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

Table of Contents

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*

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

Proof. See Proposition 7.1 in [3]. □

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 $\rho_{\pi_i',\pi_{E_{-i}}}$, we have:

$$\rho_{\pi_i',\pi_{E_{-i}}}(s,\mathbf{a}) = (\pi_i',\pi_{E_{-i}})(s,\mathbf{a}) = \pi_i'(a_i|s)\pi_{-i}(a_{-i}|s)\ , \tag{15}$$

where the second equation comes from the assumption that policies are independent. Similarly, for $\rho_{\pi_i,\pi_{E_{-i}}}$, we also have:

$$\rho_{\pi_i,\pi_{E_{-i}}}(s,\mathbf{a}) = (\pi_i,\pi_{E_{-i}})(s,\mathbf{a}) = \pi_i(a_i|s)\pi_{-i}(a_{-i}|s)\ . \tag{16}$$

Therefore, with the help of Lemma 1, we have:

$$D_f(\rho_{\pi_i',\pi_{E_{-i}}}||\rho_{\pi_i,\pi_{E_{-i}}}) = \mathbb{E}_{s_0\sim\eta(s)}[D_f(\pi_i'\pi_{-i}||\pi_i\pi_{-i})] = \mathbb{E}_{s_0\sim\eta(s)}[D_f(\pi_i'(\cdot|s_0)||\pi_i(\cdot|s_0))] \,. \tag{17}$$

□

A.2 Proof of Theorem 2

Let us restate our Theorem 2

Theorem 2. *For a given empirical payoff matrix $\mathbf{A}\in\mathbb{R}^{M\times N}$ and the reward vector $\mathbf{a}_{M+1}$ for policy π_i^{M+1}, the lower bound of $\mathrm{Div}_{\mathrm{occ}}$ is given by:*

$$\mathrm{Div}_{\mathrm{rew}}(\pi_i^{M+1}) \geq \frac{\sigma^2_{\min}(\mathbf{A})(1-\mathbf{1}^\top(\mathbf{A}^\top)^\dagger\mathbf{a}_{M+1})^2}{M} + ||(\mathbf{I}-\mathbf{A}^\top(\mathbf{A}^\top)^\dagger)\mathbf{a}_{M+1}||^2 \,, \tag{18}$$

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

Proof.

$$\begin{aligned}\min_{\substack{\mathbf{1}^\top\boldsymbol{\beta}=1\\ \boldsymbol{\beta}\geq 0}} ||\mathbf{A}^\top\boldsymbol{\beta}-\mathbf{a}_{M+1}||_2^2 &= \min_{\substack{\mathbf{1}^\top\boldsymbol{\beta}=1\\ \boldsymbol{\beta}\geq 0}} ||\mathbf{A}^\top\boldsymbol{\beta}-\mathbf{A}^\top(\mathbf{A}^\top)^\dagger\mathbf{a}_{M+1}||^2 + ||(\mathbf{I}-\mathbf{A}^\top(\mathbf{A}^\top)^\dagger)\mathbf{a}_{M+1}||^2\\
&\geq \min_{\mathbf{1}^\top\boldsymbol{\beta}=1} ||\mathbf{A}^\top\boldsymbol{\beta}-\mathbf{A}^\top(\mathbf{A}^\top)^\dagger\mathbf{a}_{M+1}||^2 + ||(\mathbf{I}-\mathbf{A}^\top(\mathbf{A}^\top)^\dagger)\mathbf{a}_{M+1}||^2\\
&= \min_{\mathbf{1}^\top\boldsymbol{\beta}=1} ||\mathbf{A}^\top(\boldsymbol{\beta}-(\mathbf{A}^\top)^\dagger\mathbf{a}_{M+1})||^2 + ||(\mathbf{I}-\mathbf{A}^\top(\mathbf{A}^\top)^\dagger)\mathbf{a}_{M+1}||^2\\
&\geq \sigma^2_{\min}(\mathbf{A}) \min_{\mathbf{1}^\top\boldsymbol{\beta}=1} ||\boldsymbol{\beta}-(\mathbf{A}^\top)^\dagger\mathbf{a}_{M+1}||^2 + ||(\mathbf{I}-\mathbf{A}^\top(\mathbf{A}^\top)^\dagger)\mathbf{a}_{M+1}||^2\\
&= \frac{\sigma^2_{\min}(\mathbf{A})(1-\mathbf{1}^\top(\mathbf{A}^\top)^\dagger\mathbf{a}_{M+1})^2}{M} + ||(\mathbf{I}-\mathbf{A}^\top(\mathbf{A}^\top)^\dagger)\mathbf{a}_{M+1}||^2 \,,\end{aligned}$$

where the first equation comes from that we decompose $\mathbf{a}_{M+1}$ into $\mathbf{A}^\top(\mathbf{A}^\top)^\dagger\mathbf{a}_{M+1} + (\mathbf{I}-\mathbf{A}^\top(\mathbf{A}^\top)^\dagger)\mathbf{a}_{M+1}$. The last equation comes from the analytic calculation of $\min_{\mathbf{1}^\top\boldsymbol{\beta}=1}||\boldsymbol{\beta}-(\mathbf{A}^\top)^\dagger\mathbf{a}_{M+1}||^2$ using Lagrangian. □

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 π in two-player symmetric zero-sum games:*

$$\phi_i(\pi,\pi)=0\,. \tag{19}$$

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

$$\phi_i(\pi_i,\pi_{-i}) = \phi_{-i}(\pi_{-i},\pi_i)\,. \tag{20}$$

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

$$\phi_{-i}(\pi_{-i},\pi_i) = -\phi_i(\pi_{-i},\pi_i)\,. \tag{21}$$

By combing Equation 20 and Equation 33, for any π_i and π_{-i}, we get:

$$\phi_i(\pi_i,\pi_{-i}) + \phi_i(\pi_{-i},\pi_i) = 0\,. \tag{22}$$

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

$$\phi_i(\pi,\pi)=0\,. \tag{23}$$

□

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 $\boldsymbol{\pi_E} = (\pi_i, \pi_{-i})$ satisfies $\pi_i = \pi_{-i}$. Therefore, with the help of Lemma 2:

$$\phi_i(\pi_i, \pi_{-i}) = \phi_{-i}(\pi_{-i}, \pi_i) = 0 \ . \tag{24}$$

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

$$\begin{aligned}
\operatorname{Expl}(\boldsymbol{\pi_E}) &= \sum_{i=1}^{2} \max_{\pi'_i} \phi_i(\pi'_i, \pi_{-i}) - \phi_i(\pi_i, \pi_{-i}) && (25)\\
&= \sum_{i=1}^{2} \max_{\pi'_i} \phi_i(\pi'_i, \pi_{-i}) && (26)\\
&= 2 \max_{\pi'_i} \phi_i(\pi'_i, \pi_{-i}) \ , && (27)
\end{aligned}$$

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

For PE, it is calculated as:

$$\begin{aligned}
\operatorname{PE}(\{\pi_i\}) &= \min_{\pi'_{-i}} \phi_i(\pi_i, \pi'_{-i}) && (28)\\
&= -\max_{\pi'_{-i}} \phi_i(\pi'_{-i}, \pi_i) && (29)\\
&= -\frac{1}{2} \operatorname{Expl}(\boldsymbol{\pi_E}) \ . && (30)
\end{aligned}$$

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

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

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

$$\operatorname{PE}(\mathfrak{Q}_i) = \min_{\pi_{-i}} \max_{\substack{\mathbf{1}^\top \boldsymbol{\alpha}=1 \\ \alpha_i \geq 0}} \sum_{k=1}^{N} \alpha_k \phi_i(\pi_i^k, \pi_{-i}) \ . \tag{31}$$

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

$$\begin{aligned}
\min_{\pi_{-i}} \max_{\substack{\mathbf{1}^\top \boldsymbol{\alpha}=1 \\ \alpha_i \geq 0}} \sum_{k=1}^{N} \alpha_k \phi_i(\pi_i^k, \pi_{-i}) &\geq \min_{\pi_{-i}} \max_{\substack{\mathbf{1}^\top \boldsymbol{\alpha}=1, \alpha_i \geq 0 \\ \alpha_i = 0 \ \forall M+1 \leq i \leq N}} \sum_{k=1}^{N} \alpha_k \phi_i(\pi_i^k, \pi_{-i}) && (32)\\
&= \min_{\pi_{-i}} \max_{\substack{\mathbf{1}^\top \boldsymbol{\alpha}'=1 \\ \alpha'_i \geq 0}} \sum_{k=1}^{M} \alpha'_k \phi_i(\pi_i^k, \pi_{-i}) && (33)\\
&= \operatorname{PE}(\mathfrak{P}_i) \ . && (34)
\end{aligned}$$

Now we conclude that:

$$\operatorname{PE}(\mathfrak{Q}_i) \geq \operatorname{PE}(\mathfrak{P}_i) \tag{35}$$

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

$$\boldsymbol{\pi}_{\boldsymbol{E}}^{\mathfrak{P}} = (\begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{bmatrix}, \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{bmatrix}) \ , \tag{36}$$

since there is only one policy in each players' population.

Now consider another two populations $\mathfrak{Q}_1 = \{ \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \}$ and $\mathfrak{Q}_2 = \mathfrak{Q}_1$. Then the Nash aggregated joint policy is given by:

$$\boldsymbol{\pi}_{\boldsymbol{E}}^{\mathfrak{Q}} = (\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}). \tag{37}$$

With simple derivations, the exploitability for $\boldsymbol{\pi}_{\boldsymbol{E}}^{\mathfrak{P}}$ and $\boldsymbol{\pi}_{\boldsymbol{E}}^{\mathfrak{Q}}$ is:

$$\mathrm{Expl}(\boldsymbol{\pi}_{\boldsymbol{E}}^{\mathfrak{P}}) = 1. \tag{38}$$

$$\mathrm{Expl}(\boldsymbol{\pi}_{\boldsymbol{E}}^{\mathfrak{Q}}) = 2. \tag{39}$$

Now we can conclude that for player 1 and player 2, even their population both get strictly enlarged ($\mathfrak{P}_1 \subseteq \mathfrak{Q}_1$ and $\mathfrak{P}_2 \subseteq \mathfrak{Q}_2$), they become more exploitable: $\mathrm{Expl}(\boldsymbol{\pi}_{\boldsymbol{E}}^{\mathfrak{Q}}) \geq \mathrm{Expl}(\boldsymbol{\pi}_{\boldsymbol{E}}^{\mathfrak{P}})$. □

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 algebric manipulations. Note that for matrix games, the reward function is given by:

$$\phi_i(\pi_i, \pi_{-i}) = \pi_i^\top \mathbf{P} \pi_{-i} \,, \tag{40}$$

where $\mathbf{P}$ is the payoff matrix. Then for population effectivity:

$$\begin{aligned} \mathrm{PE}(\{\pi_i^k\}_{k=1}^N) &= \min_{\pi_{-i}} \max_{\substack{\mathbf{1}^\top \boldsymbol{\alpha}=1 \\ \alpha_i \geq 0}} \sum_{k=1}^N \alpha_k \phi_i(\pi_i^k, \pi_{-i}) & (41) \\ &= \min_{\pi_{-i}} \max_{\substack{\mathbf{1}^\top \boldsymbol{\alpha}=1 \\ \alpha_i \geq 0}} \sum_{k=1}^N \alpha_k (\pi_i^k)^\top \mathbf{P} \pi_{-i} & (42) \\ &= \min_{\pi_{-i}} \max_{\substack{\mathbf{1}^\top \boldsymbol{\alpha}=1 \\ \alpha_i \geq 0}} \boldsymbol{\alpha}^\top (\pi_i^1, \cdots, \pi_i^N)^\top \mathbf{P} \pi_{-i} \,. & (43) \end{aligned}$$

Therefore, solving PE is still a matrix game with payoff matrix $(\pi_i^1, \cdots, \pi_i^N)^\top \mathbf{P}$. □

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

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/).

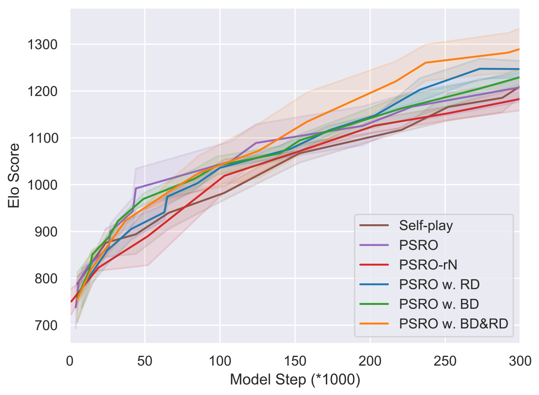


Figure 4: The Elo scores of all the models generated by different methods. Shaded areas represent the standard deviation.

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 $\mathbf{S}$ in the reward function $\phi_i(\pi_i, \pi_{-i}) = \pi_i^\top \mathbf{S} \pi_{-i} + \mathbf{1}^\top(\pi_i - \pi_{-i})$. $\mathbf{S}$ is constructed by:

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

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 reward 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.

Table 3: The hyperparameters of real-world metagames.

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
λ_1	0.2	Weight for BD
λ_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.

Table 4: The hyperparameters of non-transitive mixture model.

Parameter	Value	Description
Learning rate	0.1	Learning rate for agents
Optimizer	Adam	Gradient-based optimization
Betas	(0.9, 0.99)	Parameter for Adam
N_{train}	5	# of iterations using GD per BR
π_i	$\pi_k^i = \exp(-\left(x_i - \mu_k\right)^\top \Sigma \left(x_i - \mu_k\right)/2)$	Policy parameterization
Σ	$1/2\mathbf{I}$	Covariance of each Gaussian
u_k	$r(\cos(\frac{2\pi}{2l+1}k), \sin(\frac{2\pi}{2l+1}k))$	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	1.0	Number of learners in Pipeline-PSRO
# of iteration	50	# of training iterations for PSRO
# of seeds	5	# of trials
λ_1	1	Weight for BD
λ_2	1500	Weight for RD
Decrease rate of λ_1 and λ_2	$1 - \frac{0.7}{1+\exp(-0.25(t-25))}$	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

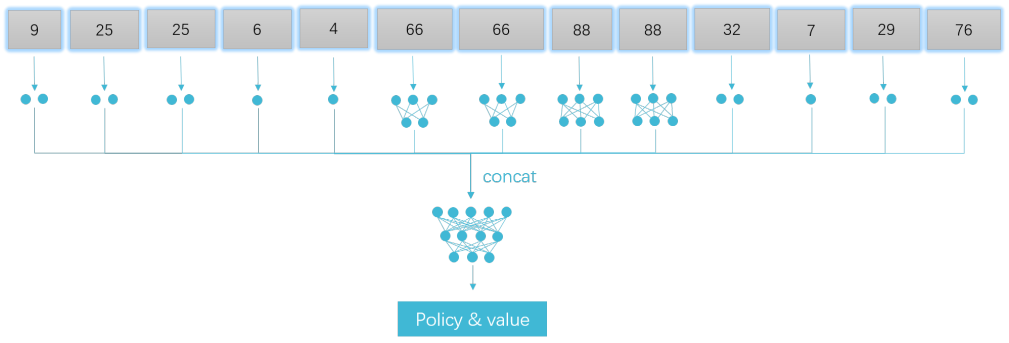


Figure 5: The shape of input states for each head and the general network structure.

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 $\Delta_{winrate} < 0.05$) or the training model step reaches an upper bound (i.e. 50000 model steps). The λ_1 and λ_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 λ_1 and λ_2 in real-world games, non-transitive mixture model, and *Google Research Football*.

F.1 Real-World Games

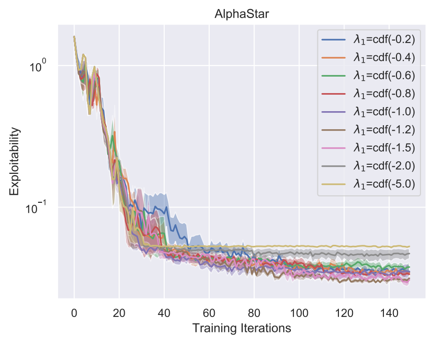
We report the exploitability and PE by varying λ_1 in Figure 6a, 6b and λ_2 in Figure 7a, 7b. It can be found that too large weights can cause the slow convergence and too small weights prevent the algorithm from finding populations with smaller exploitability and larger PE.

F.2 Non-Transitive Mixture Model

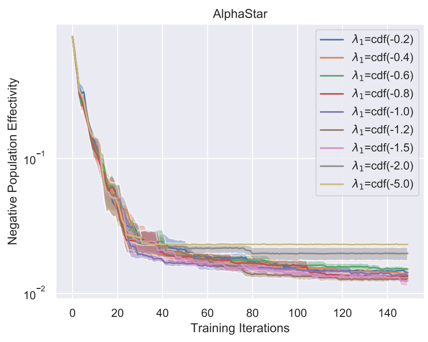
We report the exploitability of the final population generated by our algorithm with different λ_1 in Table 7 and λ_2 in Table 8. In this game, we set both λ_1 and λ_2 to decrease following the rate $1 - \frac{0.7}{1+e^{(-0.25(t-25))}}$, where t is the current iteration. We can find that in terms of 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
λ_1 (Weight for BD)	0.5
λ_2 (Weight for RD)	0.5

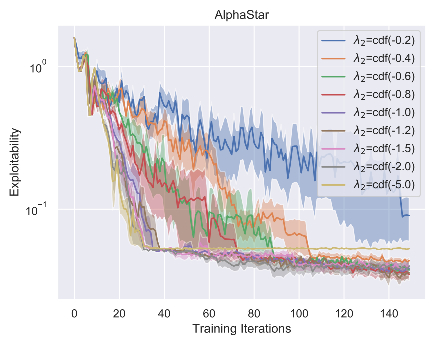


(a)

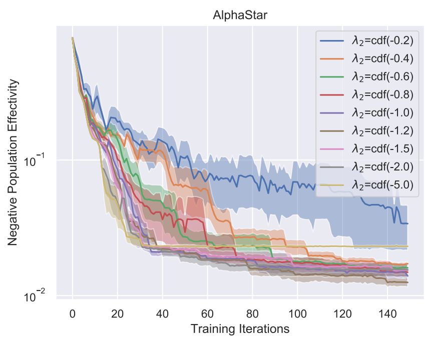


(b)

Figure 6: Ablation study on λ_1. (**a**):Exploitability *vs.* training iterations. (**b**): Negative Population Effectivity *vs.* training iterations on the AlphaStar game. $\mathrm{cdf}(k) = \int_{-\infty}^{k} \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} dx$ is the cumulative distribution function of the standard normal distribution.



(a)



(b)

Figure 7: Ablation study on λ_2. (**a**):Exploitability *vs.* training iterations. (**b**): Negative Population Effectivity *vs.* training iterations on the AlphaStar game. $\mathrm{cdf}(k) = \int_{-\infty}^{k} \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} dx$ 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 λ_1.

λ_2	7.5	15	75	750	1500	7500
Expl	$\mathbf{14.57 \pm 0.69}$	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 λ_2.

λ_2	0.5	1.0	5.0	10.0	50.0
Expl	16.23 ± 0.48	$\mathbf{14.06 \pm 1.20}$	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$_{rN}$	PSRO w. BD	PSRO w. RD	PSRO w. BD&RD
PSRO w. RD ($\lambda_2 = 1.0$)	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	$\mathbf{0.61 \pm 0.02}$	$\mathbf{0.74 \pm 0.03}$	0.54 ± 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	$\mathbf{0.74 \pm 0.02}$	$\mathbf{0.78 \pm 0.01}$	$\mathbf{0.80 \pm 0.05}$	$\mathbf{0.69 \pm 0.02}$	$\mathbf{0.57 \pm 0.02}$	-

Algorithm 3 Optimization for Matrix Games

```
1:  Input: population $\mathfrak{P}_i$ for each $i$, meta-game $\mathbf{A}_{\mathfrak{P}_i \times \mathfrak{P}_{-i}}$, weights $\lambda_1$ and $\lambda_2$, learning rate $\mu$
2:  $\sigma_i, \sigma_{-i} \leftarrow$ Nash on $\mathbf{A}_{\mathfrak{P}_i \times \mathfrak{P}_{-i}}$
3:  $\boldsymbol{\pi_E} \leftarrow$ Aggregate according to $\sigma_i, \sigma_{-i}$
4:  $\pi_i'(\theta) \leftarrow$ Initialize a new random policy for player $i$
5:  $\mathbf{BR}_{qual} \leftarrow$ 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:      $\mathbf{BR}_{occ} \leftarrow \arg\max_{s_j} D_f(s_j || \pi_i)$ for each pure strategy $s_j$
8:      $\mathbf{BR} \leftarrow$ Choose $\mathbf{BR} = \mathbf{BR}_{occ}$ with probability $\lambda_1$ else $\mathbf{BR} = \mathbf{BR}_{qual}$
9:      $\theta \leftarrow \mu\theta + (1-\mu)\theta_{\mathbf{BR}}$
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: $\mathbf{BR}_{rew} \leftarrow \arg\max_{s_j} F(s_j)$ for each pure strategy $s_j$ with probability $\lambda_2$ else $\mathbf{BR}_{qual}$
13: $\theta \leftarrow \mu\theta + (1-\mu)\theta_{\mathbf{BR}_{rew}}$
14: Output: policy $\pi_i'(\hat{\theta})$
```

F.3 Google Research Football

We also conduct an ablation study on the weight of RD λ_2 (see Table 9) in the GRF environment, where we fixed λ_1 to be 0.5 and show the results with different λ_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 ϕ_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 $\mathfrak{P}_i$ for each $i$, meta-game $\mathbf{A}_{\mathfrak{P}_i \times \mathfrak{P}_{-i}}$, weights $\lambda_1$ and $\lambda_2$, number of gradient updates $N_{train}$
2: $\sigma_i, \sigma_{-i} \leftarrow$ Nash on $\mathbf{A}_{\mathfrak{P}_i \times \mathfrak{P}_{-i}}$
3: $\boldsymbol{\pi_E} = (\pi_i, \pi_{E_{-i}}) \leftarrow$ Aggregate according to $\sigma_i, \sigma_{-i}$
4: $\pi_i'(\theta) \leftarrow$ Initialize a new random policy for player $i$
5: for $j = 1$ to $N_{train}$ do
6:     $p_j \leftarrow$ Compute payoff against the mixture of opponents $p_j = \sum_k \sigma_{-i}^k \phi_i(\pi_i', \pi_{-i}^k)$
7:     $d_j^{\text{occ}} \leftarrow$ Compute BD $d_j^{\text{occ}} = D_f(\pi_i' || \pi_i)$ as the $f$-divergence between $\pi_i$ and $\pi_i'$
8:     $\mathbf{a}_j \leftarrow$ Compute new reward vector as $\mathbf{a}_j = (\phi_i(\pi_i', \pi_{-i}^k))_{k=1}^{|\mathfrak{P}_{-i}|}$
9:     $d_j^{\text{rew}} \leftarrow$ Compute the lower bound of RD as $F(\mathbf{a}_j)$ according to Theorem 2
10:    $l_j \leftarrow -(p_j + \lambda_1 d_j^{\text{occ}} + \lambda_2 d_j^{\text{rew}})$
11:    Update $\theta$ to minimize $l_j$ by backpropagation
12: end for
13: Output: policy $\pi_i'(\theta)$
```

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