set the threshold \( q \) to 4 and 5 for the original and new environments, respectively. The initial mean field \( \mu_0 \) is set as a uniform distribution, i.e., \( \mu_0(s) = 1/|S| \) for all \( s \in S \).
D.3 Virus Infection

Model. This is a virus infection used as a case study [11]. There is a large number of agents in a building. Each of them can choose between “social distancing” (D) or “going out” (U). If a “susceptible” (S) agent chooses social distancing, they may not become “infected” (I). Otherwise, an agent may become infected with a probability proportional to the number of agents being infected. If infected, an agent will recover with a fixed chance every time step. Both social distancing and being infected have an associated negative reward. Formally, let $S = \{S, I\}$, $A = \{U, D\}$, $r(s, a, \mu_t) = -\mathbb{1}_{\{s=I\}} - 0.5 \cdot \mathbb{1}_{\{s=D\}}$. The transition probability is given by

$$p(s_{t+1} = S|s_t = I, \cdot, \cdot) = 0.3$$
$$p(s_{t+1} = I|s_t = S, a_t = U, \mu_t) = 0.9^2 \cdot \mu_t(I)$$
$$p(s_{t+1} = I|s_t = S, a_t = D, \cdot) = 0.$$

Settings. The initial mean field $\mu_0$ is set as a uniform distribution. We modify the transition function for the new dynamics as follows:

$$p(s_{t+1} = S|s_t = I, \cdot, \cdot) = 0.3$$
$$p(s_{t+1} = I|s_t = S, a_t = U, \mu_t) = 0.8^2 \cdot \mu_t(I)$$
$$p(s_{t+1} = I|s_t = S, a_t = D, \cdot) = 0.$$

D.4 Rock-Paper-Scissors

This model is adapted by [11] from the generalized non-zero-sum version of Rock-Paper-Scissors game [2]. Each agent can choose between “rock” (R), “paper” (P) and “scissors” (S), and obtains a reward proportional to double the number of beaten agents minus the number of agents beating the agent. Formally, let $S = A = \{R, P, S\}$, and for any $a \in A$, $\mu_t \in \mathcal{P}(S)$:

$$r(R, a, \mu_t) = 2 \cdot \mu_t(S) - 1 \cdot \mu_t(P),$$
$$r(P, a, \mu_t) = 4 \cdot \mu_t(R) - 2 \cdot \mu_t(S),$$
$$r(S, a, \mu_t) = 6 \cdot \mu_t(P) - 3 \cdot \mu_t(R).$$

The transition function is deterministic: $p(s_{t+1}|s_t, a_t, \mu_t) = \mathbb{1}_{\{s_{t+1}=a_t\}}$.

Settings. The initial mean field $\mu_0$ is set as a uniform distribution. Same to the setting in Left-Right, for new dynamics, we add a randomness to the transition function such that with probability 0.2 picking next state arbitrarily.

D.5 Left-Right

Model. This model is used in [11]. There is a group of agents making sequential decisions to moving “left” or “right”. At each step, each agent is at a position (state) either “left”, “right” or “center”, and can choose to move either “left” or “right”, receives a reward according the current population density (mean field) at each position, and with probability one (dynamics) they reach “left” or “right”. Once an agent leaves “center”, she can never head back and can only be in left or right thereafter. Formally, we configure the MFG as follows: $S = \{C, L, R\}$, $A = S \setminus \{C\}$, the reward

$$r(s, a, \mu_t) = -\mathbb{1}_{\{s=L\}} \cdot \mu_t(L) - \mathbb{1}_{\{s=R\}} \cdot \mu_t(R).$$

This reward setting means each agent will incur a negative reward determined by the population density at her current position. The transition function is deterministic that directs an agent to the next state with probability one:

$$p(s_{t+1}|s_t, a_t, \mu_t) = \mathbb{1}_{\{s_{t+1}=a_t\}}.$$

Settings. The initial mean field $\mu_0$ is set as $\mu_0(L) = 0.5$. For new dynamics, we add the randomness to the transition function. With probability 0.8, the agent moves to the state determined by the action, and with probability 0.2, the agent randomly moves to either “left” or “right”.

E Detailed Experiment Settings

Feature representations. We use one-hot encoding to represent states and actions. Let $\{1, 2, \ldots, |S|\}$ denote an enumeration of $S$ and $[s_1, s_2, \ldots, s_{|S|}]$ denote a vector of length $|S|$. 

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where each component stands for a state in $S$. The state $j$ is denoted by $[0, \ldots, 0, s_{[j]} = 1, 0, \ldots, 0]$. An action is represented through the same manner. A mean field $\mu$ is represented by a vector $[\mu(s_{[1]}), \mu(s_{[2]}), \ldots, \mu(s_{[|S|]})]$.

Models. The reward model $r_\omega$ takes as input the concatenation of feature vectors of $s$, $a$ and $\mu$ and outputs a scalar as the reward. The reward shaping model takes as input the concatenation of feature vectors of states and mean field. The adaptive sampler model takes as input the concatenation of feature vectors of a state and outputs a probability distribution over actions. For all models, We adopt the neural network (a four-layer perceptrons) with the Adam optimiser and the Leaky ReLU activation function. The sizes of two hidden layers are both 64. The learning rate is $10^{-4}$.

Environment Settings. We sample expert trajectories with $T = 50$ time steps, consider $N = 100$ agents and set the discounted factor $\gamma = 0.99$. In expert training, we repeat ERMFNE operator to compute the MF flow. We terminate at the $i$th iteration if the mean squared error over all steps and all state is below or equal to $10^{-10}$, i.e.,

$$\frac{1}{(T - 1)|S|} \sum_{t=1}^{T-1} \sum_{s \in S} (\mu^{(i)}(s) - \mu^{(i-1)}(s))^2 \leq 10^{-10}.$$  

Experiment Environments. We carry out experiments on a machine with 3 GHz Quad-Core Intel Core i5 CPU and 8GB RAM.