Unifying Behavioral and Response Diversity for Open-ended Learning in Zero-sum Games

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Abstract

Measuring and promoting policy diversity is critical for solving games with strong non-transitive dynamics where strategic cycles exist, and there is no consistent winner (e.g., Rock-Paper-Scissors). With that in mind, maintaining a pool of diverse policies via open-ended learning is an attractive solution, which can generate auto-curricula to avoid being exploited. However, in conventional open-ended learning algorithms, there are no widely accepted definitions for diversity, making it hard to construct and evaluate the diverse policies. In this work, we summarize previous concepts of diversity and work towards offering a unified measure of diversity in multi-agent open-ended learning to include all elements in Markov games, based on both Behavioral Diversity (BD) and Response Diversity (RD).

At the trajectory distribution level, we re-define BD in the state-action space as the discrepancies of occupancy measures. For the reward dynamics, we propose RD to characterize diversity through the responses of policies when encountering different opponents. We also show that many current diversity measures fall in one of the categories of BD or RD but not both. With this unified diversity measure, we design the corresponding diversity-promoting objective and population effectivity when seeking the best responses in open-ended learning. We validate our methods in both relatively simple games like matrix game, non-transitive mixture model, and the complex Google Research Football environment. The population found by our methods reveals the lowest exploitability, highest population effectivity in matrix game and non-transitive mixture model, as well as the largest goal difference when interacting with opponents of various levels in Google Research Football.

1 Introduction

Zero-sums games involve non-transitivity \([2, 4]\) in the policy space, and thus each player must acquire a diverse set of winning strategies to achieve high unexploitability \([33]\), which has been widely validated by recent studies of constructing AIs with superhuman performance in sophisticated tasks, such as StarCraft \([29, 27]\) and DOTA2 \([24, 36]\). The non-transitivity in games means there is not a dominating strategy and the set of strategies form a cycle (e.g., the endless cycles among Rock, Paper and Scissors). It is the presence of this special structure in games that requires players to maintain a diverse set of policies. Otherwise, we only need to seek the strongest one. Formally, the necessity of diversity for zero-sum games lies in three ways: (1) policy evaluation: with the presence of non-transitivity, one cannot justify the strength or weakness of a strategy through the outcome of the interaction with a single type of opponent; (2) avoiding being exploited \([23]\): since in non-transitive games a single strategy can be always beaten by another one, a diverse set of strategies allows players to make corresponding responses when encountering different opponents; (3) training

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adaptable strategies [31]: a diverse set of training opponents helps gradually eliminate the weakness of a strategy, which can adapt to a wide range of opponents with very few interactions at test time.

The open-ended learning framework is a promising direction towards inducing a population of distinct policies in zero-sum games via auto-curricula. Although various open-ended algorithms have been proposed to derive diverse strategies [2, 23, 6, 21], there are no consistent definitions for diversity. One of the most intuitive principles to characterize diversity is to build metrics over the trajectory or state-action distribution [6, 19]. However, this perspective only focuses on the policy behaviors and ignores the reward attributes inherited from the Markov decision process. We argue that this is not reasonable since sometimes a slight difference in the policy can result in a huge difference in the final reward like, in Maze. Contrary to this, another line of works builds the diversity measure over empirical payoffs [23, 2], thus revealing the underlying diverse behaviors of a strategy through the responses when encountering distinct opponents.

In this work, based on all previous diversity concepts, we work towards offering a unified view for diversity in an open-ended learning framework by combining both the behavioral attribute and the response attribute of a strategy. The behavioral diversity is formulated through the occupancy measure, which is an equivalent representation of a policy. We hypothesize that the diversity in policy behaviors should be revealed by differences in the state-action distribution, and we use a general divergence family \( f \)-divergence to indicate the novelty of a new policy. On the other hand, gamescape [2] has been proposed to represent the response capacity of a population of strategies. Based on gamescape, we formulate a new geometric perspective to treat the response diversity by considering the distance to the gamescape.

To summarize, in this paper, we provide the following contributions:

- We formulate the concept of behavioral diversity in the state-action space as the discrepancies of occupancy measures and analyze the optimization methods in both normal-form games and general Markov games.
- We provide a new geometric perspective on the response diversity as a form of Euclidean projection onto the convex hull of the meta-game to enlarge the gamescape directly and propose the optimization lower bound for practical implementation.
- We analyze the limitation of exploitability as the evaluation metric and introduce a new metric with theoretical soundness called population effectivity, which is a fairer way to represent the effectiveness of a population than exploitability [15].

2 Preliminaries

2.1 Markov Games

The extension of Markov decision processes (MDPs) with more than one agents is commonly modelled as Markov games [17]. A Markov game with \( N \) agents is defined by a tuple \( \langle N, S, \{A_i\}_{i=1}^N, P; \{r_i\}_{i=1}^N, \eta, \gamma \rangle \), where \( S \) denotes the state space and \( A_i \) is the action space for agent \( i \). The function \( P \) controls the state transitions by the current state and one action from each agent: \( P : S \times A_1 \times \cdots \times A_N \rightarrow P(S) \), where \( P(S) \) denotes the set of probability distributions over the state space \( S \). Given the current state \( s_t \) and the joint action \( (a_1, \ldots, a_N) \), the transition probability to \( s_{t+1} \) is given by \( P(s_{t+1} \mid s_t, a_1, \ldots, a_N) \). The initial state distribution is given by \( \eta : S \rightarrow [0, 1] \). Each agent \( i \) also has an associated reward function \( r_i : S \times A_i \times \cdots \times A_N \rightarrow \mathbb{R} \). Each agent’s goal is to maximize the \( \gamma \)-discounted expected return \( R_i = \mathbb{E}_i \left[ \sum_{t=0}^{\infty} \gamma^t r_i(s_t, a_i, a_{-i}) \right] \), where \( -i \) is a compact representation of all complementary agents of \( i \). Specifically, for zero-sum games, the rewards satisfy that \( \sum_{i=1}^N r_i(s, a) = 0 \), and players need to behave competitively to achieve higher rewards.

In multi-agent reinforcement learning (MARL) [34], each agent is equipped with a policy \( \pi_i : S \times A_i \rightarrow [0, 1] \) and the joint policy is defined by \( \pi(a) = \Pi_{i=1}^N \pi_i(a_i) \). In single-agent reinforcement learning, occupancy measure is a principle way to characterize a policy, which indicates how a policy covers the state-action space. Inspired by the definition from the single-agent setting, we define the joint occupancy measure in MARL induced by the joint policy \( \pi(a) \) as:
Then the distribution of state-action pairs \( \rho(\cdot) : \mathcal{S} \times \mathcal{A} \to \mathbb{R} \) denote the normalized distribution of state visitation by following the joint policy \( \pi = (\pi_i, \pi_{-i}) \) in the environment:

\[
\rho(\pi \cdot)(s, a) = \frac{1}{\sum a : \rho(\pi \cdot)(s, a)}
\]

Then the distribution of state-action pairs \( \rho(\pi \cdot)(s, a) = \rho(\pi \cdot)(s, a) \) is called occupancy measure of the joint policy \( \pi \).

### 2.2 Policy Space Response Oracle

Adapted from double oracle [22], policy space response oracle (PSRO) [15, 5] has been serving as a powerful tool to solve the nash equilibrium (NE) in zero-sum games. In PSRO, each player maintains a pool of policies, say \( \Psi_i = \{\pi^1_i, \ldots, \pi^M_i\} \) for player \( i \) and \( \Psi_{-i} = \{\pi^1_{-i}, \ldots, \pi^N_{-i}\} \) for player \(-i\). The so-called meta game \( A_{\Psi_i \times \Psi_{-i}} \) has its \((k, j)\) entry as \( \phi_k(\pi^k_i, \pi^j_{-i}) \), where the function \( \phi_k \) encapsulates the reward outcome for player \( i \) like the winning rate or expected return. When player \( i \) adds a new policy \( \pi^M_i \), it will compute the best response to the mixture of its opponents:

\[
\text{Br}(\Psi_{-i}) = \max_{\pi_{-i}^{M+1}} \sum_{j} \sigma^j \pi_{-i}^{M+1} \mathbb{E}_{\pi^j_i, \pi_{-i}^{M+1}} \left[ r_i(s, a) \right].
\]

where \( \sigma = (\sigma_i, \sigma_{-i}) \) is a distribution over policies in \( \Psi_i \) and \( \Psi_{-i} \), which is usually a NE of \( A_{\Psi_i \times \Psi_{-i}} \).

The empirical gamescape is introduced by [2] to represent the expressiveness of a population \( \Psi_i \) in the reward outcome level given the opponent population \( \Psi_{-i} \):

**Definition 2.** Given population \( \Psi_i \) and \( \Psi_{-i} \) with evaluation matrix \( A_{\Psi_i \times \Psi_{-i}} \), the corresponding empirical gamescape (EGS) for \( \Psi_i \) is defined as

\[
G_{\Psi_i, \Psi_{-i}} := \{\text{convex mixtures of rows of } A_{\Psi_i \times \Psi_{-i}}\}.
\]

### 2.3 Existing Diversity Measures

As the metric to measure the differences between models, diversity is an important topic in many fields of machine learning, including generative modelling [6], latent variable models [32], and robotics [1]. Specifically, in reinforcement learning (RL), diversity is a useful tool for learning transferable skills [7], boosting explorations [26], or collecting near-optimal policies that are distinct. Thanks to the tools of empirical game theory analysis, diversity can be modeled as the average total variation distance of two action distributions under certain sampled states. Considering the geometric perspective that the determinant of the kernel matrix represents the volume of a parallelepiped spanned by feature maps, DvD [25] proposed the concept of population diversity using the determinant of the kernel matrix composed by the behavioral embeddings by multiple policies. Thanks to the tools of empirical game theory analysis, diversity can be modeled from the perspective of the empirical game. Effective diversity [2] is formulated as the weighted \( L_{1,1} \) norm of the empirical payoff matrix, which emphasizes what opponents a policy can win against. Also inspired by determinantal point process (DPP) [13, 35], [23] uses the expected cardinality to measure the diversity of a population.

| Method          | Tool for Diversity       | BD | RD | Game Type               |
|-----------------|--------------------------|----|----|-------------------------|
| DvD             | Determinant              | ✓  |    | Single-agent            |
| PSRO \(_N\)     | None                     | ×  |    | n-player general-sum game |
| PSRO \(_N\)     | \( L_1 \) norm           | ×  | ✓  | 2-player zero-sum game   |
| DPP-PSRO        | Determinantal point process | ×  | ✓  | 2-player general-sum game |
| Our Methods     | Occupancy measure & convex hull | ✓  | ✓  | n-player general-sum game |

Table 1: Comparisons of Different Algorithms.
3 A Unified Diversity Measure

Motivated by bisimulation metric [8] to measure the similarity of two states in MDPs: $d(s_i, s_j) = \max_{a \in A}(1 - c) \cdot |R^a_{s_i} - R^a_{s_j}| + c \cdot W_1(P^n_{s_i}, P^n_{s_j}; d)$, which considers both the immediate reward and the following transition dynamics, we want to build the metric to measure the similarity of two policies in a given Markov game through the task-specific reward attributes and the interaction between policy behaviors and transition dynamics. We will firstly model the interaction between policy behaviors and transition dynamics through the principled occupancy measure in MDPs, which encodes how a policy behaves in a given state and how the state will transit. On the reward side, the interaction responses with different opponents feature a policy, which can be used for common diversity measures like DPP [23] and rectified Nash [2].

3.1 Behavioral Diversity via Occupancy Measure Mismatching

One fundamental way to characterize a policy in MDPs is through the distribution of the state-action pair $(s, a)$. Formally, we define the occupancy measure in multi-agent learning as the distribution of the joint state-action distribution. It has been shown that there is a one-to-one correspondence between the joint policy $\pi$ and the occupancy measure $\rho_\pi$.

**Proposition 1** (Theorem 2 of [28]). If $\rho$ is valid occupancy measure, then $\rho$ is the occupancy measure for $\pi_\rho(a | s) = \rho(s, a) / \sum_a \rho(s, a')$, and $\pi_\rho$ is the only policy whose occupancy measure is $\rho$.

Usually, the policy $\pi$ is parameterized as a neural network, and tackling the policy in the parameter space is intractable. However, due to the one-to-one correspondence between the policy and occupancy measure, the occupancy measure $\rho_\pi$ serves as a unique and informative representation for the policy $\pi$. Therefore, we are justified in considering diversity from a perspective of the occupancy measure.

Next, we will consider how to promote diversity in the framework of policy space response oracle. Suppose after $t$ iterations of PSRO, the joint policy aggregated according the distribution of nash is $\pi_E = (\pi_i, \pi_{E_{-i}})$. The occupancy measure is given by $\rho_{\pi_E}$. For player $i$ in the $t + 1$ iteration, it will seek the new policy $\pi'_i$, which can maximize the discrepancy between old $\rho_{\pi_E}$ and $\rho_{\pi'_i, \pi_{E_{-i}}}$.

$$\max_{\pi'_i} \text{Div}_{occ}(\pi'_i) = D_f(\rho_{\pi'_i, \pi_{E_{-i}}} \| \rho_{\pi_i, \pi_{E_{-i}}}) ,$$

where we use the general $f$-divergence to measure the discrepancy of two distributions.

We firstly investigate the objective under the one-step game by giving the following theorem:

**Theorem 1.** By assuming the game is a one-step game (normal-form games, functional-form games, etc.) and policies among players are independent, the behavioral diversity can be simplified by:

$$D_f(\rho_{\pi'_i, \pi_{E_{-i}}} \| \rho_{\pi_i, \pi_{E_{-i}}}) = E_{s_0 \sim \eta(s)}[D_f(\pi'_i(\cdot | s_0) || \pi_i(\cdot | s_0))] .$$

**Proof.** See Appendix A.1.

For more general Markov games, computing the exact occupancy measure is intractable. However, notice that we are maximizing a $f$-divergence objective of occupancy measures, while occupancy measure matching algorithms in imitation learning try to minimize the same objective [12, 10, 9]. Leveraging the powerful tool from occupancy measure matching, we here propose an approximate method to maximize $\text{Div}_{occ}$.

**Prediction Error for Approximate Optimization.** Inspired by random expert distillation [30], a neural network $f_\theta(s, a)$ is trained to fit a randomly initialized fixed network $f_0(s, a)$ on the dataset of state-action pair $(s, a) \sim \rho_{\pi_E}$. Then we can assign an intrinsic reward $r^\text{intr}_{\pi_E}(s, a) = \| f_\theta(s, a) - f_0(s, a) \|$ to the player, which will encourage the agent to visit the state-action with large prediction errors, thus pushing occupancy measure of the new policy to be different from the old one.

**Alternative Solutions.** There are also many other practical occupancy measure matching algorithms. One popular paradigm is learning a discriminator $D(s, a)$ to classify the state-action pair $(s, a)$ from the distribution $\rho_{\pi'_i, \pi_{E_{-i}}}$ and the distribution $\rho_{\pi_E}$. Then the trained $D(s, a)$ can be used to construct
different intrinsic rewards, which will correspond to different choices of \( f \)-divergence [12, 10, 9]. One major drawback of this paradigm is that the discriminator depends on the new policy \( \pi_i' \) and needs re-training once the policy \( \pi_i' \) is updated. Another popular paradigm is to learn an intrinsic reward directly from the target distribution \( \rho_{\pi E} \) like the prediction error. Besides using the prediction error, there are also other choices, including energy-based model (EBM) [18] and expert variance [3]. However, those methods usually require specialized training techniques.

3.2 Response Diversity via Convex Hull Enlargement

Take the two-player game for an example. In games with more than two players, one can simply denote players other than player \( i \) as player \(-i\). Thanks to the empirical payoff matrix, another fundamental way to characterize the diversity of a new policy is through the reward outcome from the interaction with many different opponents. Each row in the empirical payoff matrix embeds how the corresponding row policy behaves against different opponent policies. We are therefore justified in using the row vector of the empirical payoff matrix to represent the corresponding row policy.

Formally, assume the row player maintains a pool of policies \( \Psi_i = \{\pi_i^1, \ldots, \pi_i^M\} \) and the column player maintains a pool of policies \( \Psi_{-i} = \{\pi_{-i}^1, \ldots, \pi_{-i}^N\} \). The induced \((k, j)\) entry in the empirical payoff matrix \( A_{\pi_i^k \times \pi_{-i}^j} \) is given by \( \phi_k(\pi_i^k, \pi_{-i}^j) \), where the function \( \phi_k \) encapsulates the reward outcome for player \( i \) given the joint policy \((\pi_i^k, \pi_{-i}^j)\). Now we can define the diversity measure induced by the reward representations:

\[
\text{Div}_{\text{rew}}(\pi_i^{M+1}) = D(a_{M+1} \| A_{\pi_i^1 \times \Psi_{-i}}) \quad \text{(4)}
\]

\[
a_{M+1} := (\phi_k(\pi_i^k, \pi_{-i}^j))_{k=1}^N. \quad \text{(5)}
\]

\(D(a_{M+1} \| A_{\pi_i^1 \times \Psi_{-i}})\) essentially measures the diversity of the new vector \( a_{M+1} \) given the presence of row vectors in \( A_{\pi_i^1 \times \Psi_{-i}} \).

Inspired by the intuition of the convex hull that indicates the representational capacity of a pool of policies, the diverse new policy should seek to enlarge the convex hull of reward vectors as large as possible. To characterize the contribution of a vector to the enlargement of the convex hull directly, we define the novel diversity measure as a form of Euclidean projection:

\[
\text{Div}_{\text{rew}}(\pi_i^{M+1}) = \min_{x \in \mathbb{R}^M, \beta \geq 0} \| A_{\pi_i^1 \times \Psi_{-i}} \beta - a_{n+1} \|_2^2. \quad \text{(6)}
\]

Unfortunately, there is no closed-form solution to this optimization problem. To facilitate the optimization, we propose a practical and differential lower bound:

**Theorem 2.** For a given empirical payoff matrix \( A \) and the reward vector \( a_{n+1} \), the lower bound of \( \text{Div}_{\text{occ}} \) is given by:

\[
\text{Div}_{\text{rew}}(\pi_i^{M+1}) \geq \sigma_{\min}(A)(1 - 1^T(A^T)^\dagger a_{n+1})^2 + \|\| (I - A^T(A^T)^\dagger) a_{n+1} \|_2^2, \quad \text{(7)}
\]

where \((A^T)^\dagger\) is the Moore–Penrose pseudoinverse of \( A^T \), and \( \sigma_{\min}(A) \) is the minimum singular value of \( A \).

**Proof.** See Appendix A.2. \(\square\)

Let \( F(\pi_i^{M+1}) \) be the right hand of the inequality. Then \( F(\pi_i^{M+1}) \) serves as a lower bound of \( \text{Div}_{\text{rew}}(\pi_i^{M+1}) \).

4 A Unified Diverse Objective for Best Response

Equipped with the unified diversity measure, we are ready to propose the diversity-aware response during each iteration of PSRO:

\[
\arg \max_{\pi_i'} E_{s, a \sim \rho_{\pi_{i'}^i \times \rho_{-i}}} [r(s, a)] + \lambda_1 \text{Div}_{\text{occ}}(\pi_i') + \lambda_2 \text{Div}_{\text{rew}}(\pi_i'). \quad \text{(8)}
\]

If both \( \lambda_1 \) and \( \lambda_2 \) are 0, then objective is a normal best response.
Algorithm 1: Gradient-based Optimization for Unified Diverse Response

1: Input: population \( \mathcal{P}_i \) for each \( i \), meta-game \( \mathbf{A}_{\mathcal{P}_i \times \mathcal{P}_{-i}} \), state-action dataset \( \{(s, a)\} \), weights \( \lambda_1 \) and \( \lambda_2 \)
2: \( \sigma_i, \sigma_{-i} \leftarrow \text{Nash on } \mathbf{A}_{\mathcal{P}_i \times \mathcal{P}_{-i}} \)
3: \( \pi_{E_i} \leftarrow \text{Aggregate according to } \sigma_i, \sigma_{-i} \)
4: \( r_{i}^{\text{int}}(s, a) \leftarrow \text{Train fixed reward from distribution } (s, a) \sim \rho_{\pi_{E_i}} \text{ by EBM or prediction errors.} \)
5: \( \theta^* \leftarrow \text{Train } \pi_i'(\theta) \text{ against fixed opponent policies } \pi_{E_{-i}} \text{ by single-agent RL algorithm with } \)
6: \( \partial F_{\sigma_{n+1}} \leftarrow \text{Simulate the reward row vector } \mathbf{a}_{n+1} \text{ using new } \pi_i'(\theta) \text{ and compute } \partial F_{\sigma_{n+1}} \text{ analytically.} \)
7: \( \hat{\theta} \leftarrow \text{Train } \pi_i'(\theta^*) \text{ against a new mixture distribution } \sigma_{-i} + \lambda_2 \partial F_{\sigma_{n+1}} \text{ of opponent policies.} \)
8: Output: policy \( \pi_i'(\hat{\theta}) \)

4.1 On the Optimization of Diverse Regularizers

Discussions on Optimizing BD. As discussed in Section 3.1, diversity in the occupancy measure level is fully compatible with the reinforcement learning task since the agent can get an intrinsic reward \( r_{i}^{\text{int}}(s, a) \) to indicate the novelty of a state-action pair \( (s, a) \). Therefore, to optimize the first two items in the objective, we only need to add the original reward by the \( \lambda_1 \)-weighted intrinsic reward. Another issue we need to address is to sample \( (s, a) \) from the distribution \( \rho_{\pi_{E_i}} \), which has been mentioned in Section 3. Since \( \pi_{E_i} \) is not a true policy but only a hypothetical policy aggregated according to the mixture \( (\sigma_i, \sigma_{-i}) \), sampling from \( \rho_{\pi_{E_i}} \) is equivalent to sampling from \( \rho_{\pi_{i}^1, \pi_{i}^2} \) with probability \( \sigma_i^1 \sigma_{-i}^2 \).

Discussions on Optimizing RD. Optimizing \( \text{Div}_{\text{rew}} \) is not so easy since it involves an inner minimization problem. Fortunately, we have derived a closed-form low-bound \( F \), which can serve as a surrogate for the outer maximization.

Assume the policy \( \pi_i' \) is parameterized by \( \theta \) as \( \pi_i'(\theta) \). Then the gradient of \( F \) with respect to \( \theta \) is given by:

\[
\frac{\partial F(\pi_i'(\theta))}{\partial \theta} \Bigg|_{\theta} = \frac{\partial F}{\partial \theta} \bigg|_{\theta} \frac{\partial F}{\partial \mathbf{a}_{n+1}} = \left( \frac{\partial \phi_i(\pi_i'(\theta), \pi_{i-1})}{\partial \theta}, \ldots, \frac{\partial \phi_i(\pi_i'(\theta), \pi_{N-i})}{\partial \theta} \right) \frac{\partial F}{\partial \mathbf{a}_{n+1}}.
\]

\( \frac{\partial F}{\partial \mathbf{a}_{n+1}} \) controls weights of the policy gradient backpropagated from different opponents policies \( \pi_{-i} \).

For practical implement, we sample an opponent \( j \) according to the absolute values of \( \frac{\partial F}{\partial \mathbf{a}_{n+1}} \) and then train \( \pi_i' \) against the opponent \( \pi_{i-1} \) using gradient descent or ascent, which depends on the sign of the \( j_{\text{th}} \) entry of \( \frac{\partial F}{\partial \mathbf{a}_{n+1}} \).

Joint Optimization. One issue worth our notice is that the update direction of \( \text{Div}_{\text{rew}} \) will heavily rely on the initialization of \( \pi_i'(\theta) \). A bad initialization of \( \theta \) will make the response diversity tell \( \pi_i' \) to update toward worse rewards. Therefore, we propose to first optimize the first two items in the objective jointly and then optimize \( \pi_i' \) using \( \text{Div}_{\text{rew}} \). The final unified diverse response with gradient-based optimization is described in Algorithm 1.

In addition to the gradient-based optimization, we also provide other kinds of optimization oracles suitable for different games. Pseudocodes can be found in Appendix G.

4.2 Evaluation Metrics

Exploitability. Exploitability [15] measures the distance of a joint policy from the Nash equilibrium. It shows how much each player gains by deviating to their best responses:

\[
\text{Exp}(\pi) = \sum_{i=1}^{N} \left( \max_{\pi_i} \phi_i(\pi_i, \pi_{-i}) - \phi_i(\pi_i, \pi_{-i}) \right).
\]

Therefore, the smaller exploitability means the joint policy is closer to the Nash equilibrium.
**Population Effectivity.** Note the limitation of exploitability is that it only measures how exploitable a single joint policy is. Therefore, to evaluate the effectiveness of a population, we first need to get an aggregated policy from a population, and we usually use the Nash aggregated policy output by PSRO. Since the Nash is computed over the meta game, which varies with the opponents, the aggregation may be sub-optimal and cannot be used to represent a population. Intuitively, the aggregation weights, and further, the evaluation of a population should not be determined by the population that a specific opponent holds. To address this issue, we propose a generalized opponent-free concept of exploitability called Population Effectivity (PE) by looking for the optimal aggregation in the worst cases:

\[
PE(\{\pi^k\}_{k=1}^N) = \min_{\pi^0} \max_{\alpha \geq 0} \sum_{k=1}^N \alpha_k \phi_i(\pi^k_1, \pi^k_{-i}).
\] (10)

PE is again a NE over a two-player zero-sum game, where the player owning the population optimizes towards an optimal aggregation denoted by \(\alpha\), while the opponent can search over the entire policy space. Next, we offer a simple example to further illustrate the limitations of exploitability and superiority of PE.

**Example 1.** Consider the matrix game Rock-Scissor-Paper, where \(\phi_1(\pi_1, \pi_2) = \pi_1^\top A \pi_2\) and \(\phi_2(\pi_2, \pi_1) = \pi_2^\top B \pi_1\), \(\pi_1 \in \mathbb{R}^3, \pi_2 \in \mathbb{R}^3, A = \begin{bmatrix} 0 & 1 & -1 \\ -1 & 0 & 1 \\ 1 & -1 & 0 \end{bmatrix}, B = -A^\top\). Suppose player 1 holds the population \(\mathcal{P}_1 = \{\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}\}\), i.e. \{Rock, Scissor, Paper\} and \(\mathcal{P}_2 = \{\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}\}\), i.e. \{Rock\}. Then the meta-game \(A_{\mathcal{P}_1 \times \mathcal{P}_2} = \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix}\). The Nash aggregated joint policy \((\pi_1, \pi_2) = (\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix})\). Now we can compute \(\text{Expl}((\pi_1, \pi_2))\) as:

\[
\text{Expl}((\pi_1, \pi_2)) = \max_{\pi_1} \phi_1(\pi_1^t, \pi_2) - \phi_1(\pi_1, \pi_2) + \max_{\pi_2} \phi_2(\pi_2^t, \pi_1) - \phi_2(\pi_2, \pi_1)
\] (11)

\[= \max_{\pi_1} \phi_1(\pi_1^t, \pi_2) + \max_{\pi_2} \phi_2(\pi_2^t, \pi_1) = 2.\] (12)

Now notice that the contribution of player 1 to the exploitability is \(\max_{\pi_1^t} \phi_1(\pi_2^t, \pi_1)\), which equals 1. However, it is not reasonable that player 1 and 2 have the same contribution to the exploitability since player 1 has a perfect diverse policy set. Instead, if we use PE as the metric:

\[PE(\mathcal{P}_1) = 0,\] (13)

which justifies that player 1 has already found a perfect population.

In the following theorem, we show that PE is a generalized notion of exploitability under certain conditions and has some desirable properties:

**Theorem 3.** Population effectivity has the following properties:

**P1. Equivalence:** If \(N = 1\) and the underlying game \(\phi_i(\cdot, \cdot)\) is a symmetric two-player zero-sum game, PE is equivalent to exploitability.

**P2. Monotonicity:** If there are two populations \(\mathcal{P}_i, \Omega_i\) and \(\mathcal{P}_i \subseteq \Omega_i\), then \(PE(\mathcal{P}_i) \leq PE(\Omega_i)\), while the relationship for exploitability of the Nash aggregated policies of \(\mathcal{P}_i\) and \(\Omega_i\) may or may not hold.

**P3. Tractability:** If the underlying game \(\phi_i(\cdot, \cdot)\) is a matrix game, then computing PE is still solving a matrix game.

**Proof.** See Appendix A.3.
We firstly visualize the exploration trajectories during different algorithms solving the game in Figure 2. It shows that the best response algorithm regularized by both BD and RD achieves the most diverse trajectories. Although our algorithm finds the most diverse trajectories, such superiority is not revealed by the metric of exploitability in the last row of Table 2. On the other hand, we also report the PE values for the final population generated by different algorithms in Table 2. It can found that our unified diversity regularizer can always help PSRO dominate other baselines in terms of values of exploitability and PE during the growth of the population in Figure 1a and Figure 1b. The result shows that with our unified diversity regularizer, our methods achieve the smallest exploitability and largest population effectivity, while most baselines fail to recover the diverse strategies and are easily exploited.

**Non-Transitive Mixture Games.** This zero-sum two-player game consists of $2l+1$ equally-distanced Gaussian humps on the 2D plane. Each player chooses a point in the 2D plane, which will be translated into a $(2l+1)$-dimensional vector $\pi_i$ with each coordinate being the density in the corresponding Gaussian distribution. The payoff of the game is given by $\phi_i(\pi_i, \pi_{-i}) = \pi_i^\top \mathbf{S} \pi_{-i} + 1^\top (\pi_i - \pi_{-i})$. According to the delicately designed $\mathbf{S}$, this game involves both the transitive component and non-transitive component, which means the optimal strategy should stay close to the center of the Gaussian and explore all the Gaussian distributions equally.

We firstly visualize the exploration trajectories during different algorithms solving the game in Figure 2. It shows that the best response algorithm regularized by both BD and RD achieves the most diverse trajectories. Although our algorithm finds the most diverse trajectories, such superiority is not revealed by the metric of exploitability in the last row of Table 2. On the other hand, we also report the PE values for the final population generated by different algorithms in Table 2. It can found that our unified diversity regularizer can always help PSRO dominate other baselines in terms of values of exploitability and PE during the growth of the population in Figure 1a and Figure 1b. The result shows that with our unified diversity regularizer, our methods achieve the smallest exploitability and largest population effectivity, while most baselines fail to recover the diverse strategies and are easily exploited.

**Real-World Games.** [4] studies the properties of some complex real-world games, including AlphaStar and AlphaGO. We test our method on the empirical games generated through the process of solving these real-world games. In Figure 1a, we report the exploitabilities of different algorithms solving the AlphaStar game, which contains the meta-payoffs for 888 RL policies. We report values of exploitability and PE during the growth of the population in Figure 1a and Figure 1b. The result shows that with our unified diversity regularizer, our methods achieve the smallest exploitability and largest population effectivity, while most baselines fail to recover the diverse strategies and are easily exploited.

5 Experiments

To verify that our diversity-regularized best response algorithm can induce a diverse and less exploitable population, we compare our methods with state-of-the-art game solvers including Self-play [11], PSRO [15], PSRO-rN [2], Pipeline-PSRO (P-PSRO) [20], DPP-PSRO [23]. In this section, we want to demonstrate the effectiveness of our method to tackle the non-transitivity of zero-sum games, which can be shown via higher PE, lower exploitability, and diverse behaviors. Beyond the simple games, we also have the results on the complex Google Research Football game, and our methods can still work. In all the following experiments, we choose the appropriate diversity weights $\lambda_1$ and $\lambda_2$ by extensive hyper-parameter tuning. We also conduct ablation study by choosing different $\lambda_1$ and $\lambda_2$ in Appendix F. The environment details are in Appendix D, and the hyper-parameter settings for each experiment are in Appendix E.3.
population effectivity, which also justifies why PE is a better metric to evaluate diverse populations. The details of computing approximate PE using PSRO can be found in Appendix B.

**Google Research Football**. In addition to the experiments on relatively simple games, we also evaluate our methods on a challenging real-world game named Google Research Football (GRF) [14]. GRF simulates a complete football game under standard rules with 11 players on each team, and a normal match lasts for 30,000 steps. The enormous exploration spaces, the long-time horizon, and the sparse rewards problems in this game make it a challenging environment for modern reinforcement learning algorithms. In such complex scenarios, the exploitability of a certain policy or PE of a certain population would be hard to calculate because both metrics involve a max or min operator, and the approximate best response can be quite inaccurate for this complex game. Since our goal is to find robust policies with strong capabilities in real-world games, we compare the average goal differences between the aggregated policies of different methods and the built-in bots with various difficulty levels of GRF. The models within each aggregated policies are trained for 300000 steps under the generalized framework of Self-play [11] by selecting opponents according to the probabilities output by different methods.

As depicted in Figure 3, policies trained by PSRO with both BD and RD achieve the largest goal differences when playing against the built-in bots. Moreover, they have an average of 60% win-rate over other baseline methods (see the table in the Appendix C). We do not report the results of DPP-PSRO since it needs evolutionary updates and cannot scale to such a complex setting. We also abandon the pipeline trick for ease of implement since it does not affect the relative performance among algorithms. Additionally, the discussion of robustness of policies trained with different methods, the network architectures, the hyperparameters, and other detailed experimental setups can also be found in Appendix C.

### 6 Conclusions

This paper investigated a new perspective on unifying diversity measures for open-ended learning in zero-sum games, which shapes an auto-curriculum to induce diverse yet effective behaviors. To this end, we decomposed the similarity measure of MDPs into behavioral and response diversity and showed the most of the existing diversity measures for RL can be concluded into one of the categories of them. We also provided the corresponding diversity-promoting objective and optimization methods, which consist of occupancy measure mismatching and convex hull enlargement. Finally, we proposed population effectivity to overcome the limitation of exploitability in measuring diverse policies for open-ended algorithms. Experimental results demonstrated our method is robust to both highly non-transitive games and complex games like the Google Research Football environment.
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Appendix for "Unifying Behavioral and Response Diversity for Open-ended Learning in Zero-sum Games"

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A Full Proof of Theorems

A.1 Proof of Theorem 1

To prove Theorem 1, we need the help of the following Lemma

**Lemma 1.** If \( P_{X,Y} = P_X P_{Y|X} \) and \( Q_{X,Y} = Q_X P_{Y|X} \) then

\[
D_f(P_{X,Y} \| Q_{X,Y}) = D_f(P_X \| Q_X).
\] (14)

**Proof.** See Proposition 7.1 in [3]. \(\square\)

Now we can prove our Theorem 1.

**Proof.** For games with only one step (normal-form games, functional-form games), there is only one fixed state. Therefore, the distribution of state-action is equivalent to the distribution of the action. Formally, for \( \rho_{\pi'_i, \pi_{E \sim i}} \), we have:

\[
\rho_{\pi'_i, \pi_{E \sim i}}(s, a) = (\pi'_i, \pi_{E \sim i})(a) = \pi'_i(a_i)\pi_{-i}(a_{-i}) ,
\] (15)

where the second equation comes from the assumption that policies are independent. Similarly, for \( \rho_{\pi_i, \pi_{E \sim i}} \), we also have:

\[
\rho_{\pi_i, \pi_{E \sim i}}(s, a) = (\pi_i, \pi_{E \sim i})(a) = \pi_i(a_i)\pi_{-i}(a_{-i}) .
\] (16)
Therefore, with the help of Lemma 1, we have:
\[
D_f(\rho_{\pi^*_i, \pi_{E-i}} \| \rho_{\pi_i, \pi_{E-i}}) = D_f(\pi^*_i \| \pi_i) = D_f(\pi_i^* \| \pi_i) .
\]  
(17)

\[\square\]

A.2 Proof of Theorem 2

Let us restate our Theorem 2

**Theorem 2.** For a given empirical payoff matrix \(A \in \mathbb{R}^{M \times N}\) and the reward vector \(a_{M+1}\) for policy \(\pi_{M+1}\), the lower bound of Divocc is given by:

\[
\text{Div}_{\text{occ}}(\pi_{M+1}) \geq \frac{\sigma_{\text{min}}^2(A)(1 - I^T(A^T)^+a_{M+1})^2}{M} + ||(I - A^T(A^T)^+)a_{M+1}||^2,
\]

where \((A^T)^+\) is the Moore–Penrose pseudoinverse of \(A^T\), and \(\sigma_{\text{min}}(A)\) is the minimum singular value of \(A\).

**Proof.**

\[
\min_{1^T \beta = 1} \min_{\beta \geq 0} ||A^T \beta - a_{M+1}||^2 
\geq \min_{1^T \beta = 1} \min_{\beta \geq 0} ||A^T \beta - A^T (A^T)^+a_{M+1}||^2 + ||(I - A^T (A^T)^+)a_{M+1}||^2 
= \min_{1^T \beta = 1} ||A^T (\beta - (A^T)^+a_{M+1})||^2 + ||(I - A^T (A^T)^+)a_{M+1}||^2 
\geq \sigma_{\text{min}}^2(A) \min_{1^T \beta = 1} ||\beta - (A^T)^+a_{M+1}||^2 + ||(I - A^T (A^T)^+)a_{M+1}||^2 
\geq \frac{\sigma_{\text{min}}^2(A)(1 - I^T(A^T)^+a_{M+1})^2}{M} + ||(I - A^T (A^T)^+)a_{M+1}||^2,
\]

where the first equation comes from that we decompose \(a_{M+1}\) into \(A^T(A^T)^+a_{M+1} + (I - A^T(A^T)^+)a_{M+1}\). The last equation comes from the analytic calculation of \(\min_{1^T \beta = 1} ||\beta - (A^T)^+a_{M+1}||^2\) using Lagrangian.

\[\square\]

A.3 Proof of Theorem 3

Now let us first restate the propositions.

**Proposition 1.** If \(N = 1\) and the underlying game \(\phi_i(\cdot, \cdot)\) is a symmetric two-player zero-sum game, PE is equivalent to exploitability.

To prove this, let us prove the following Lemma 2.

**Lemma 2.** For any policy \(\pi\) in two-player symmetric zero-sum games:

\[
\phi_i(\pi, \pi) = 0 .
\]

**Proof.** To begin with, due to the assumption that the game is symmetric, we get:

\[
\phi_i(\pi_i, \pi_{-i}) = \phi_{-i}(\pi_{-i}, \pi_i) .
\]

(20)

Since the game is also zero-sum, we have:

\[
\phi_{-i}(\pi_{-i}, \pi_i) = -\phi_i(\pi_{-i}, \pi_i) .
\]

(21)

By combing Equation 20 and Equation 33, for any \(\pi_i\) and \(\pi_{-i}\), we get:

\[
\phi_i(\pi_i, \pi_{-i}) + \phi_i(\pi_{-i}, \pi_i) = 0 .
\]

(22)

Let \(\pi_i = \pi_{-i} = \pi\), we get what we need to prove:

\[
\phi_i(\pi, \pi) = 0 .
\]

(23)

\[\square\]
Now we can begin proof of our proposition.

**Proof.** To prove this theorem, we need a further assumption that PSRO maintains only one population for two-player symmetric game, which is a quite common practice. Therefore, the joint Nash aggregated policy satisfies that \( \pi_E = (\pi_i, \pi_{-i}) \) satisfies \( \pi_i = \pi_{-i} \). Therefore, with the help of Lemma 2:

\[
\phi_i(\pi_i, \pi_{-i}) = \phi_{-i}(\pi_{-i}, \pi_i) = 0 .
\]

Furthermore, exploitability for symmetric zero-sum game can be written as:

\[
\text{Exp}_E(\pi_E) = \sum_{i=1}^{2} \max_{\pi_i} \phi_i(\pi_i', \pi_{-i}) - \phi_i(\pi_i, \pi_{-i}) \tag{25}
\]

\[
= \sum_{i=1}^{2} \max_{\pi_i} \phi_i(\pi_i', \pi_{-i}) \tag{26}
\]

\[
= 2 \max_{\pi_i} \phi_i(\pi_i', \pi_{-i}) , \tag{27}
\]

where the last equation comes from the symmetry of the game and \( \pi_i = \pi_{-i} \).

For PE, it is calculated as:

\[
\text{PE}(\{\pi_i\}) = \min_{\pi_{-i}} \phi_i(\pi_i, \pi_{-i}) \tag{28}
\]

\[
= - \max_{\pi_{-i}} \phi_i(\pi_{-i}', \pi_i) \tag{29}
\]

\[
= -\frac{1}{2} \text{Exp}_E(\pi_E) . \tag{30}
\]

The second to last equation comes from Equation 22, and the last equation is due to the assumption that \( \pi_i = \pi_{-i} \). \( \square \)

**Proposition 2.** If there are two populations \( \mathcal{P}_i, \mathcal{Q}_i \) and \( \mathcal{P}_i \subseteq \mathcal{Q}_i \), then \( \text{PE}(\mathcal{P}_i) \leq \text{PE}(\mathcal{Q}_i) \), while the relationship for exploitability of the Nash aggregated policies of \( \mathcal{P}_i \) and \( \mathcal{Q}_i \) may or may not hold.

**Proof.** We begin with proof of the monotonicity of PE. W.o.l.g, let us assume that \( \mathcal{P}_i = \{\pi_i^k\}_{k=1}^M \), \( \mathcal{Q}_i = \{\pi_i^k\}_{k=1}^N \), where \( M \leq N \). Then for the population effectivity of \( \mathcal{Q}_i \):

\[
\text{PE}(\mathcal{Q}_i) = \min_{\pi_{-i}} \max_{\alpha \geq 0} \sum_{k=1}^N \alpha_k \phi_i(\pi_i^k, \pi_{-i}) . \tag{31}
\]

where \( \alpha = (\alpha_1, \cdots, \alpha_N)^T \). Let \( \alpha_i = 0 \) for \( M + 1 \leq i \leq N \), then we get:

\[
\min_{\pi_{-i}} \max_{\alpha \geq 0} \sum_{k=1}^M \alpha_k \phi_i(\pi_i^k, \pi_{-i}) \geq \min_{\pi_{-i}} \max_{\alpha \geq 0} \sum_{k=1}^N \alpha_k \phi_i(\pi_i^k, \pi_{-i}) \geq \min_{\pi_{-i}} \max_{\alpha \geq 0} \sum_{k=1}^M \alpha_k \phi_i(\pi_i^k, \pi_{-i}) \tag{32}
\]

\[
= \min_{\pi_{-i}} \max_{\alpha' \geq 0} \sum_{k=1}^M \alpha'_k \phi_i(\pi_i^k, \pi_{-i}) \tag{33}
\]

\[
= \text{PE}(\mathcal{Q}_i) . \tag{34}
\]

Now we conclude that:

\[
\text{PE}(\mathcal{Q}_i) \geq \text{PE}(\mathcal{P}_i) \tag{35}
\]

Regarding exploitability, the analysis comes from our Example 1. Suppose player 1 holds the population \( \mathcal{P}_1 = \{ \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{bmatrix} \} \) and \( \mathcal{P}_2 = \mathcal{Q}_1 \). Apparently, the Nash aggregated joint policy is

\[
\pi_E^{\mathcal{Q}} = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{bmatrix}, \tag{36}
\]

\[
\pi_E^{\mathcal{P}} = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{bmatrix},
\]

3
since there is only one policy in each players’ population.

Now consider another two populations \(q_1 = \{ \begin{bmatrix} 1/2 \\ 1/2 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \} \) and \(q_2 = \Omega_1\). Then the Nash aggregated joint policy is given by:

\[
\pi_E^Q = \left( \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \right).
\] (37)

With simple derivations, the exploitability for \(\pi_{PE}^Q\) and \(\pi_{PE}^Q\) is:

\[
\text{Expl}(\pi_{PE}^Q) = 1.
\] (38)

\[
\text{Expl}(\pi_{PE}^Q) = 2.
\] (39)

Now we can conclude that for player 1 and player 2, even their population both get strictly enlarged (\(P_1 \subseteq \Omega_1\) and \(P_2 \subseteq \Omega_2\)), they become more exploitable:

\[
\text{Expl}(\pi_{PE}^Q) \geq \text{Expl}(\pi_{PE}^Q).
\] (40)

**Proposition 3.** If the underlying game \(\phi_i(\cdot, \cdot)\) is a matrix game, then computing PE is still solving a matrix game.

**Proof.** The proof follows some simple algebraic manipulations. Note that for matrix games, the reward function is given by:

\[
\phi_i(\pi_i, \pi_{-i}) = \pi_i^T P \pi_{-i},
\] (40)

where \(P\) is the payoff matrix. Then for population effectivity:

\[
\text{PE}\left(\{\pi_i^k\}_{k=1}^N\right) = \min_{\pi_{-i}} \max_{\alpha_i \geq 0} \sum_{k=1}^N \alpha_k \phi_i(\pi_i^k, \pi_{-i})
\] (41)

\[
= \min_{\pi_{-i}} \max_{\alpha_i \geq 0} \sum_{k=1}^N \alpha_k (\pi_i^k)^T P \pi_{-i}
\] (42)

\[
= \min_{\pi_{-i}} \max_{\alpha_i \geq 0} \alpha^T (\pi_i^1, \cdots, \pi_i^N)^T P \pi_{-i}.
\] (43)

Therefore, solving PE is still a matrix game with payoff matrix \((\pi_i^1, \cdots, \pi_i^N)^T P\).

**B PE Approximation via PSRO**

We have already mentioned the tractability for PE of matrix games in Theorem 3. However, for more general games, solving exact PE is still very hard. Since PE is still computing an NE, we here propose using PSRO again as the approximate solver. The only difference is that population of player \(i\) is already fixed by \(\pi_i = \{\pi_i^k\}_{k=1}^N\). Therefore, during iterations of PSRO, only player \(-i\) needs to enlarge its population. We now outline the algorithm PE(\(n\)) in Algorithm 2. The intuition behind this algorithm is that the opponent is enlarging its population gradually and trying to exploit \(\pi_i\). Therefore, the metric of PE is actually testing how exploitable a population is by gradually constructing a real adversarial. The opponent strength \(n\) essentially represents how accurate each best response is.

**C Additional Experimental Results on Google Research Football**

In real world games, we expect our models are robust enough to defeat all the previous models in the model pool and show diverse behaviors to better exploit the opponents. To further evaluate the performance of all the models generated with different methods during the training process, we rank all the models with the Elo rating system [2], and the results are shown in Figure 4. It can be found
Algorithm 2 PE(n)

1: Input: Population $\mathcal{P}_i = \{\pi_k^i\}_{k=1}^N$, Opponent Strength $n$, Number of iterations $T$
2: $\mathcal{P}_{-i} \leftarrow$ Initialize opponent population with one random policy
3: $A_{\mathcal{P}_i \times \mathcal{P}_{-i}} \leftarrow$ Initialize empirical payoff matrix
4: for $t = 1$ to $T$ do
5: $\sigma_i, \sigma_{-i} \leftarrow$ Nash Equilibrium on $A_{\mathcal{P}_i \times \mathcal{P}_{-i}}$
6: $\pi_{t-i}(\theta) \leftarrow$ Initialize a new opponent policy
7: $\theta^* \leftarrow$ Train $\pi_{t-i}(\theta)$ against mixture of $\sum_j \sigma_j^i \pi_j^i$ with $n$ gradient steps
8: $\mathcal{P}_{-i} \leftarrow \mathcal{P}_{-i} \cup \{\pi_{t-i}(\theta^*)\}$
9: Compute missing entries in the evaluation matrix $A_{\mathcal{P}_i \times \mathcal{P}_{-i}}$
10: end for
11: Output: Nash value on $A_{\mathcal{P}_i \times \mathcal{P}_{-i}}$

that models generated by PSRO w. BD&RD outperform other methods and reaches an Elo score of around 1300. This implies that a combination of BD and RD will essentially contribute to the generation of diverse opponents during the training, so that the final models will be more robust and less exploitable since they are more likely to be offered strong diverse opponents and have the chance to learn to defeat them. Additionally, we also visualize the policies of our methods when playing against other baseline methods and verify our methods truly generate diverse behaviors (see https://sites.google.com/view/diverse-psro/).

Figure 4: The Elo scores of all the models generated by different methods. Shaded areas represent the standard deviation.

D Environment Details

D.1 Environment Details of Non-Transitive Mixture Model

In our experiments, we set $l = 4$ and use 9 Gaussian distributions in the plane. This environment involves both transitivity and non-transitivity because of the delicately designed $S$ in the reward function $\phi_i(\pi_i, \pi_{-i}) = \pi_i^t S \pi_{-i} + 1$ $\pi_i - \pi_{-i})$. $S$ is constructed by:

$$S[i][k] = \begin{cases} 0 & k = i \\ 1 & 0 < (k - i) \mod (2l + 1) \leq l \\ -1 & \text{otherwise} \end{cases}$$

D.2 Environment Details of Google Research Football

Google Research Football (GRF) [4] is a physics-based 3D simulator where agents can be trained to play football. The engine implements a full football game under standard rules (such as goal kicks, side kicks, corner kicks, etc.), with 11 players on each team and 3000 steps duration for a full game. It offers several state wrappers (such as Pixels, SMM, Floats) and the players can be controlled
with 19 discrete actions (such as move in 8 directions, high pass, long pass, steal, etc.). The rewards include both the scoring reward (+1 or −1) and the checkpoint reward, where the checkpoint reward means that the agent will be rewarded with +0.1 if it is the first time that the agent’s team possesses the ball in each of the checkpoint regions.

E Hyperparameter Settings

E.1 Hyperparameter Settings for Real-World Games

We report our hyperparameter setting for real-world metagames in Table 3.

| Parameter                               | Value   | Description                  |
|-----------------------------------------|---------|------------------------------|
| Learning rate                           | 0.5     | Learning rate for agents     |
| Improvement threshold                   | 0.03    | Convergence criteria         |
| Metasolver                              | Fictitious play | Method to compute NE |
| Metasolver iterations                   | 1000    | # of iterations of metasolver |
| Metasolver iterations for PE            | 2000    | # of iterations to compute PE |
| # of threads in pipeline                | 1.0     | Number of learners in Pipeline-PSRO |
| # of seeds                              | 5       | # of trials                  |
| $\lambda_1$                             | 0.2     | Weight for BD                |
| $\lambda_2$                             | 0.2     | Weight for RD                |

E.2 Hyperparameter Settings for Non-Transitive Mixture Model

We report our hyperparameter setting for non-transitive mixture model in Table 4.

| Parameter                               | Value   | Description                  |
|-----------------------------------------|---------|------------------------------|
| Learning rate                           | 0.1     | Learning rate for agents     |
| Optimizer                               | Adam    | Gradient-based optimization  |
| Bezas                                   | (0.9, 0.99) | Parameter for Adam        |
| $N_{\text{train}}$                      | 5       | # of iterations using GD per BR |
| $\pi_i$                                 | $\pi'_i = \exp((- (x_i - \mu_k) \Sigma (x_i - \mu_k) / 2)$ | Policy parameterization |
| $\Sigma$                                | Covariance of each Gaussian |
| $u_k$                                   | Center of each Gaussian |
| $l$                                     | 4       | 9 Gaussian distributions    |
| $r$                                     | 5       | Radius of each Gaussian     |
| Metasolver                              | Fictitious play | Method to compute NE |
| Metasolver iterations                   | 1000    | # of iterations of metasolver |
| # of threads in pipeline                | 1       | Number of learners in Pipeline-PSRO |
| # of iteration                         | 50      | # of training iterations for PSRO |
| # of seeds                              | 5       | # of trials                  |
| $\lambda_1$                             | 1       | Weight for BD                |
| $\lambda_2$                             | 1500    | Weight for RD                |
| Decrease rate of $\lambda_1$ and $\lambda_2$ | $1 - \frac{t^2}{1500^2}$ | The weights will decrease as the iteration progresses, where $t$ is the current iteration |
| # of iteration for PE                   | 30      | # of training iterations using PSRO for PE |

E.3 Hyperparameter Settings for Google Research Football

States and Network Architecture. For GRF, we use a structured multi-head vector as the states input. The information of each head is listed in Table 5:

The network structure is shown in Figure 5. The shapes of the fully-connected layers for the input heads are: $[32, 64, 64, 16, 16, 128 \times 64, 128 \times 64, 128 \times 128, 128 \times 128, 64, 16, 64, 64]$, followed by three fully-connected layers (i.e. $[512 \times 256 \times 128]$) and finally output the policy and value.

Hyperparameter Settings for Reinforcement Learning Oracle. We use IMPALA [1] as the reinforcement learning algorithm to approximate the best response for each opponent selected by different methods during the training process. The hyperparameters are listed in Table 6.
Table 5: The states input for Google Research Football.

| Head index | Length | Information                                                                 |
|------------|--------|-----------------------------------------------------------------------------|
| 0          | 9      | Ball information (position, direction, rotation)                            |
| 1          | 25     | Ball owner information (ball owned team id, ball owned player id)           |
| 2          | 25     | Active player information (id, position, direction, area of the field)      |
| 3          | 6      | Active player vs. ball (distance, 1/distance)                               |
| 4          | 4      | Active player vs. ball player (distance, 1/distance)                         |
| 5          | 66     | Active player vs. self-team players (position, distance, 1/distance, position cosine, direction cosine) |
| 6          | 66     | Active player vs. oppo-team players (position, distance, 1/distance, position cosine, direction cosine) |
| 7          | 88     | Self-team information (position, direction, tired factor, yellow card, active player, offside flag) |
| 8          | 88     | Oppo-team information (position, direction, tired factor, yellow card, active player, offside flag) |
| 9          | 32     | Goal keeper information (distance to self-player/oppo-player, nearest/farthest player information) |
| 10         | 7      | Game mode information (one-hot)                                             |
| 11         | 29     | Legal action and sticky action information                                   |
| 12         | 76     | History (one-hot) actions of last four steps                                |

Figure 5: The shape of input states for each head and the general network structure.

Network Training Details. We carry out the experiments on six servers (CPU: AMD EPYC 7542 128-Core Processor, RAM: 500G), with each one corresponding to one of six methods (i.e. Self-play, PSRO, PSROrN, PSRO w. BD, PSRO w. RD, PSRO w.BD&RD). For each experiment, the approximated best response (i.e. checkpoint) is saved only when the win-rate against corresponding opponent is stable during two checks (check frequency = 1000 model steps, and \( \Delta_{\text{winrate}} < 0.05 \)) or the training model step reaches an upper bound (i.e. 50000 model steps). The \( \lambda_1 \) and \( \lambda_2 \) we used for both coefficients are 0.5. For the Google Research Football environment settings, we use both scoring reward and checkpoint reward for the training.

F Ablation Studies

We also conduct ablation study on the sensitivity of the diversity weights \( \lambda_1 \) and \( \lambda_2 \) in real-world games, non-transitive mixture model, and Google Research Football.

F.1 Real-World Games

We report the exploitability and PE by varying \( \lambda_1 \) in Figure 6a, 6b and \( \lambda_2 \) in Figure 7a, 7b. It can be found that too large weights can cause the slow convergence and too small weights prevent the algorithm from finding populations with smaller exploitability and larger PE.

F.2 Non-Transitive Mixture Model

We report the exploitability of the final population generated by our algorithm with different \( \lambda_1 \) in Table 7 and \( \lambda_2 \) in Table 8. In this game, we set both \( \lambda_1 \) and \( \lambda_2 \) to decrease following the rate \( 1 - \frac{0.7}{1 + e^{(-0.25\cdot(t-25))}} \), where \( t \) is the current iteration. We can find that in terms of exploitability, PSRO with only BD cannot help the population to achieve lower exploitability.
Table 6: The hyperparameters of the IMPALA algorithm.

| Parameter                        | Value          |
|----------------------------------|----------------|
| Batch Size                       | 1024           |
| Discount Factor (γ)              | 0.993          |
| Learning Rate                    | 0.00019896     |
| Number of Actors                 | 100            |
| Optimizer                        | Adam           |
| Unroll Length/n-step             | 1.0            |
| Entropy Coefficient              | 0.0001         |
| Value Function Coefficient       | 1.0            |
| Grad Clip Norm                   | 0.5            |
| Rho (for V-Trace)                | 1.0            |
| C (for V-Trace)                  | 1.0            |
| λ₁ (Weight for BD)               | 0.5            |
| λ₂ (Weight for RD)               | 0.5            |

Figure 6: Ablation study on λ₁. (a): Exploitability vs. training iterations. (b): Negative Population Effectivity vs. training iterations on the AlphaStar game. \( \text{cdf}(k) = \int_{-\infty}^{k} \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} dx \) is the cumulative distribution function of the standard normal distribution.

Figure 7: Ablation study on λ₂. (a): Exploitability vs. training iterations. (b): Negative Population Effectivity vs. training iterations on the AlphaStar game. \( \text{cdf}(k) = \int_{-\infty}^{k} \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} dx \) is the cumulative distribution function of the standard normal distribution.
Table 7: Exploitability $\times 10^2$ for populations generated by PSRO only with BD with varied diversity weight $\lambda_1$.

| $\lambda_1$ | 7.5  | 15   | 75   | 750  | 1500 | 7500 |
|------------|------|------|------|------|------|------|
| Expl       | 14.57 ± 0.69 | 14.93 ± 1.87 | 14.64 ± 1.48 | 42.37 ± 10.12 | 33.39 ± 5.71 | 62.69 ± 10.90 |

Table 8: Exploitability $\times 10^2$ for populations generated by PSRO only with RD with varied diversity weight $\lambda_2$.

| $\lambda_2$ | 0.5  | 1.0  | 5.0  | 10.0 | 50.0 |
|-----------|------|------|------|------|------|
| Expl       | 16.23 ± 0.48 | 14.06 ± 1.20 | 14.77 ± 0.09 | 15.60 ± 1.11 | 31.29 ± 12.93 |

Table 9: The win-rate between the final policies of different methods after trained for 300000 model steps. (We set $\lambda_1 = \lambda_2 = 0.5$ as default values for PSRO w. RD and PSRO w. BD&RD)

| Method                  | Self-play | PSRO | PSRO, $N$ | PSRO w. BD | PSRO w. RD | PSRO w. BD&RD |
|-------------------------|-----------|------|-----------|------------|------------|--------------|
| PSRO w. RD ($\lambda_1$) | 0.62 ± 0.01 | 0.49 ± 0.03 | 0.65 ± 0.02 | 0.47 ± 0.01 | 0.28 ± 0.04 | 0.33 ± 0.02 |
| PSRO w. RD ($\lambda_2$ = 0.5) | 0.68 ± 0.03 | 0.61 ± 0.02 | 0.74 ± 0.03 | 0.54 ± 0.02 | 0.43 ± 0.02 | 0.43 ± 0.02 |
| PSRO w. RD ($\lambda_2$ = 0.2) | 0.63 ± 0.02 | 0.48 ± 0.02 | 0.68 ± 0.02 | 0.50 ± 0.01 | 0.45 ± 0.03 | 0.28 ± 0.03 |
| PSRO w. BD&RD            | 0.74 ± 0.02 | 0.78 ± 0.01 | 0.80 ± 0.05 | 0.69 ± 0.02 | 0.57 ± 0.02 | -             |

Algorithm 3 Optimization for Matrix Games

1: **Input**: population $\Psi_i$ for each $i$, meta-game $A_{\Psi_i \times \Psi_{-i}}$, weights $\lambda_1$ and $\lambda_2$, learning rate $\mu$
2: $\sigma, \sigma_{-i} \leftarrow$ Nash on $A_{\Psi_i \times \Psi_{-i}}$
3: $\pi \leftarrow$ Aggregate according to $\sigma, \sigma_{-i}$
4: $\pi_i(\theta) \leftarrow$ Initialize a new random policy for player $i$
5: $\text{BR}_{\text{qual}} \leftarrow$ Compute best response against mixture of opponents $\sum_k \sigma_{-i}^k \phi_i(\cdot, \pi_{-i}^k)$
6: **while** the reward $p$ improvement does not meet the threshold **do**
7: $\text{BR}_{\text{occ}} \leftarrow \text{arg}\ max_s D_f(s_j || \pi_i)$ for each pure strategy $s_j$
8: $\text{BR} \leftarrow$ Choose $\text{BR} = \text{BR}_{\text{occ}}$ with probability $\lambda_1$ else $\text{BR} = \text{BR}_{\text{qual}}$
9: $\theta \leftarrow \mu \theta + (1 - \mu) \theta_{\text{BR}}$
10: $p \leftarrow$ Compute the payoff $p$ after the update according to $\sum_k \sigma_{-i}^k \phi_i(\pi_i(\theta), \pi_{-i}^k)$
11: **end while**
12: $\text{BR}_{\text{rew}} \leftarrow \text{arg}\ max_{s_j} F(s_j)$ for each pure strategy $s_j$ with probability $\lambda_2$ else $\text{BR}_{\text{qual}}$
13: $\theta \leftarrow \mu \theta + (1 - \mu) \theta_{\text{BR}_{\text{rew}}}$
14: **Output**: policy $\pi_i(\theta)$

F.3 Google Research Football

We also carry out an ablation study on the weight of RD $\lambda_2$ (see Table 9) in the GRF environment, where we fixed $\lambda_1$ to be 0.5 and show the results with different $\lambda_2$.

G Simplified Optimization Method for Unified Diverse Response

In Algorithm 1, we have outlined using RL as the optimization oracle for approximate best response. However, computing best response in real-world metagames (matrix games) or non-transitive mixture model (differential games) can be simplified, since the $f$-divergence objective can be simplified according to Theorem 1 or the reward function $\phi_i$ is analytically accessible. Now we provide the simplified optimization methods separately for matrix games in Algorithm 3 and differential games in Algorithm 4.
Algorithm 4 Optimization for Differential Games

1: **Input:** population $\mathcal{P}_i$ for each $i$, meta-game $A_{\mathcal{P}_i \times \mathcal{P}_{-i}}$, weights $\lambda_1$ and $\lambda_2$, number of gradient updates $N_{\text{train}}$

2: $\sigma_i, \sigma_{-i} \leftarrow \text{Nash on } A_{\mathcal{P}_i \times \mathcal{P}_{-i}}$

3: $\pi_E = (\pi_i, \pi_{E_{-i}}) \leftarrow \text{Aggregate according to } \sigma_i, \sigma_{-i}$

4: $\pi'_i(\theta) \leftarrow \text{Initialize a new random policy for player } i$

5: for $j = 1$ to $N_{\text{train}}$ do

6: $p_j \leftarrow \text{Compute payoff against the mixture of opponents } p_j = \sum_k \sigma_{-i}^k \phi_i(\pi'_i, \pi_{-i}^k)$

7: $d_{\text{occ}}^j \leftarrow \text{Compute } \text{BD } d_{\text{occ}}^j = D_f(\pi'_i || \pi_i)$ as the $f$-divergence between $\pi_i$ and $\pi_i'$

8: $a_j \leftarrow \text{Compute new reward vector as } a_j = (\phi_i(\pi'_i, \pi_{-i}^k))_{k=1}^{\mathcal{P}_{-i}}$

9: $d_{\text{rew}}^j \leftarrow \text{Compute the lower bound of RD as } F(a_j)$ according to Theorem 2

10: $l_j \leftarrow -(p_j + \lambda_1 d_{\text{occ}}^j + \lambda_2 d_{\text{rew}}^j)$

11: Update $\theta$ to minimize $l_j$ by backpropagation

12: end for

13: **Output:** policy $\pi'_i(\theta)$

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