Generating Diverse Teammates to Train Robust Agents For Ad Hoc Teamwork

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Abstract

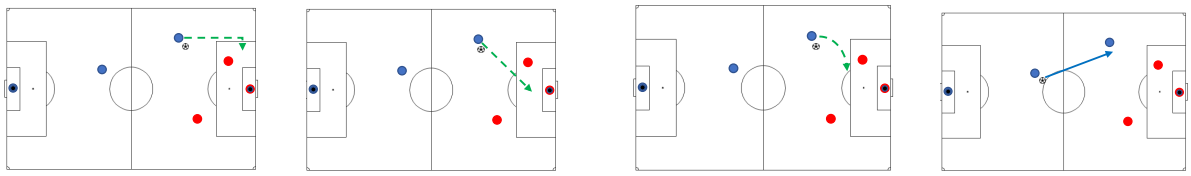
Ad hoc teamwork (AHT) is the challenge of designing a learner that effectively collaborates with unknown teammates without prior coordination mechanisms. Early approaches address the AHT challenge by training the learner with a diverse set of handcrafted teammate policies, usually designed based on an expert's domain knowledge about the policies the learner may encounter. However, implementing teammate policies for training based on domain knowledge is not always feasible. In such cases, recent approaches attempted to improve the robustness of the learner by training it with teammate policies generated by optimising information-theoretic diversity metrics. However, optimising information-theoretic diversity metrics may generate teammates with superficially different behaviours, which does not necessarily result in a robust learner that can effectively collaborate with unknown teammates. In this paper, we present an automated teammate policy generation method optimising the Best-Response Diversity (BRDiv) metric, which measures diversity based on the compatibility of teammate policies in terms of returns. We evaluate our approach in environments with multiple valid coordination strategies, comparing against methods optimising information-theoretic diversity metrics and an ablation not optimising any diversity metric. Our experiments indicate that optimising BRDiv yields a diverse set of training teammate policies that improve the learner's performance relative to previous teammate generation approaches when collaborating with near-optimal previously unseen teammate policies.

1 Introduction

Ad hoc teamwork (AHT) is the challenging problem of creating a single agent, called the *learner*, which can collaborate with a set of unknown teammates without prior coordination mechanisms (Stone et al., 2010). While in AHT all teammates are assumed to be working together to achieve a common goal, they may exhibit different behaviours or take different roles in the team. Consequently, the learner may need to use distinct policies to collaborate optimally with the different encountered teammates. A robust AHT learner should be able to adapt their own policy based on teammates' displayed behaviour and a team's composition to achieve optimal collaboration.

Prior AHT approaches produce robust learners by interacting with teammate policies encountered during training. During training, AHT approaches learn the best response policy for the different encountered teammate policies alongside unique characteristics that differentiate their behaviour. After training is finished, the learner infers whether encountered unknown teammates display these learned characteristics based on their observed behaviour. Based on inferred characteristics of the unknown teammates, the learner then computes an approximate best response policy for effective collaboration. Prior AHT methods often use policy mixtures (Albrecht et al., 2016; Barrett et al., 2017) or neural networks (Rahman et al., 2021; Papoudakis et al., 2021; Zintgraf et al., 2021) to generalise the best responses for training teammates towards new teammates with unknown policies.

Designing a collection of teammate policies that covers the myriad of useful cooperation strategies is essential for ensuring the robustness of learners in AHT. The design of an appropriate set of training teammate policies is especially crucial in AHT environments with multiple valid cooperation strategies. By only training a



(a) First dribbling style. (b) Second dribbling style. (c) Third dribbling style. (d) Best-response policy.

Figure 1: **Potential teammate policies generated from information-theoretic diversity maximisation.** In Figure 1a- 1c, we provide three example teammate behaviours with high information-theoretic diversity in a 3 vs 3 soccer environment. Each of these three visualisations highlights the behaviour of a teammate that favours dribbling and shooting, with the favoured dribbling trajectory of each teammate indicated by the green dashed arrow. Figure 1d then shows the behaviour acquired by a learner that encounters the previously mentioned teammates during training. Despite the diversity in these teammates' trajectories, an AHT learner will only acquire the skill to pass the ball to teammates, which is indicated by the blue solid line, since it is sufficient for effective collaboration with all three teammates.

learner against teammate policies that behave according to a subset of the valid strategies, the learner may not acquire policies for collaborating with teammates that adopt different cooperation strategies unseen during training. This issue resembles the failure of jointly trained agents to collaborate with other agents that were not co-trained alongside them (Hu et al., 2020; Vezhnevets et al., 2020; Rahman et al., 2021).

In previous AHT works, approaches to design teammate policies for AHT training fall into two categories. First, early AHT approaches (Barrett et al., 2014; Albrecht et al., 2016; Barrett et al., 2017) formulate training teammate policies based on experts' knowledge regarding reasonable teammate behaviours an agent may encounter in an environment. Second, more recent AHT approaches (Xing et al., 2021; Lupu et al., 2021; Lucas & Allen, 2022) generate diverse teammate policies for training by optimising information-theoretic diversity metrics, which encourage an increased difference of the trajectory or action distribution of different generated teammate policies.

Existing methods to generate AHT training teammate policies face challenging problems in their goal to produce robust learners. The reliance on experts' domain knowledge regarding teammate policies that an agent may encounter is problematic since such information is often unavailable or difficult to elicit in many real-world problems. Meanwhile, merely encouraging different training teammate policies to have distinct trajectory or action distributions may produce teammates with superficial differences (Lupu et al., 2021), which do not encourage the emergence of robust AHT learners. As an example of behaviour with superficial differences, consider the problem of creating training teammate policies for a soccer game. Under this environment, a teammate generation method potentially produces superficial differences when it creates teammate policies displaying different trajectories to execute the same style of play. Figure 1 exemplifies this as three teammate policies that like to dribble with different trajectories on the pitch.

Superficially different behaviours provide a challenge to AHT training since they do not encourage improved learner robustness. In the example in Figure 1, effective collaboration with all generated teammate policies can be achieved by passing the ball to the teammate. A learner trained to collaborate with these policies will only acquire expertise in passing the ball to teammates, while neglecting other essential skills in soccer. This prevents the emergence of effective collaboration when the learner has to interact with teammates where passing skills alone are insufficient, such as when interacting with a teammate that likes to pass.

A teammate generation method aiming to improve the robustness of a learner should avoid the emergence of superficial differences between generated teammates and instead produce teammate policies that force the learner to learn a broader range of cooperation strategies during training. In this work, we present a teammate generation method which prevents the emergence of teammate policies with superficial differences by optimising a diversity metric called **B**est-**R**esponse **Div**ersity (BRDiv). Instead of assessing diversity in terms of information-theoretic measures like previous approaches, BRDiv measures diversity based on the returns of generated teammate policies when cooperating with best-response policies for other generated teammate policies. We empirically demonstrate that BRDiv prevents the emergence of teammate policies

with superficial differences in their behaviour by forcing the best-response policy for a teammate policy to be ineffective when collaborating with other teammate policies. The BRDiv metric can then be optimised using off-the-shelf MARL techniques to produce teammate policies with minimal superficial differences. Our experiments compare the returns of a learner trained with teammate policies generated by BRDiv, previous teammate generation approaches based on action and trajectory diversity maximisation (Lupu et al., 2021; Lucas & Allen, 2022), and an ablation of BRDiv. We empirically demonstrate the robustness of a learner trained with teammate policies generated by BRDiv by showing its higher returns than other evaluated baselines when dealing with near-optimal previously unseen teammate policies.

2 Related Work

Ad Hoc Teamwork (AHT). AHT was defined as a formal challenge of developing a learner capable of collaborating with unknown teammates by Stone et al. (2010). Since then, previous works (Mirsky et al., 2022) have explored AHT under different application areas and alternative names, such as zero-shot coordination (ZSC) (Hu et al., 2020) which explores AHT in problems where unknown teammates are optimal agents optimising the same reward function as the learner. Many of these works utilise type-based methods (Albrecht et al., 2016; Barrett et al., 2017; Rahman et al., 2021). A limitation of type-based approaches is that they assume access to predefined teammate policies for learning. This entails the manual specification of all possible types, which is often an infeasible process. Our work seeks to bridge this gap by providing ways to automatically generate teammates.

Multi-agent Reinforcement Learning (MARL). The objective of MARL is to jointly train a set of agents to maximise their returns in the presence of each other (Papoudakis et al., 2020; Zhang et al., 2021). Unlike ad hoc teamwork, these methods assume full control of all members of the team. Current methods in the literature have shown great success in solving complex tasks (Vinyals et al., 2019; Christianos et al., 2021), and have been shown to be able to adapt to novel tasks (Schäfer et al., 2022). However, a drawback of joint training is that the resulting agents have low performance when interacting with agents that are not encountered during the joint training process (Vezhnevets et al., 2020; Hu et al., 2020; Rahman et al., 2021).

Teammate Policy Generation. Diverse teammate policy generation has been previously explored in problems that are closely related to AHT, such as in zero-shot coordination (ZSC) (Hu et al., 2020). Several works in this area formulate diversity in terms of information-theoretic measures defined over the generated policies' trajectories (Xing et al., 2021; Lupu et al., 2021; Lucas & Allen, 2022). Despite its prevalence, previous works (Lupu et al., 2021; Liu et al., 2021) highlighted that training with teammates generated by trajectory diversity-based methods does not always lead to improved learner's robustness, which we also demonstrate through our experiments. This is because many teammate behaviours producing distinct trajectories entail the same learner's best-response policy. While Liu et al. (2021) also proposed an approach based on the best-response policies' performance, their approach is limited to zero-sum games.

Diversity in Reinforcement Learning. In single-agent reinforcement learning, diversity maximisation is mainly utilised as a way for agents to increase exploration (Pathak et al., 2017; Hong et al., 2018; Parker-Holder et al., 2020) or discover reusable skills (Eysenbach et al., 2019). For example, Eysenbach et al. (2019) proposed a method to learn a diverse set of reusable skills by only maximising an information-theoretic objective. Similarly, in multi-agent reinforcement learning (MARL), works such as MAVEN (Mahajan et al., 2019), have aided exploration by maximising a mutual-information metric between the trajectories and a latent space. Another recent work also utilised reward randomisation to achieve diverse behaviours in multi-agent settings (Tang et al., 2021). As another application of diversity optimisation in RL, Li et al. (2021) proposed a method optimising an information-theoretic objective to facilitate agents' specialisation towards a diverse range of roles for solving a MARL problem. Note that unlike when inducing diversity for teammate policy generation, these techniques are not designed to create a diverse set of teammates to improve the robustness of a learner.

Population-based Training (PBT). Our method aims to train a population of agent policies that optimise a specific metric, similar to existing works on population-based training. Population based training was proposed by Jaderberg et al. (2017) as a way to speed up the optimisation process of neural networks. This asynchronous algorithm jointly optimises a population of models and their respective hyperparameters,

through an alternating process of parallel training and hyperparameter tuning. Further work from Li et al. (2019) then introduced a framework that enables population-based training in more general settings. Unlike our method which optimises the diversity of the entire population, note that PBT methods optimise an objective function defined over a single individual. PBT then uses its population of agents to iteratively generate new population members having more optimal objective function values, which is different from our method's use of MARL techniques for optimisation.

3 Background & Setting

In this section, we formalises the problem of teammate policy generation. We first start by formalising the interaction between agents in our AHT problem. We then provide details on the main objective of a teammate generation process given our previous formulation of agents' interaction.

3.1 Decentralised Partially Observable Markov Decision Process

We model the interaction between agents in a AHT environment as a decentralised partially observable Markov decision process (Dec-POMDP) (Bernstein et al., 2002). Dec-POMDPs are formally defined as an 8-tuple, $\langle N, S, \{\mathcal{A}^i\}_{i=1}^{|N|}, P, R, \{\Omega^i\}_{i=1}^{N}, O, \gamma\rangle$. Within a Dec-POMDP, N, $\mathcal{S}$, and γ denote the set of agents, state space, and discount rate, respectively. $\mathcal{A}^i$ and Ω^i represent the action and observation space of agent i, respectively. The transition function of a Dec-POMDP is denoted by $P : S \times \mathcal{A}^1 \times \cdots \times \mathcal{A}^{|N|} \mapsto \Delta S$, where ΔS represents the set of all possible probability distributions over S. Similarly, the reward function is denoted by $R : S \times \mathcal{A}^1 \times \cdots \times \mathcal{A}^{|N|} \mapsto \mathbb{R}$, and the observation function as $O : S \mapsto \Delta(\Omega^1 \times \cdots \times \Omega^{|N|})$.

Each episode in a Dec-POMDP starts from an initial state, $s_0 \in \mathcal{S}$. At timestep t, each agent $i \in \{1, \ldots, N\}$ receives an observation $o_t^i \sim O(s_t)$ and selects an action a_t^i according to its policy $\pi^i(H_t^i)$, which is conditioned on its observation-action history $H_t^i = \left\{o_{\leq t}^i, a_{<t}^i\right\}$ containing the sequence of observation and actions observed up to timestep t. Each agent then jointly executes their selected action in the environment. After execution of the joint action $\boldsymbol{a}_t$, the state of the environment changes according to the transition function $s_{t+1} \sim P(s_t, \boldsymbol{a}_t)$, and each agent is rewarded with $\mathcal{R}(s_t, \boldsymbol{a}_t)$. This reward is common to all agents due to the cooperative nature of AHT problems.

3.2 Teammate Policy Generation

A teammate generation process aims to design a set of teammate policies, $\Pi^{\text{train}} = \{\pi^1, \pi^2, \ldots, \pi^K\}$, that when being used for AHT training maximises the robustness of the learner. Formalising this goal as a quantitative learning objective requires a measure of robustness for a given Dec-POMDP. Once such a robustness measure is formally defined, a learning objective can be formulated by defining how the generated teammate training policies affect the learner's robustness.

We characterise a learner policy as *robust* if it achieves high returns when collaborating with teammates from an unknown evaluation set, Π^{eval}. Given a Dec-POMDP and a learner policy π^i, our proposed measure of robustness is defined below:

$$M_{\Pi^{\text{eval}}}(\pi^i) = \mathbb{E}_{\boldsymbol{\pi}^{-i} \sim U(\Pi^{\text{eval}}), a_t^i \sim \pi^i, a_t^{-i} \sim \boldsymbol{\pi}^{-i},\, P, O}\left[\sum_{t=0}^{\infty} \gamma^t R(s_t, a_t)\right], \tag{1}$$

where $U(X)$ and $\boldsymbol{\pi}^{-i}$ denote a uniform distribution over a set X and the joint policy of agents other than the learner respectively. It is important to note that Π^{eval} in Equation 1 may consist of policies not encountered during AHT training, highlighting the need for a robust learner for effective collaboration.

Since the proposed measure of robustness depends on the set of policies in Π^{eval}, we outline assumptions regarding the policies that can appear in Π^{eval}. As formulated by Stone et al. (2010), we assume that Π^{eval} consists of feasible teammate policies that can achieve a minimum threshold expected performance in the Dec-POMDP used in training. This assumption reflects how an encounter with highly suboptimal teammate policies is very unlikely in many practical applications of AHT.

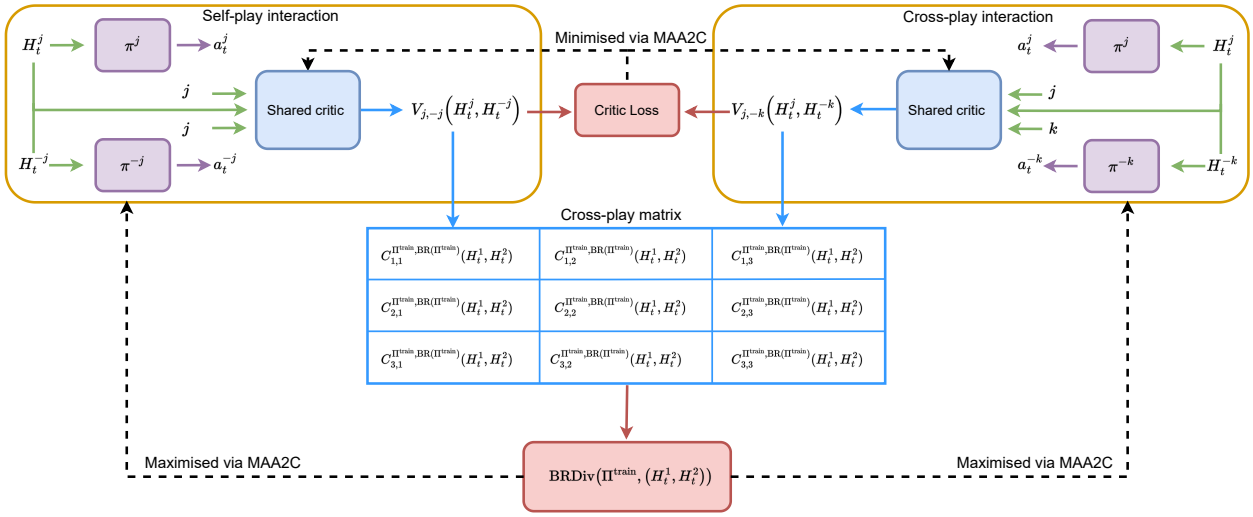


Figure 2: **Teammate Generation By Optimising BRDiv.** This figure visualises our teammate generation method assuming that we are generating $|\Pi^{\text{train}}| = 3$ for AHT environments with two players. Our method utilises MAA2C (Papoudakis et al., 2020) to generate a set of teammates that maximises the BRDiv diversity metric. The MAA2C algorithm trains a separate *actor network* (purple rectangles) to represent the policies of each generated teammate, $\pi^j \in \Pi^{\text{train}}$, and their associated best response policies, π^{-j}. Assuming $\pi^j, \pi^k \in \Pi^{\text{train}}$, a *shared critic network* (green box) is trained to estimate expected returns from the interaction between any possible pairs of (π^j, π^{-k}). The shared critic network's return estimates for all pairs are then compiled into a cross-play matrix (blue bordered box), which serves as a basis to compute the BRDiv diversity metric (red box). Finally, a diverse Π^{train} is produced by optimising the actor networks to maximise the cross-play matrix-based BRDiv metric by minimizing the actor loss outlined in Equation 9.

As the missing piece to formalise the goal of the teammate generation process, we now define how Π^{train} affects the robustness of a learner produced by AHT methods based on $M_{\Pi^{\text{eval}}}$. Given an AHT method to train a learner, Π^{train} is utilised to learn an optimal AHT policy, $\pi^{*,i}(\Pi^{\text{train}})$ that maximises the expected returns of the learner when collaborating with teammates from Π^{train}. Given a Dec-POMDP, the optimal policy given Π^{train} is defined below:

$$\pi^{*,i}(\Pi^{\text{train}}) = \underset{\pi^i}{\text{argmax}}\ \mathbb{E}_{\pi^{-i}\sim U(\Pi^{\text{train}}), a_t^i\sim\pi^i, a_t^{-i}\sim\boldsymbol{\pi}^{-i},\, P,\, O}\left[\sum_{t=0}^{\infty}\gamma^t R(s_t, a_t)\right]. \tag{2}$$

Later during the AHT evaluation process, $\pi^{*,i}(\Pi^{\text{train}})$ is the policy whose robustness when collaborating with teammates from Π^{eval} will be measured.

Based on the definition of $\pi^{*,i}(\Pi^{\text{train}})$, the goal of a teammate generation process is to find an optimal set of training teammates, $\Pi^{*,\text{train}}$, that maximises the robustness of an AHT agent. Given a Dec-POMDP and an unknown Π^{eval}, $\Pi^{*,\text{train}}$ is formally defined as:

$$\Pi^{*,\text{train}} = \underset{\Pi^{\text{train}}}{\text{argmax}}\ M_{\Pi^{\text{eval}}}\left(\pi^{*,i}(\Pi^{\text{train}})\right). \tag{3}$$

While setting $\Pi^{*,\text{train}} = \Pi^{\text{eval}}$ provides an optimal solution to the above objective, note that the teammate generation problem operates in a setup where Π^{eval} is unknown during training. Therefore, the main challenge in the teammate generation problem arises as a result of optimising for $\Pi^{*,\text{train}}$ without knowing Π^{eval}.

4 Best-Response Diversity-based Teammate Generation

This section provides the details of **B**est-**R**esponse **Div**ersity (BRDiv), the diversity metric that is optimised by our teammate generation method. Section 4.1 starts by outlining a desirable characteristic for Π^{train}, a

set of teammates policies generated for AHT training. Section 4.2 then formally defines BRDiv as a diversity metric optimised by our teammate generation approach to encourage the creation of a desirable Π^{train}.

4.1 Desirable Diversity for AHT

Our teammate generation method is based on the idea that a suitable Π^{train} for AHT must avoid having multiple policies that can be effectively collaborated with by the same best-response policy. Assuming a sufficiently small number ϵ, this characteristic can be formally written as:

$$\exists \pi^i, \pi^j \in \Pi^{\text{train}},\ \pi^i \neq \pi^j\ \wedge \left|\text{Returns}(\pi^i, \pi^{-i}) - \text{Returns}(\pi^j, \pi^{-i})\right| \leq \epsilon,$$

with π^{-i} being the best-response policy to π^i and $\text{Returns}(\pi^i, \pi^j)$ defined as:

$$\mathbb{E}_{a_t^1 \sim \pi^i, a_t^2 \sim \boldsymbol{\pi}^j,\, P,\, O}\left[\sum_{t=0}^{\infty} \gamma^t R(s_t, a_t)\right],$$

for a given Dec-POMDP. This characteristic we impose in Π^{train} is motivated by the need to avoid generating teammates with superficial differences. As we illustrated in the example provided in Figure 1, a superficial difference between generated teammate policies is characterised by the existence of a common best-response policy that can be utilised to facilitate effective collaboration with these different teammate policies.

We argue that AHT training with Π^{train} requiring different best-response policies facilitates the design of a more robust learner. Through the interaction with each $\pi^j \in \Pi^{\text{train}}$, the learner will learn different best-response policies to interact with a possible teammate. This equips the learner with a more comprehensive library of behaviours to effectively collaborate with any teammate type, which should improve the learner's robustness by reducing the likelihood of it having no adequate strategies to effectively collaborate with an unknown teammate from Π^{eval}.

4.2 BRDiv Metric

This section defines a diversity metric that can be maximised to generate Π^{train} requiring different best-response policies for effective collaboration. The description of BRDiv assumes that only two agents exist in the environment. Extending our proposed diversity metric and optimisation method to environments with more than two agents is straightforward.

BRDiv aims to generate a set of diverse policies for AHT training, $\Pi^{\text{train}} = \{\pi^1, \pi^2, ..., \pi^K\}$, where similar best-response policies cannot be used to effectively collaborate with different generated teammate types from Π^{train}. Therefore, defining a metric that quantifies the effectiveness of two agents' policies when collaborating with each other is a crucial first step in formulating our diversity metric. We measure the effectiveness of two policies when collaborating via their expected returns, which is inspired by our notion of robust collaboration introduced in Section 3.2. Assuming that agent j and k are interacting with each other based on policies, $\pi^j(a^j|H_t^j)$ and $\pi^k(a^k|H_t^k)$, that are conditioned on their respective observation-action history H_t^j and H_t^k, this return-based effectiveness measure is defined as:

$$V_{j,k}(H_t^j, H_t^k) = \mathbb{E}_{a_T^1 \sim \pi^j, a_T^2 \sim \pi^k}\left[\sum_{T=t}^{\infty} \gamma^{T-t} R(s_T, \langle a_T^1, a_T^2 \rangle)\middle| H_t^j, H_t^k\right]. \tag{4}$$

This return-based effectiveness measure provides a foundation for defining an optimised diversity metric to achieve the goal of BRDiv. Denoting the best-response policy to π^k by $\pi^{-k,*}$, and the set of best response policies to each policy in Π^{train} by $\text{BR}(\Pi^{\text{train}})$, we use Equation 4 to evaluate the effectiveness of $\pi^{-k,*} \in \text{BR}(\Pi^{\text{train}})$ when collaborating with $\pi^j \in \Pi^{\text{train}}$. Given a pair of observation-action histories, H_t^1 and H_t^2, we arrange the measured cooperative effectiveness between all possible $(\pi^j, \pi^{-k,*}) \in \Pi^{\text{train}} \times \text{BR}(\Pi^{\text{train}})$ into a $K \times K$ cross-play matrix, $C^{\Pi^{\text{train}}, \text{BR}(\Pi^{\text{train}})}(H_t^1, H_t^2)$. Elements of this cross-play matrix are defined as:

$$\forall j, k \in \{1, 2, ..., K\}, C_{j,k}^{\Pi^{\text{train}}, \text{BR}(\Pi^{\text{train}})}(H_t^1, H_t^2) = V_{j,(-k,*)}(H_t^1, H_t^2). \tag{5}$$

$C^{\Pi^{\text{train}},\text{BR}(\Pi^{\text{train}})}_{j,k}(H^1_t, H^2_t)$ then provides the necessary information to compute the BRDiv metric.

The BRDiv metric is based on the intuition that a good Π^{train} to ensure the learner's robustness must possess two characteristics. First, the cross-play matrix of Π^{train} must have high values on its diagonal elements to ensure that each $\pi^j \in \Pi^{\text{train}}$ interacts effectively with its associated best-response policy, $\pi^{-j} \in \text{BR}(\Pi^{\text{train}})$. This characteristic also prevents the emergence of teammate policies producing low returns, which no reward-optimising agent would have a reason to use in an environment. Second, the off-diagonal elements of $C^{\Pi^{\text{train}},\text{BR}(\Pi^{\text{train}})}$ must also have low values to discourage a best-response policy $\pi^{-j} \in \text{BR}(\Pi^{\text{train}})$ from being effective for collaborating with $\pi^k \in (\Pi^{\text{train}} - \{\pi^j\})$. By optimising the incompatibility of a best-response policy when dealing with other policies in Π^{train}, we aim to induce the need for different collaboration strategies to deal with each policy in Π^{train}.

Based on these two characteristics, we define our diversity metric as:

$$\begin{aligned}\text{BRDiv}(\Pi^{\text{train}}, (H^1_t, H^2_t)) = \text{Tr}\left(C^{\Pi^{\text{train}},\text{BR}(\Pi^{\text{train}})}(H^1_t, H^2_t)\right) \\ + \sum_{\substack{i,j\in\{1,\ldots,K\},\\ i\neq j}} \left(C^{\Pi^{\text{train}},\text{BR}(\Pi^{\text{train}})}_{i,i}(H^1_t, H^2_t) - C^{\Pi^{\text{train}},\text{BR}(\Pi^{\text{train}})}_{i,j}(H^1_t, H^2_t)\right) \\ + \sum_{\substack{i,j\in\{1,\ldots,K\},\\ i\neq j}} \left(C^{\Pi^{\text{train}},\text{BR}(\Pi^{\text{train}})}_{i,i}(H^1_t, H^2_t) - C^{\Pi^{\text{train}},\text{BR}(\Pi^{\text{train}})}_{j,i}(H^1_t, H^2_t)\right).\end{aligned} \tag{6}$$

The maximisation of the first term in Equation 6 enforces the first characteristic. Meanwhile, maximising the remaining terms produces a cross-play matrix with low off-diagonal values, encouraging the generated policies to fulfil the previously mentioned second desired characteristic.

5 MAA2C-Based Diversity Optimisation

We now describe an optimisation technique that maximises BRDiv to generate Π^{train}. Although a wide range of multi-agent RL algorithms can be used to maximise BRDiv, we propose an optimisation technique based on the Multi-Agent A2C (MAA2C) algorithm (Papoudakis et al., 2020) due to the straightforward modifications required to utilise it for maximising BRDiv. We use the centralised critic of MAA2C to estimate the elements of the cross-play matrix defined in Equation 5. Meanwhile, the policies in Π^{train} alongside their associated best response policies in $\text{BR}(\Pi^{\text{train}})$ are treated as actors that MAA2C trains. A detailed pseudocode of our MARL-based diversity optimisation technique is provided in Algorithm 1 in Appendix C. A visualisation that summarises our proposed teammate generation method is also provided in Figure 2.

Data Collection. Our optimisation technique separately collects two types of interaction data for training the actors and the centralised critic. First, we collect *self-play experiences* where we let a policy, $\pi^k \in \Pi^{\text{train}}$, interact with its associated best-response policy, $\pi^{-k} \in \text{BR}(\Pi^{\text{train}})$. The second type of data is *cross-play experiences* which we collect by letting a policy, $\pi^j \in \Pi^{\text{train}}$, interact with the best-response policy of a different policy, $\pi^{-k} \in \text{BR}(\Pi^{\text{train}} - \{\pi^j\})$. Both self-play and cross-play interaction data are then stored in separate storage denoted by $\mathcal{D}^{\text{SP}}$ and $\mathcal{D}^{\text{XP}}$ respectively. Note that assuming we also record the identity of the agents generating the experience, which is j and $-k$, each experience stored in the storage is then defined as a 7-tuple, $\langle (H^1_t, H^2_t), a^j_t, a^{-k}_t, \{R_t\}, (H^1_{t+1}, H^2_{t+1}), j, -k\rangle$ with H^1_t and H^2_t denoting the observation-action history from using policies π^j and π^{-k} up to timestep t.

Actor and Centralised Critic Architecture. As we mentioned at the beginning of Section 5, the trained actors in our optimisation method correspond to the generated teammate policies in Π^{train} and their associated best-response policies. For each $\pi^i \in (\Pi^{\text{train}} \cup \text{BR}(\Pi^{\text{train}}))$, this policy is represented as a neural network parameterised by θ^i. In the remainder of our description of BRDiv, note that we denote the set of actor parameters from $\Pi^{\text{train}} \cup \text{BR}(\Pi^{\text{train}})$ as Θ.

Like the actor networks, the centralised critic used in this optimisation process is also implemented as a neural network. The centralised critic network is specifically responsible for estimating elements of the cross-play

matrix, $C^{\Pi^{\text{train}},\text{BR}(\Pi^{\text{train}})}$, based on Equation 5. As shown in Figure 2, the shared critic network input consists of a sequence of observation-action history from both players in the environment. In the remainder of this document, note that we drop Π^{train} as parameters to the cross-play matrix since evaluating each element of this matrix at row i and column j does not involve π^i and $\pi^{-j,*}$. Instead, we evaluate $V^{\phi}_{i,-j}(H^i_t, H^{-j}_t)$ by also concatenating a one-hot identification of i and $-j$ to the centralised critic's input as indicated by Figure 2.

Learning Objective. The centralised critic network is trained to minimise the n-step return loss. As in many deep RL methods, we incorporate a target critic network parameterised by $\bar{\phi}$ to compute the target values for the critic network. Using the collected experiences from $\mathcal{D}^{\text{SP}}$ and $\mathcal{D}^{\text{XP}}$, the centralised critic loss function is defined below:

$$L_{\phi}(\mathcal{D}^{\text{SP}}, \mathcal{D}^{\text{XP}}) = \sum_{\mathcal{D}^{\text{SP}} \cup \mathcal{D}^{\text{XP}}} \frac{1}{2} \left(V^{\phi}_{i,-j}(H^1_t, H^2_t) - \sum_{k=0}^{n-1} \gamma^k R_{t+k} - \gamma^n V^{\bar{\phi}}_{i,-j}(H^1_{t+n}, H^2_{t+n}) \right)^2. \tag{7}$$

Given a stored experience from $\mathcal{D}^{\text{SP}}$ or $\mathcal{D}^{\text{XP}}$, the actor networks in Π^{train} and $\text{BR}(\Pi^{\text{train}})$ are trained to maximise the BRDiv-based advantage function, $A^{\phi}_{i,-j}(H^1_t, H^2_t, \{R_{t+k}\}_{k=0}^{n-1}, H^1_{t+n}, H^2_{t+n})$, defined below:

$$\text{BRDiv}(C^{\text{pred},\phi}_{i,-j}(H^1_t, H^2_t, \{R_{t+k}\}_{k=0}^{n-1}, H^1_t, H^2_t)) - \text{BRDiv}(C^{\text{base},\phi}(s_t)). \tag{8}$$

In the above expression, $C^{\text{pred},\phi}_{i,-j}(H^1_t, H^2_t, \{R_{t+k}\}_{k=0}^{n-1}, H^1_t, H^2_t)$ is a cross-play matrix which has its entry at row i and column j replaced by an n-step return estimate resulting from the interaction between π^i and π^{-j}. We use an n-step return-based estimate for one of the elements of this cross-play matrix to reduce the bias of gradients associated with the actor loss updates, which is a commonly used method in single-agent actor-critic methods. Meanwhile, $C^{\text{base},\phi}(s_t)$ is a baseline cross-play matrix whose elements only depend on H^1_t and H^2_t. The role of this baseline in the advantage function is to reduce the variance of the gradient updates for the actor networks. Given stored experiences from $\mathcal{D}^{\text{SP}}$ and $\mathcal{D}^{\text{XP}}$, this results in the use of the following loss function to optimise the actor networks:

$$\begin{aligned} L_{\theta}(\mathcal{D}^{\text{SP}}, \mathcal{D}^{\text{XP}}) = \sum_{\mathcal{D}^{\text{SP}} \cup \mathcal{D}^{\text{XP}}} \Bigg(& -\log\Big(\pi(a^i_t|H^1_t;\theta_i)\pi(a^{-j}_t|H^2_t;\theta_{-j})\Big) \\ & A^{\phi}_{i,-j}(H^1_t, H^2_t, \{R_{t+k}\}_{k=0}^{n-1}, H^1_{t+n}, H^2_{t+n})\Bigg), \end{aligned} \tag{9}$$

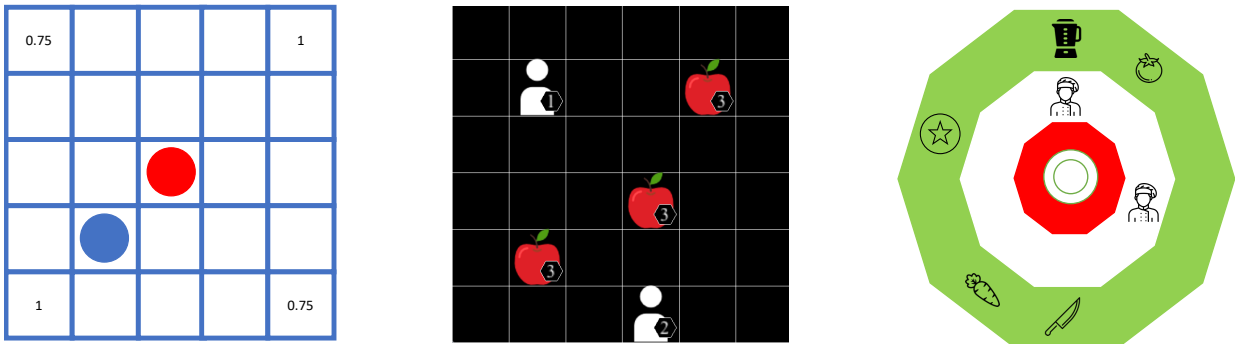
where,

$$\begin{aligned} C^{\text{pred},\phi}_{i,-j,p,q}(H^1_t, H^2_t, \{R_{t+k}\}_{k=0}^{n-1}, H^1_{t+n}, H^2_{t+n}) &= \begin{cases} V^{\phi}_{p,-q}(H^1_t, H^2_t), & \text{if } (p,q) \neq (i,j) \\ \sum_{k=0}^{n-1} \gamma^k R_{t+k} + \gamma^n V^{\phi}_{i,-j}(H^1_{t+n}, H^2_{t+n}), & \text{otherwise} \end{cases} \\ C^{\text{base},\phi}_{m,n}(H^1_t, H^2_t) &= V^{\phi}_{m,-n}(H^1_t, H^2_t). \end{aligned} \tag{10}$$

Minimising Equation 9 updates the actor networks to maximise $C^{\text{pred},\phi}_{i,-j}(H^1_t, H^2_t, \{R_{t+k}\}_{k=0}^{n-1}, H^1_t, H^2_t)$. This effectively encourages the emergence of actor networks that assign high probabilities towards actions leading towards trajectories with higher BRDiv values.

6 Experiments

We present the experiments we conduct to demonstrate the effectiveness of BRDiv in improving the robustness of an AHT learner when dealing with previously unseen teammate types in this section. First, we provide details of the environments used in our teammate generation experiments in Section 6.1. This is followed by an overview of our experiments' AHT training and evaluation process in Section 6.2. Section 6.3 then details the baseline approaches we compare BRDiv against. We then present and analyse the results of the teammate generation experiments in Section 6.4. Finally, Section 6.5 ends this chapter by describing the behaviours of teammate types generated by BRDiv.



(a) Cooperative Reaching. (b) Level-Based Foraging. (c) Simple Cooking.

Figure 3: **Environments for Teammate Generation Experiments.** Figure 3a visualizes an example state of the Cooperative Reaching environment. In this visualisation, the red circle, blue circle, and grids with texts denote the teammate, learner, and reward-providing coordinates. Meanwhile, an example state of level-based foraging environment is visualised in Figure 3b. The white and red icons represent the players and the objects that exist in the environment. The level of each player and object is then visualised in the bottom right corner of their respective icons. Finally, an example environment state for the Simple Cooking environment is provided in Figure 3c. The kitchen layout in this environment is such that the chefs are inside a decagon kitchen with a table in the middle, symbolised by the red decagon with a plate on top of it. The required cooking items and ingredients to finish the recipe are then placed on top of the green counters in this kitchen. To finish the task, all processed ingredients and the plate must be placed on the serving counter which is visualised as a green side of a decagon with a star on top.

6.1 Environments

Our experiments evaluate BRDiv and the baseline approaches in three multi-agent environments. All environments used in our experiments have two agents, one of which will be controlled by a teammate policy during an interaction episode. A visualisation of an example state from each environment is shown in Figure 3. Further details of the environments used in our experiments are provided below:

Cooperative Reaching. Cooperative reaching is a simple environment situated in a 5×5 grid world. Each agent has five actions corresponding to staying at a particular grid and moving into the four cardinal directions. The goal of all agents is to reach and jointly stay in a grid cell whose location belongs to the set of reward-providing coordinates, $F = \{(0,0),(0,4),(4,0),(4,4)\}$. Within these reward-providing coordinates, $(0,0)$ and $(4,4)$ provide a reward of 1 to both agents once they are in the same grid cell with this coordinate. Meanwhile, the grid in $(0,4)$ and $(4,0)$ only provide a reward of 0.75 once both agents arrive. In this environment, the collaboration strategies correspond to the distinct ways a teammate may select a destination grid within F. A robust AHT learner should ideally learn to follow their teammates towards any reward-providing coordinates.

Level-based Foraging (LBF): In this environment, agents must retrieve three objects that are randomly scattered in a 6×6 grid world. Agents can move in either of the four cardinal directions and have a special action that allows them to collect adjacent objects. At the beginning of each episode, each object and each agent are assigned a level that determines whether an agent may collect an object. To successfully pick up an object, the total level of agents choosing the object collection action next to the object must be at least the same as the level of the collected object. We then enforce the need for collaboration between agents by setting the level of each object as the total level of agents in the environment. For every successful collection of an object, agents will then be given a reward of 0.33.

Simple Cooking: Simple Cooking is an environment where two chefs must collaborate to create a simple dish with chopped tomatoes and blended carrots. Following Figure 3c, the two chefs can only be positioned on 10 empty spaces between the cooking counter and the table in the middle of the kitchen. Each chef is then

equipped with eight actions that enable them to (i) stay still, (ii) move clockwise, (iii) move anti-clockwise, (iv) retrieve an ingredient from a counter, (v) put an ingredient to a counter, (vi) retrieve an ingredient in the middle table, (vii) put an ingredient on the middle table, or (viii) use cooking tools placed on a counter. A chef must be positioned in the space closest to the target counter to collect or put an ingredient from or to a counter. On the other hand, a chef can put or collect items on the table at any time. Using a blender or knife to blend carrots or chop tomatoes requires an agent to be positioned in the space closest to the tool and have the right ingredient placed on the same counter as the tool. In this environment, a reward of 0.25 is provided to both agents right after (i) the tomato is chopped, (ii) the carrot is blended, (iii) both chopped tomato and blended carrot are placed on a plate, and (iv) a plate containing chopped tomatoes and blended carrots has been placed on top of the serving counter.

6.2 Experiment Protocol

Our process to evaluate the compared teammate generation methods can be divided into three stages. In the first stage, we run BRDiv and other baseline teammate generation methods to create a set of training teammates Π^{train}. The second stage utilises the resulting teammates from the first stage to train an AHT learner. We then evaluate the performance of the robustness of the learner when collaborating with a set of previously unseen teammate types from Π^{eval}.

In the first stage, we run each evaluated teammate generation method to produce K teammate types. Each teammate generation method is run for five experiment seeds and learns for T total timesteps. We utilised different K and T for each evaluated environment. In Cooperative Reaching, each teammate generation method is trained for 16 million timesteps to produce four teammate types due to the simplicity of the environment. Meanwhile, each method for 200 million timesteps to produce six and eight different teammate types for LBF and Simple Cooking. Under each experiment seed, we save Π^{train} produced by each compared algorithm at the end of the teammate generation process.

The second stage utilises Π^{train} generated from the first stage to train a learner policy through AHT training. To enable a fair comparison between results from each teammate generation method, our evaluation protocol uses the same AHT algorithm to train a learner based on each Π^{train}. We specifically use the PLASTIC Policy algorithm (Barrett et al., 2017) due to its ease of use for computing a learner policy given Π^{train} produced by our teammate generation methods. In particular, a PLASTIC Policy agent's decision-making process only requires the policy of each teammate and their associated best-response policies, both being a by-product of the teammate generation process contained in the resulting Π^{train} and $\text{BR}(\Pi^{\text{train}})$.

Using learners produced from the previous stage, our experiment protocol's final stage evaluates the learner's robustness when dealing with agents from Π^{eval}. Π^{eval} consists of policies generated by the teammate generation methods evaluated in this work or policies following predefined heuristics defined in Appendix B. Note that when evaluating the learner's robustness against teammates generated by the same teammate generation method, we also measure the learner's robustness against teammate policies generated from different experiment seeds. Such evaluation remains a challenge since teammates generated by the same method under different seeds may have different behaviours that cause difficulties in effective collaboration.

As a measure of robustness, our evaluation process proceeds by evaluating the mean returns of an AHT learner when dealing with teammate policies in Π^{eval}. For each teammate generation method, the mean returns from the learner produced by each experiment seed are logged. Using the reported returns from the five experiments for each compared method, we compute a 95% confidence interval over the returns of AHT learners when dealing with each unknown teammate policy type from Π^{train}. This confidence interval allows us to argue over the significance of the difference in robustness between teammate generation methods. The resulting returns of a learner trained through generated teammate types produced by BRDiv and baseline approaches are reported and analysed in Section 6.4.

6.3 Baselines

Our experiments compared BRDiv with two types of baselines. The first type of baseline comprises previous methods for automatically generating teammates in AHT or related problems, such as zero-shot coordination.

Meanwhile, the second type of baseline consists of an ablation of BRDiv, which removes parts of BRDiv responsible for encouraging ineffective collaboration between a generated teammate policy and the best response policy associated with another generated teammate type. Details of these methods and their implementation are provided below. Appendix C then provides the value of each methods' hyperparameters used in our experiments.

Prior teammate generation methods. Among methods under this category, we choose TrajeDi (Lupu et al., 2021) and Any-Play (Lucas & Allen, 2022) as representative baselines. We choose TrajeDi following its usage of the *action discounting term*, which provides additional flexibility when defining the optimised information-theoretic diversity metric. Prior teammate generation methods other than TrajeDi define their optimised diversity metric in terms of an agent's overall trajectory or its selected action at each timestep, which both have their drawbacks. TrajeDi's action discounting term enables users to tune the resemblance of its optimised diversity metric to an action diversity and trajectory diversity-based approach. In the plots that we report in this work, we denote these TrajeDi-based baselines as **TrajeDi0**, **TrajeDi025**, **TrajeDi05**, **TrajeDi075**, and **TrajeDi1**, which use the action discounting term of 0, 0.25, 0.5, 0.75, and 1 respectively.

We also add Any-Play as a baseline following the results from Lucas & Allen (2022) that demonstrated its improved performance over TrajeDi in a few environments. This baseline will be denoted in our analysis as **AnyPlay**. Unlike BRDiv and TrajeDi, Any-Play's teammate generation process adds an intrinsic reward that the actor networks also attempt to maximise aside from the original rewards from the environment. This intrinsic reward is specifically an information-theoretic diversity metric computed based on a classifier that distinguishes the different policies in Π^{train}. Thus, comparing BRDiv's performance against Any-Play also delivers insights regarding the gains from using a different optimisation technique to induce diversity.

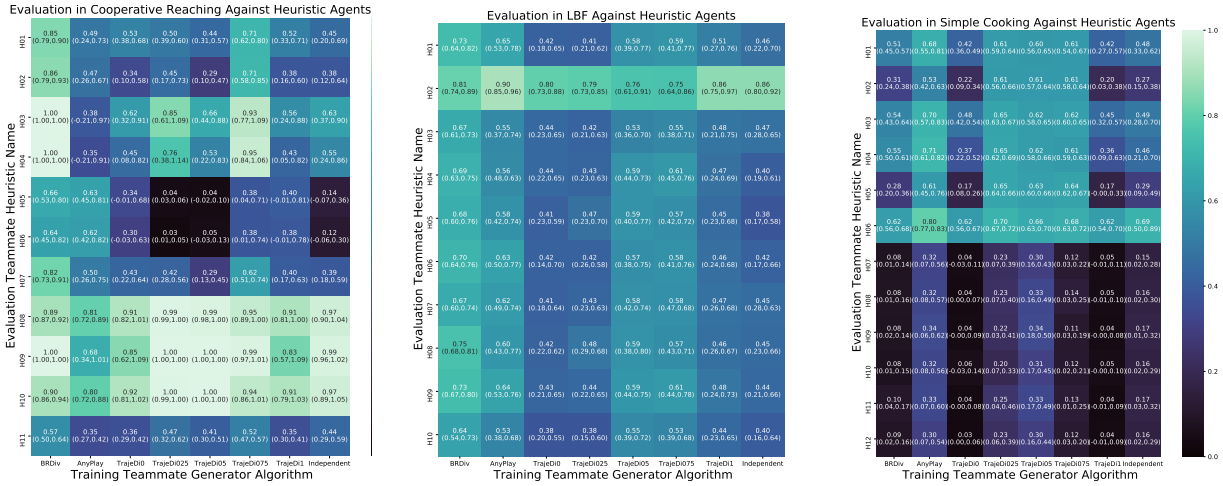
Implementing TrajeDi and Any-Play based on our MAA2C-based teammate generation method is straightforward. First, we remove all loss functions evaluated based on cross-play data since TrajeDi and Any-Play only rely on self-play data for training. This is effectively done by subtracting $\mathcal{L}_{\phi}^{\text{XP}}$ and $\mathcal{L}_{\Theta}^{\text{XP}}$ from the loss function returned by Algorithm 2. Using $\mathcal{D}^{\text{SP}}$ for its evaluation, we also add the negative of the information-theoretic diversity metric maximised by TrajeDi to the loss function returned by Algorithm 2. Meanwhile, for Any-Play we also add a loss function that trains a classifier that identifies the population a teammate belongs to based on an observed state and its action. The output of this classifier is then used at each timestep to compute an intrinsic reward that is added on top of the environment rewards during training. These straightforward changes enable us to generate teammates with TrajeDi and Any-Play using our proposed BRDiv pseudocode.

Ablations of BRDiv. We also compare BRDiv against an ablation which independently trains K teammate policies with MAA2C (Papoudakis et al., 2020) without maximising BRDiv's proposed diversity metric outlined in Equation 6. Our experiments denote this baseline as **Independent**. Comparing BRDiv's resulting performance against this ablation helps us identify the impact of optimising our proposed diversity metric on the resulting learner's robustness when dealing with previously unseen teammates. Similar to our TrajeDi baseline, we implement this ablation with our pseudocode by first subtracting $\mathcal{L}_{\phi}^{\text{XP}}$ and $\mathcal{L}_{\Theta}^{\text{XP}}$ from BRDiv's original loss function. Furthermore, when computing MAA2C's actor loss, we use a modified diversity metric that subtracts all terms on the right-hand side of Equation 6 except for the first term. This modification ensures that all K generated policies are only trained to maximise their performance when collaborating with its best response policy.

6.4 AHT Evaluation

This section provides the results of using the generated teammate policies for training an AHT learner, following the experimental protocol outlined in Section 6.2. Figure 4 show the performance of a PLASTIC Policy-based learner when interacting with teammates that follow one of the previously unseen heuristics defined in Appendix B. The performance of the same learner when dealing with previously unseen teammates generated by different teammate generation methods is then provided in Figure 5.

As shown in Figure 4a and Figure 4b, BRDiv provides a more reliable way to generate robust learners than the baseline methods when collaborating with unseen heuristics that are near optimal. When comparing the resulting returns between BRDiv-based learners with the Independent baseline, we see that BRDiv achieves

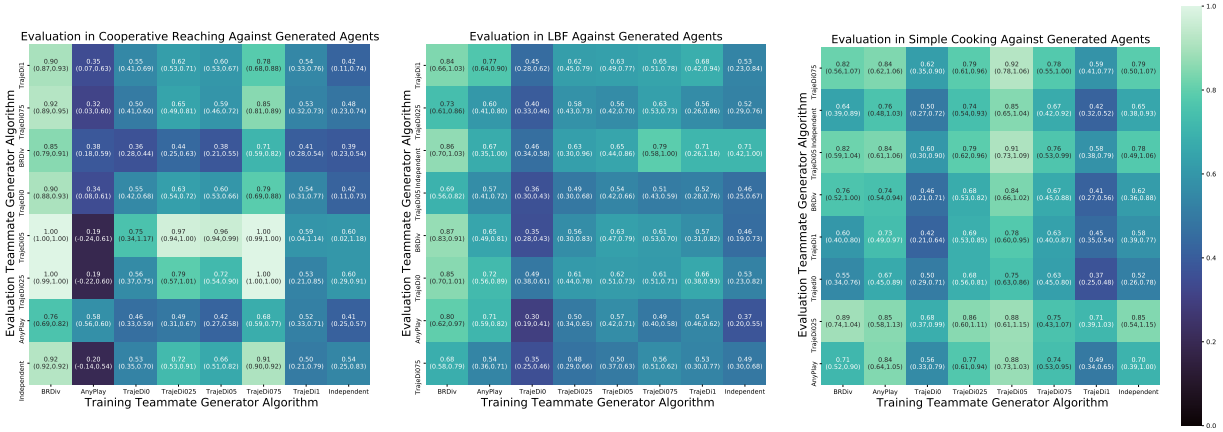


(a) Cooperative Reaching (b) LBF (c) Simple Cooking

Figure 4: **AHT Evaluation Results Against Heuristic-based Teammates.** We provide the average returns resulting from the interaction between Π^{eval} consisting of heuristic-based teammates and the learner, which is trained using PLASTIC Policy (Barrett et al., 2017) and Π^{train} produced by the evaluated teammate generation methods. Labels on the x-axis of the heatmap visualisation indicate the teammate generation method used to produce Π^{train}. Labels on the y-axis highlight the heuristics followed by agent policies from Π^{eval}. Within each entry of the heatmap, the first number provides the average returns from the collaboration between learners trained with Π^{train} generated by the method indicated in the x-axis and teammates following heuristics labelled in the y-axis. The numbers in the parentheses provide a 95% confidence interval of the returns based on teammate generation experiments conducted across five seeds. Figure 4a show the results in the Cooperative Reaching environment where training a learner with BRDiv-based teammates produces more robust agents that can deliver higher returns than the baselines, except for interactions against H08 and H10. Meanwhile, the results in the LBF environment also mirrors the general findings from the Cooperative Reaching environment where a BRDiv-based learner yields higher average returns than all baselines with the exception for interactions against H02. Finally, Figure 4c show the results in the Simple Cooking environment where BRDiv did not achieve the best performance compared to other methods due to its inadequacy when dealing with suboptimal teammate heuristics.

higher returns in all but three heuristics throughout the entire types of teammates used in the evaluation process. Except for interactions against teammates using heuristics H08 and H10, a learner trained with BRDiv-based teammates consistently achieves the highest average returns compared to the other evaluated teammate generation methods in Cooperative Reaching. Meanwhile, BRDiv also consistently yields more robust learners than compared baselines in LBF except for interactions against teammates using heuristic H02. In experiments against teammates using policies generated by other teammate generation methods which results are provided by Figures 5a and 5b, learners trained using BRDiv-based teammates consistently achieve the highest average returns compared to other baseline methods in all environments. Finally, note that in cases where specific baseline methods outperform a BRDiv-based learner in terms of the resulting average returns, the difference in performance between BRDiv and these baselines is insignificant.

Another substantial evidence of BRDiv's reliability in training robust learners can be found by comparing the confidence interval of returns between compared methods. In Figures 4 and 5, we observe BRDiv's tendency to produce more compact confidence intervals in its returns, which indicates lower variance in a BRDiv-based learner's returns across different training seeds. The baseline methods' larger variance in returns results from their generated Π^{train} having high variance in Best-Response Diversity across different experiment seeds. Across some seeds, the baseline methods still discover Π^{train} with a high BRDiv value even without optimising BRDiv. These baseline methods can discover Π^{train} with high BRDiv values since policies in Π^{train} with high BRDiv also exhibit high diversity in the trajectories they generate. However, since high trajectory diversity does not imply high BRDiv, a few seeds of the baseline methods also discover Π^{train} with



(a) Cooperative Reaching (b) LBF (c) Simple Cooking

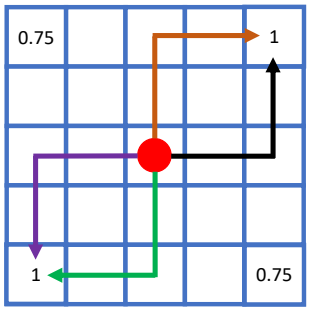
Figure 5: **AHT Evaluation Results Against Previously Unseen Generated Teammates.** Given Π^{train} generated by a teammate generation method, we also report the average returns achieved by the learner when dealing with Π^{eval} consisting of teammates generated by the different evaluated teammate generation methods. In the figures above, the labels on the x-axis, y-axis, and numbers within the heatmap have similar semantics with their respective counterparts in Figure 4. Note that when dealing with Π^{eval} generated by the same algorithm producing Π^{train}, it is possible that effective collaboration cannot be achieved since Π^{eval} also consists of policies generated through experiments using different seeds from which is being used to produce Π^{train}. In Cooperative Reaching and LBF, BRDiv-based learners produce higher average returns when dealing with its previously unseen teammates. For certain teammate generation methods, the difference between a BRDiv-based learner's and its mean returns is even statistically significant. For Simple Cooking, our method occasionally struggles to deal with suboptimal teammate policies generated by some teammate generation methods. Further discussions regarding the suboptimality of policies produced by certain methods are provided in Section 6.5.

lower BRDiv that yields learners with lower returns due to superficial differences between generated policies. While TrajeDi has an action discounting hyperparameter that can be tuned to minimise the emergence of Π^{train} with superficial differences (Lupu et al., 2021), our results indicate that tuning this hyperparameter is less effective in preventing the emergence of superficial differences between generated teammates compared to directly optimising BRDiv.

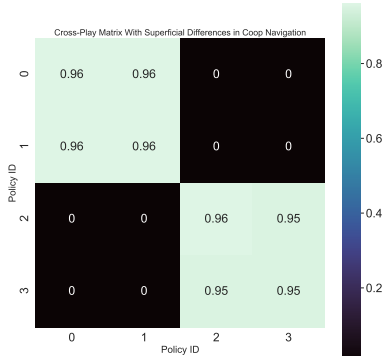
Important insights are also obtained from evaluating learners when collaborating with more suboptimal teammates. Against teammate-following heuristics H08 and H10 in Cooperative Reaching, BRDiv ceased to become the best-performing teammate generation method to improve the robustness of the learner. The same trend is seen in Figure 4c where the learner must collaborate with H01-H12 whose expertise only spans parts of tasks in the environment, such as processing the ingredients, assembling them into a dish, and delivering it to a serving counter. This echoes with the results of BRDiv when dealing with other Simple Cooking teammate policies generated by other baseline teammate generation methods, which we discuss in Section 6.5 to have generated suboptimal policies. All these results point towards the inadequacy of BRDiv-based generated policies to improve learner robustness when dealing with suboptimal teammates.

6.5 Behaviour Evaluation

In this section, we provide additional empirical evidence regarding the effectiveness of BRDiv in generating Π^{train} for AHT training. First, we show an example of Π^{train} exhibiting superficial differences based on the results of running one of our baseline teammate generation methods in the Cooperative Reaching environment. We then show how BRDiv successfully avoids generating Π^{train} exhibiting superficial differences, which then leads to improved learner robustness when Π^{train} is used for AHT training.

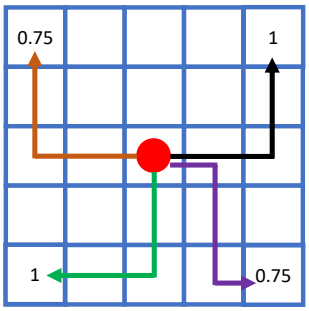


(a) Example of superficial differences between generated teammates.

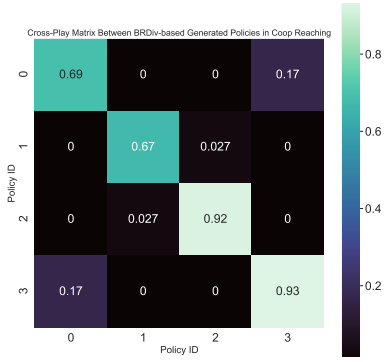


(b) Cross-play matrix between policies generated following Figure 6a.

Figure 6: **Example of Superficial Policy Differences in Cooperative Reaching.** From one of the Π^{train} resulting from a baseline teammate generation method in our experiments, we see an example of teammates with superficial differences in Cooperative Reaching. Figure 6a show that superficial difference is characterised by different teammate policies that move a teammate towards the same reward-providing corner. Since an effective collaboration with teammates having superficial differences can be achieved using the same best response policy, the cross-play matrix from Figure 6b demonstrates the compatibility of some best response policies with multiple policies from Π^{train}.



(a) Π^{train} generated by BRDiv in Cooperative Reaching.

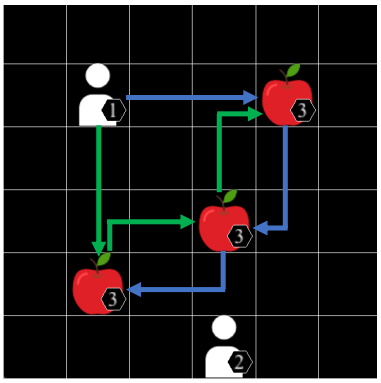


(b) Cross-play matrix between the policies generated by BRDiv in Figure 7a.

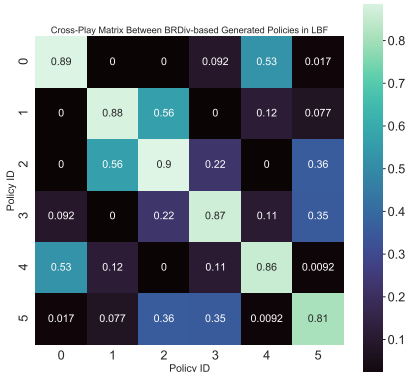
Figure 7: **Ideal Π^{train} for Cooperative Reaching.** An example Π^{train} generated by maximising BRDiv is provided in Figure 7a. A robust learner is more likely to be produced from training with this Π^{train} since it contains different policies that move teammates towards all the reward-providing coordinates in Cooperative Reaching. Following Figure 7b, this Π^{train} is characterised by the distinct best response policies required for effective collaboration against each generated policy.

An example of Π^{train} with superficial differences discovered by one of our baseline methods can be seen in Figure 6a. In this visualisation, multiple policies in Π^{train} move towards the same reward-providing coordinates. Effective collaboration with these policies can be achieved through the same best response policy of moving towards a reward-providing grid the teammate moves towards. This commonality in best response policies is reflected in Figure 6b, which shows the cross-play matrix resulting from the interaction between the policies in Π^{train} and $\text{BR}(\Pi^{\text{train}})$.

Training a Cooperative Reaching learner based on Π^{train} in Figure 6a will not provide a robust learner. This is because certain teammate behaviours are not present in the training set, such as teammates that move



(a) Trajectories produced by two randomly sampled policies from Π^{train}.



(b) Cross-play matrix from Π^{train} produced by BRDiv.

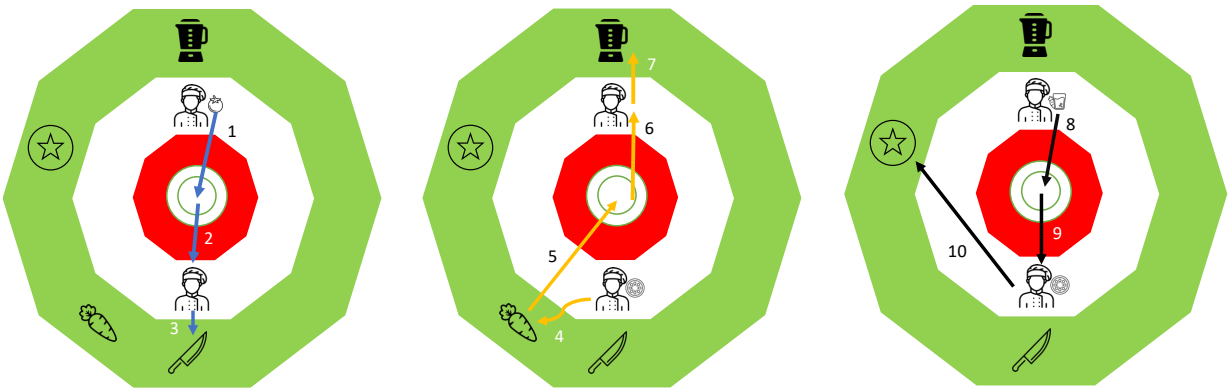
Figure 8: Π^{train} **Generated by Optimising BRDiv in LBF.** Assuming that the level one agent is the teammate, example trajectories from two randomly sampled policies generated by optimising BRDiv for LBF are displayed in Figure 8a. In this visualisation, each sequence of the same coloured arrows starting from the teammate's position corresponds to a trajectory of a single policy from Π^{train}. Different policies in Π^{train} specifically correspond to the distinct orderings that a teammate may follow to collect objects in the environment. Since an effective collaboration with teammates that follow a specific object collection ordering requires best response policies that follow the same object collection ordering, the best response to every policy in Π^{train} is distinct and incompatible for collaboration with other policies. This results in the cross-play matrix displayed in Figure 8b.

towards the upper-left or bottom-right reward-providing corners. A better Π^{train} for training learners in Cooperative Reaching is visualised by the BRDiv-based teammate policies in Figure 7a. In this case, Π^{train} produces a more robust learner by equipping it with a more comprehensive set of strategies against teammates moving towards any reward-providing grid. We can consistently find this desirable Π^{train} since each policy in Π^{train} requires different best response policies, which makes it highly likely to be discovered by optimising BRDiv.

Optimising BRDiv also enables the discovery of a Π^{train} that encourages the emergence of robust learners in the LBF environment. As seen in Figure 8a, each policy in Π^{train} generated by optimising BRDiv for LBF corresponds to the distinct orderings that an optimal agent may take to collect objects in the environment. Since any optimal or near-optimal teammate should follow one of the six possible orderings when collecting objects, the discovery of Π^{train} containing policies that follow each ordering prevents the learner from not having an adequate strategy to deal with optimal or near-optimal teammates. As in the case with Cooperative Reaching, note that the discovery of good quality teammate policies for LBF is made possible by each policy in Π^{train} requiring different best response policies, which makes it highly likely to be discovered by optimising BRDiv.

Besides highlighting why optimising BRDiv facilitates improved learner robustness in Cooperative Reaching and LBF, analysing the behaviour of policies generated by our method and the baselines also provides insights into why our method does not yield the most robust learner in Simple Cooking. As displayed by Figure 9, teammate policies generated by optimising BRDiv are highly optimal. The generated policies alongside its best-response policy quickly learn to divide and execute the available subtasks among themselves. Between different generated policies in Π^{train}, a difference emerges due to different task assignments between agents and different orderings to complete the subtasks. In general, BRDiv-based generated policies and their best-response policies tend to finish an episode of Simple Cooking in 17-20 timesteps. Learning from such highly optimal policies makes a learner unprepared when facing highly suboptimal policies during evaluation.

This result from BRDiv highly contrasts with the results from optimising alternative diversity metrics tested in this work. A detailed breakdown of the number of timesteps required by each compared teammate generation method to solve Simple Cooking in self-play is provided in Table 1. The better-performing baselines



(a) Tomato Preparation. (b) Carrot Preparation. (c) Food Assembly & Delivery.

Figure 9: **Teammate Policy Generated By Optimising BRDiv & Its Best-Response Policy.** From left to right, we show an example of a teammate policy alongside its best-response policy generated by optimising BRDiv. The generated policy and its best-response policy learn to quickly divide the ingredient preparation, dish assembly, and delivery tasks between themselves. In Figure 9a, the generated policy collects the tomato and puts it on the table so another teammate closer to the knife and positioned on the opposite side of the kitchen can retrieve and chop it. After chopping the tomato, Figure 9b then shows that the best-response policy learns to move towards the carrot and puts it on the table so that the agent controlled by the generated policy can collect and blend it. After the generated policy puts the blended carrot on the table, the best-response policy collects the plate and carrot to combine it with its chopped tomatoes. The best-response policy eventually delivers this combined food to the serving counter as seen in Figure 9c.

for generating robust learners for Simple Cooking against heuristic-based teammates particularly produce suboptimal teammate policies that solve the environment in 30-195 timesteps. Throughout interaction, Any-Play and TrajeDi-based policies often exhibit suboptimal behaviour such as (i) going back and forth between putting an item on the counter and retrieving it again or (ii) stopping working on subtasks and doing nothing. The availability of such suboptimal policies in Π^{train} makes the learner more prepared to complete a task on its own in case teammates are performing poorly in the task. While this inability to deal with highly suboptimal teammates presents potential research directions to further improve BRDiv, note that such suboptimal teammates are rarely encountered in many realistic applications of AHT. As originally formulated by (Stone et al., 2010), encountered teammates are normally assumed to be capable of achieving a specific return threshold at the given task.

Table 1: **Required Timesteps to Solve Simple Cooking In Self-Play.** The number of timesteps required by each method to solve Simple Cooking is provided in their respective entries in the second row.

BRDiv	Any-Play	TrajeDi0	TrajeDi025	TrajeDi05	TrajeDi075	TrajeDi1	Independent
17-20	30-35	18-25	65-158	85-233	53-161	20-28	18-29

7 Conclusion & Future Work

In this work, we discussed the importance of generating a collection of training teammate policies, Π^{train}, that require different best-response policies to improve the robustness of an AHT agent. To achieve this, we proposed a teammate generation method that optimises BRDiv, a diversity metric designed to prevent the emergence of superficial differences between policies in Π^{train}. Based on a comparison against TrajeDi (Lupu et al., 2021), Any-Play (Lucas & Allen, 2022), and a baseline that independently trains different teammate policies via MARL, our experiments show that optimising BRDiv achieves higher average returns when dealing with near-optimal previously unseen teammate policies. At the same time, we also see a smaller variance in the returns produced by learners trained with Π^{train} produced by optimising BRDiv.

Further analysis of the generated teammates' behaviour shows that optimising BRDiv avoids generating teammates with superficial differences. At the same time, Π^{train} generated by optimising BRDiv covers a comprehensive set of reward-maximising teammate behaviours. Training against this set of teammates eventually produced teammates that can perform a wider range of strategies to collaborate against previously unseen teammate policies.

Although our results in the teammate generation experiments show that optimising BRDiv can generate teammate policies that require different strategies for effective collaboration, we note that this is not the only type of diversity displayed by decision-making agents in real-world problems. In many applications of AHT, a learner also has to deal with teammates that vary in their ability to maximise the teams' returns. For example, even with different teammates that prefer a specific role such as being a striker, we see a wide range of skill levels between potential teammates in a pick-up soccer game. A teammate's ability may range from having the skills of an amateur player to possessing elite skills displayed by top-division professional players. Currently, this diversity cannot be discovered solely based on optimising BRDiv. The first term on the right-hand side of Equation 6 encourages the creation of teammates with near-optimal policies when we optimise BRDiv. By only training a learner against teammates generated by optimising BRDiv, this limitation potentially results in a learner yielding suboptimal returns when dealing with teammates with a low skill level. The results of our experiments in the Simple Cooking environment also confirmed the need for further improvements under this direction.

The proposed method to optimise BRDiv also faces challenges when dealing with problems other than two-player games. In many real-world problems such as those addressed in open ad hoc teamwork (Rahman et al., 2021), generating a team of multiple agents with different policies is desirable. While our proposed optimisation method can be modified to generate a team of teammates, many such teams must be generated at once to improve the robustness of the learner. After all, the number of generated training teams must match the exponential increase in the space of possible team configurations. Since training agents via MARL may require millions of experiences even in simple domains, the computational resources required by our proposed method to generate a large collection of teams can quickly grow impractical as the size of a generated team increases.

References

Stefano V. Albrecht, Jacob W. Crandall, and Subramanian Ramamoorthy. Belief and truth in hypothesised behaviours. *Artificial Intelligence*, 235:63–94, 2016.

Samuel Barrett, Noa Agmon, Noam Hazon, Sarit Kraus, and Peter Stone. Communicating with unknown teammates. In *Proceedings of the 2014 International Conference on Autonomous Agents and Multi-Agent Systems*, AAMAS '14, pp. 1433–1434, Richland, SC, 2014. International Foundation for Autonomous Agents and Multiagent Systems. ISBN 9781450327381.

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

Daniel S Bernstein, Robert Givan, Neil Immerman, and Shlomo Zilberstein. The complexity of decentralized control of markov decision processes. *Mathematics of operations research*, 27(4):819–840, 2002.

Filippos Christianos, Georgios Papoudakis, Arrasy Rahman, and Stefano V. Albrecht. Scaling multi-agent reinforcement learning with selective parameter sharing. In *International Conference on Machine Learning (ICML)*, 2021.

Benjamin Eysenbach, Abhishek Gupta, Julian Ibarz, and Sergey Levine. Diversity is all you need: Learning skills without a reward function. In *International Conference on Learning Representations*, 2019. URL `https://openreview.net/forum?id=SJx63jRqFm`.

Zhang-Wei Hong, Tzu-Yun Shann, Shih-Yang Su, Yi-Hsiang Chang, Tsu-Jui Fu, and Chun-Yi Lee. Diversity-driven exploration strategy for deep reinforcement learning. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett (eds.), *Advances in Neural Information Processing Systems*,

volume 31. Curran Associates, Inc., 2018. URL https://proceedings.neurips.cc/paper/2018/file/a2802cade04644083dcde1c8c483ed9a-Paper.pdf.

Hengyuan Hu, Adam Lerer, Alex Peysakhovich, and Jakob Foerster. "other-play" for zero-shot coordination. In *International Conference on Machine Learning*, pp. 4399–4410. PMLR, 2020.

Max Jaderberg, Valentin Dalibard, Simon Osindero, Wojciech M. Czarnecki, Jeff Donahue, Ali Razavi, Oriol Vinyals, Tim Green, Iain Dunning, Karen Simonyan, Chrisantha Fernando, and Koray Kavukcuoglu. Population based training of neural networks. *CoRR*, abs/1711.09846, 2017. URL http://arxiv.org/abs/1711.09846.

Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.

Ang Li, Ola Spyra, Sagi Perel, Valentin Dalibard, Max Jaderberg, Chenjie Gu, David Budden, Tim Harley, and Pramod Gupta. A generalized framework for population based training. In *Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, KDD 2019, pp. 1791–1799, New York, NY, USA, 2019. Association for Computing Machinery. ISBN 9781450362016. doi: 10.1145/3292500.3330649. URL https://doi.org/10.1145/3292500.3330649.

Chenghao Li, Tonghan Wang, Chengjie Wu, Qianchuan Zhao, Jun Yang, and Chongjie Zhang. Celebrating diversity in shared multi-agent reinforcement learning. In A. Beygelzimer, Y. Dauphin, P. Liang, and J. Wortman Vaughan (eds.), *Advances in Neural Information Processing Systems*, 2021. URL https://openreview.net/forum?id=C087OIEOGU8.

Xiangyu Liu, Hangtian Jia, Ying Wen, Yujing Hu, Yingfeng Chen, Changjie Fan, ZHIPENG HU, and Yaodong Yang. Towards unifying behavioral and response diversity for open-ended learning in zero-sum games. In M. Ranzato, A. Beygelzimer, Y. Dauphin, P.S. Liang, and J. Wortman Vaughan (eds.), *Advances in Neural Information Processing Systems*, volume 34, pp. 941–952. Curran Associates, Inc., 2021. URL https://proceedings.neurips.cc/paper/2021/file/07bba581a2dd8d098a3be0f683560643-Paper.pdf.

Keane Lucas and Ross E Allen. Any-play: An intrinsic augmentation for zero-shot coordination. *arXiv preprint arXiv:2201.12436*, 2022.

Andrei Lupu, Brandon Cui, Hengyuan Hu, and Jakob Foerster. Trajectory diversity for zero-shot coordination. In *Proceedings of the 38th International Conference on Machine Learning*, 2021.

Anuj Mahajan, Tabish Rashid, Mikayel Samvelyan, and Shimon Whiteson. Maven: Multi-agent variational exploration. In *Advances in Neural Information Processing Systems*, pp. 7611–7622, 2019.

Reuth Mirsky, Ignacio Carlucho, Arrasy Rahman, Elliot Fosong, William Macke, Mohan Sridharan, Peter Stone, and Stefano V Albrecht. A survey of ad hoc teamwork research. *European Conference on Multi-Agent Systems (EUMAS)*, 2022.

Georgios Papoudakis, Filippos Christianos, Lukas Schäfer, and Stefano V Albrecht. Benchmarking multi-agent deep reinforcement learning algorithms in cooperative tasks. *arXiv preprint arXiv:2006.07869*, 2020.

Georgios Papoudakis, Filippos Christianos, and Stefano Albrecht. Agent modelling under partial observability for deep reinforcement learning. *Advances in Neural Information Processing Systems*, 35, 2021.

Jack Parker-Holder, Aldo Pacchiano, Krzysztof Choromanski, and Stephen Roberts. Effective diversity in population based reinforcement learning. In *Proceedings of the 34th International Conference on Neural Information Processing Systems*, NIPS'20, Red Hook, NY, USA, 2020. Curran Associates Inc. ISBN 9781713829546.

Deepak Pathak, Pulkit Agrawal, Alexei A. Efros, and Trevor Darrell. Curiosity-driven exploration by self-supervised prediction. In *Proceedings of the 34th International Conference on Machine Learning - Volume 70*, ICML'17, pp. 2778–2787. JMLR.org, 2017.

Arrasy Rahman, Niklas Höpner, Filippos Christianos, and Stefano V. Albrecht. Towards open ad hoc teamwork using graph-based policy learning. In *International Conference on Machine Learning*, volume 139. PMLR, 2021.

Lukas Schäfer, Filippos Christianos, Amos Storkey, and Stefano V. Albrecht. Learning task embeddings for teamwork adaptation in multi-agent reinforcement learning, 2022.

Peter Stone, Gal A. Kaminka, Sarit Kraus, and Jeffrey S. Rosenschein. Ad hoc autonomous agent teams: Collaboration without pre-coordination. In *AAAI Conference on Artificial Intelligence*, pp. 1504–1509, 2010.

Zhenggang Tang, Chao Yu, Boyuan Chen, Huazhe Xu, Xiaolong Wang, Fei Fang, Simon Du, Yu Wang, and Yi Wu. Discovering diverse multi-agent strategic behavior via reward randomization, 2021. URL https://arxiv.org/abs/2103.04564.

Alexander Vezhnevets, Yuhuai Wu, Maria Eckstein, Rémi Leblond, and Joel Z Leibo. Options as responses: Grounding behavioural hierarchies in multi-agent reinforcement learning. In *International Conference on Machine Learning*, pp. 9733–9742. PMLR, 2020.

Oriol Vinyals, Igor Babuschkin, Wojciech M. Czarnecki, Michaël Mathieu, Andrew Dudzik, Junyoung Chung, David H. Choi, Richard Powell, Timo Ewalds, Petko Georgiev, Junhyuk Oh, Dan Horgan, Manuel Kroiss, Ivo Danihelka, Aja Huang, Laurent Sifre, Trevor Cai, John P. Agapiou, Max Jaderberg, Alexander S. Vezhnevets, Rémi Leblond, Tobias Pohlen, Valentin Dalibard, David Budden, Yury Sulsky, James Molloy, Tom L. Paine, Caglar Gulcehre, Ziyu Wang, Tobias Pfaff, Yuhuai Wu, Roman Ring, Dani Yogatama, Dario Wünsch, Katrina McKinney, Oliver Smith, Tom Schaul, Timothy Lillicrap, Koray Kavukcuoglu, Demis Hassabis, Chris Apps, and David Silver. Grandmaster level in StarCraft II using multi-agent reinforcement learning. *Nature*, 575(7782):350–354, November 2019. ISSN 1476-4687. doi: 10.1038/s41586-019-1724-z. URL https://www.nature.com/articles/s41586-019-1724-z. Number: 7782 Publisher: Nature Publishing Group.

Dong Xing, Qianhui Liu, Qian Zheng, and Gang Pan. Learning with generated teammates to achieve type-free ad-hoc teamwork. In *IJCAI*, pp. 472–478, 2021.

Kaiqing Zhang, Zhuoran Yang, and Tamer Başar. *Multi-Agent Reinforcement Learning: A Selective Overview of Theories and Algorithms*, pp. 321–384. Springer International Publishing, Cham, 2021. ISBN 978-3-030-60990-0. doi: 10.1007/978-3-030-60990-0_12. URL https://doi.org/10.1007/978-3-030-60990-0_12.

Luisa Zintgraf, Sam Devlin, Kamil Ciosek, Shimon Whiteson, and Katja Hofmann. Deep interactive bayesian reinforcement learning via meta-learning. *arXiv preprint arXiv:2101.03864*, 2021.

A BRDiv Pseudocode

We complete the description of our method by providing a pseudocode for the teammate generation process undergone in BRDiv, shown in in Algorithm 1. An essential part of Algorithm 1 is a call to the **COMPUTE_LOSS** function that evaluates the loss functions minimised by BRDiv. How BRDiv utilises the gathered self-play and cross-play experience to compute the minimised loss functions is then described in Algorithm 2.

B Heuristic-based Teammates

As we mentioned in Section 6.2, we use Π^{eval} consisting of heuristic-based policies to evaluate the methods used in our experiments. The details of heuristics followed by each policy for the Cooperative Reaching environment are provided in Section B.1. Meanwhile, Section B.2 outlines the heuristics followed by the policies in Π^{eval} for LBF.

Algorithm 1 BRDiv-based Teammate Generation Process

Require:
Number of training episodes, n_{eps}.
Episode length, T.
Update period, t_{update}.
Number of generated teammate types, K.
Initial population actor network parameters, $\Theta = \{\theta_1, \theta_2, ..., \theta_K\}$.
Initial centralised critic parameters, ϕ.
Target centralised critic parameters, $\bar{\phi}$.
Learning Rate, α.
Target network update coefficient, $\bar{\alpha}$.
Environment for SP and XP interaction, env^{SP} & env^{XP}.

for $i = 1$ to n_{eps} **do**
  $t \leftarrow 0$
  $\mathcal{D}^{\text{SP}}, \mathcal{D}^{\text{XP}} \leftarrow \{\}, \{\}$
  $\text{ID}^{\text{SP}} \sim \text{Uniform}(\{1, \ldots, K\})$ ▷ Sample Population ID for SP
  $\text{ID}_1^{\text{XP}}, \text{ID}_2^{\text{XP}} \sim \text{Uniform}(\{(i,j) | i, j \in 1, \ldots, K,\ i \neq j\})$ ▷ Sample Population ID for XP
  Observe $\boldsymbol{H}_0^{SP} = (o_0^{1,\text{SP}}, o_0^{2,\text{SP}})$ and $\boldsymbol{H}_0^{\text{XP}} = (o_0^{1,\text{XP}}, o_0^{2,\text{XP}})$ from env^{SP} and env^{XP} respectively.
  $H_0^{1,SP}, H_0^{2,SP}, H_0^{1,XP}, H_0^{2,XP} \leftarrow \{o_0^{1,\text{SP}}\}, \{o_0^{2,\text{SP}}\}, \{o_0^{1,\text{XP}}\}, \{o_0^{2,\text{XP}}\}$
  while $t < T$ **do**
    // Self-Play Data Collection
    $a_t^{1,\text{SP}} \sim \pi\left(a_t^{1,\text{SP}} | H_t^{1,\text{SP}}; \theta^{\text{ID}^{\text{SP}}}\right)$ and $a_t^{2,\text{SP}} \sim \pi\left(a_t^{2,\text{SP}} | H_t^{2,\text{SP}}; \theta^{\text{ID}^{\text{SP}}}\right)$
    $r_{t+1}^{\text{SP}}, \boldsymbol{H}_{t+1}^{\text{SP}} \leftarrow \text{env}^{\text{SP}}\left(\boldsymbol{H}_t^{\text{SP}}, \boldsymbol{a}_t^{\text{SP}}\right)$
    $\mathcal{D}^{\text{SP}} \leftarrow \mathcal{D}^{\text{SP}} || \langle \boldsymbol{H}_t^{\text{SP}}, \boldsymbol{a}_t^{\text{SP}}, r_{t+1}^{\text{SP}}, \boldsymbol{H}_{t+1}^{\text{SP}}, \text{ID}^{\text{SP}} \rangle$
    // Cross-Play Data Collection
    $a_t^{1,\text{XP}} \sim \pi\left(a_t^{1,\text{XP}} | H_t^{1,\text{XP}}; \theta_{\text{ID}_1^{\text{XP}}}\right)$ and $a_t^{2,\text{XP}} \sim \pi\left(a_t^{2,\text{XP}} | H_t^{2,\text{XP}}; \theta_{\text{ID}_2^{\text{XP}}}\right)$
    $r_{t+1}^{\text{XP}}, \boldsymbol{H}_t^{\text{XP}} \leftarrow \text{env}^{\text{XP}}\left(\boldsymbol{H}_t^{\text{XP}}, \boldsymbol{a}_t^{\text{XP}}\right)$
    $\mathcal{D}^{\text{XP}} \leftarrow \mathcal{D}^{\text{XP}} || \langle \boldsymbol{H}_t^{\text{XP}}, \boldsymbol{a}_t^{\text{XP}}, r_{t+1}^{\text{XP}}, \boldsymbol{H}_{t+1}^{\text{XP}}, \text{ID}_1^{\text{XP}}, \text{ID}_2^{\text{XP}} \rangle$
    if $t \bmod t_{\text{update}} = 0$ **then**
      // Parameter Update
      $\mathcal{L}_{\Theta,\phi}(\mathcal{D}^{\text{SP}}, \mathcal{D}^{\text{XP}}) \leftarrow$ **COMPUTE_LOSS**$(\mathcal{D}^{\text{SP}}, \mathcal{D}^{\text{XP}}, \Theta, \phi, \bar{\phi})$
      for $\theta_i \in \Theta$ **do**
        $\theta_i \leftarrow$ **GRADIENT_DESCENT**$(\theta_i, \alpha, \nabla_{\theta_i} \mathcal{L}_{\Theta,\phi}(\mathcal{D}^{\text{SP}}, \mathcal{D}^{\text{XP}}))$
      end for
      $\phi \leftarrow$ **GRADIENT_DESCENT**$(\phi, \alpha, \nabla_{\theta_i} \mathcal{L}_{\Theta,\phi}(\mathcal{D}^{\text{SP}}, \mathcal{D}^{\text{XP}}))$
      $\bar{\phi} \leftarrow (1 - \bar{\alpha})\phi + \bar{\alpha}\phi$
      $\mathcal{D}^{\text{SP}} \leftarrow \{\}$
      $\mathcal{D}^{\text{XP}} \leftarrow \{\}$
    end if
    $t \leftarrow t + 1$
  end while
end for
Return: Θ

B.1 Cooperative Reaching

For Cooperative Reaching, we implement 11 heuristics as part of Π^{eval}. Each heuristic differs from others in terms of their way of selecting which reward-providing coordinates to move towards. Some heuristics also encourage teammates to follow the learner towards one of the existing reward-providing coordinates. The details of each heuristic used in Cooperative Reaching are provided below:

Algorithm 2 Loss Computation

Require:
Self-play and cross-play data, $\mathcal{D}^{\text{SP}}$ & $\mathcal{D}^{\text{XP}}$.
Population actor network parameters, Θ.
Centralised critic parameters, ϕ.
Target centralised critic parameters, $\bar{\phi}$

function COMPUTE_LOSS$(\mathcal{D}^{\text{SP}}, \mathcal{D}^{\text{XP}}, \Theta, \phi, \bar{\phi})$
  $t_{\text{start}} \leftarrow$ first time in the buffers $\mathcal{D}^{\text{SP}}, \mathcal{D}^{\text{XP}}$
  $t_{\text{end}} \leftarrow$ latest time in the buffers $\mathcal{D}^{\text{SP}}, \mathcal{D}^{\text{XP}}$
  $V_{\text{target}} \leftarrow V(\boldsymbol{H}^{\text{SP}}_{t_{\text{end}}+1}, \text{ID}^{\text{SP}}, \text{ID}^{\text{SP}}; \bar{\phi})$
  $\mathcal{L}^{\text{SP}}_{\phi} \leftarrow 0$ ▷ Compute Self-Play Critic Loss
  for $t = t_{\text{end}}$ to t_{start} **do**
    $V_{\text{pred}} \leftarrow V(\boldsymbol{H}^{\text{SP}}_{t}, \text{ID}^{\text{SP}}, \text{ID}^{\text{SP}}; \phi)$
    $V_{\text{target}} \leftarrow \begin{cases} r^{\text{SP}}_t, & \text{if episode terminates at } t \\ r^{\text{SP}}_t + \gamma V_{\text{target}}, & \text{otherwise.} \end{cases}$
    $\mathcal{L}^{\text{SP}}_{\phi} \leftarrow \mathcal{L}^{\text{SP}}_{\phi} + \frac{1}{2}(V_{\text{pred}} - V_{\text{target}})^2$
  end for
  $V_{\text{target}} \leftarrow V(\boldsymbol{H}^{\text{XP}}_{t_{\text{end}}+1}, \text{ID}^{\text{XP}}_1, \text{ID}^{\text{XP}}_2; \bar{\phi})$
  $\mathcal{L}^{\text{XP}}_{\phi} \leftarrow 0$ ▷ Compute Cross-Play Critic Loss
  for $t = t_{\text{end}}$ to t_{start} **do**
    $V_{\text{pred}} \leftarrow V(\boldsymbol{H}^{\text{XP}}_{t}, \text{ID}^{\text{XP}}_1, \text{ID}^{\text{XP}}_2; \phi)$
    $V_{\text{target}} \leftarrow \begin{cases} r^{\text{XP}}_t, & \text{if episode terminates at } t \\ r^{\text{XP}}_t + \gamma V_{\text{target}}, & \text{otherwise.} \end{cases}$
    $\mathcal{L}^{\text{XP}}_{\phi} \leftarrow \mathcal{L}^{\text{XP}}_{\phi} + \frac{1}{2}(V_{\text{pred}} - V_{\text{target}})^2$
  end for
  $V_{\text{bootstrap}} \leftarrow V(\boldsymbol{H}^{\text{SP}}_{t_{\text{end}}+1}, \text{ID}^{\text{SP}}, \text{ID}^{\text{SP}}; \phi)$
  $\mathcal{L}^{\text{SP}}_{\Theta} \leftarrow 0$ ▷ Compute Self-Play Actor Loss
  for $t = t_{\text{end}}$ to t_{start} **do**
    $M_{\text{baseline}} \leftarrow$ **TO_XP_MATRIX**$\big(\{V(\boldsymbol{H}^{\text{SP}}_{t}, i, j; \phi) | i, j \in 1, \ldots, N\}\big)$
    $V_{\text{bootstrap}} \leftarrow \begin{cases} r^{\text{SP}}_t, & \text{if episode terminates at } t \\ r^{\text{SP}}_t + \gamma V_{\text{bootstrap}}, & \text{otherwise.} \end{cases}$
    $M_{\text{pred}} \leftarrow M_{\text{baseline}}$
    $M_{\text{pred},\text{ID}^{\text{SP}},\text{ID}^{\text{SP}}} \leftarrow V_{\text{bootstrap}}$ ▷ Replace matrix element of interacting populations
    $\mathcal{L}^{\text{SP}}_{\Theta} \leftarrow \mathcal{L}^{\text{SP}}_{\Theta} - \log(\pi(a^{1,\text{SP}}_t | H^{1,\text{SP}}_t; \theta_{\text{ID}^{\text{SP}}})\pi(a^{2,\text{SP}}_t | H^{2,\text{SP}}_t; \theta_{\text{ID}^{\text{SP}}}))(\text{BRDiv}(M_{\text{pred}}) - \text{BRDiv}(M_{\text{baseline}}))$
  end for
  $V_{\text{bootstrap}} \leftarrow V(\boldsymbol{H}^{\text{XP}}_{t_{\text{end}}+1}, \text{ID}^{\text{XP}}_1, \text{ID}^{\text{XP}}_2; \phi)$
  $\mathcal{L}^{\text{XP}}_{\Theta} \leftarrow 0$ ▷ Compute Cross-Play Actor Loss
  for $t = t_{\text{end}}$ to t_{start} **do**
    $M_{\text{baseline}} \leftarrow$ **TO_XP_MATRIX**$\big(\{V(\boldsymbol{H}^{\text{XP}}_{t}, i, j; \phi) | i, j \in 1, \ldots, N\}\big)$
    $V_{\text{bootstrap}} \leftarrow \begin{cases} r^{\text{XP}}_t, & \text{if episode terminates at } t \\ r^{\text{XP}}_t + \gamma V_{\text{bootstrap}}, & \text{otherwise.} \end{cases}$
    $M_{\text{pred}} \leftarrow M_{\text{baseline}}$
    $M_{\text{pred},\text{ID}^{\text{XP}}_1,\text{ID}^{\text{XP}}_2} \leftarrow V_{\text{bootstrap}}$ ▷ Replace matrix element of interacting populations
    $\mathcal{L}^{\text{XP}}_{\Theta} \leftarrow \mathcal{L}^{\text{XP}}_{\Theta} - \log(\pi(a^{1,\text{XP}}_t | H^{1,\text{XP}}_t; \theta_{\text{ID}^{\text{XP}}_1})\pi(a^{2,\text{XP}}_t | H^{2,\text{XP}}_t; \theta_{\text{ID}^{\text{XP}}_2}))(\text{BRDiv}(M_{\text{pred}}) - \text{BDiv}(M_{\text{baseline}}))$
  end for
  Return: $\mathcal{L}^{\text{SP}}_{\phi} + \mathcal{L}^{\text{XP}}_{\phi} + \mathcal{L}^{\text{SP}}_{\Theta} + \mathcal{L}^{\text{XP}}_{\Theta}$
end function

- **Heuristic H01.** This heuristic selects the action that gets a teammate closer to the closest reward-providing coordinate.
- **Heuristic H02.** This heuristic selects the action that gets a teammate closer to the furthest reward-providing coordinate from its initial position at the beginning of the episode.
- **Heuristic H03.** A teammate under this heuristic moves towards the closest optimal reward-providing coordinate.
- **Heuristic H04.** H4 moves an agent towards the furthest optimal reward-providing coordinate from a teammate's initial location in an episode.
- **Heuristic H05.** Same as H4, except that the learner only considers the suboptimal reward-providing coordinates instead of the optimal ones.
- **Heuristic H06.** Same as H5, except the teammate goes towards the closest suboptimal reward-providing coordinate.
- **Heuristic H07.** At the beginning of the episode, agents under this heuristic randomly select a reward-providing coordinate and move towards it.
- **Heuristic H08.** This heuristic moves a teammate towards the reward-providing coordinate closest to its counterpart agent's location.
- **Heuristic H09.** Same as H8, but only optimal reward-providing coordinates are considered as the teammate's destination.
- **Heuristic H10.** This heuristic moves the teammate towards its counterpart agent's location.
- **Heuristic H11.** This heuristic always randomly selects an action from the teammate's possible actions.

B.2 LBF

Like Cooperative Reaching, we create diverse teammate heuristics requiring a learner to adapt their policies to achieve optimal collaboration. The ten heuristics used for LBF generally correspond to different ways of deciding the ordering to collect objects scattered in LBF's grid world. Details of each heuristic are provided below:

- **Heuristic H01.** The teammate attempts to collect whichever object is closest to its current location.
- **Heuristic H02.** At each timestep, the teammate computes the midpoint between the learner and its location. This teammate then attempts to collect whichever object is closest to this midpoint.
- **Heuristics H03-H08.** For heuristics H03 to H08, we assign a distinct random index from $\{1, 2, 3\}$ to each object at the beginning of each episode. Heuristics H03-H08 then collect the objects according to one of the 6 distinct possible orderings of the object index.
- **Heuristic H09.** The teammate always attempts to collect food closest to the learner's location.
- **Heuristic H10.** At the beginning of each episode, H10 identifies the object furthest from its location and attempts to collect it. Each time its target item is collected, H10 then attempts to collect the remaining object at the furthest distance from the current location of the controlled teammate.

B.3 Simple Cooking

As the layout of our Simple Cooking is a ring, we consider two movement directions around the ring: clockwise and anti-clockwise. Each heuristic agent has a goal, such as "seek and process the nearest food." Once their goal has been completed, the heuristic agent finds a counter without any tools on it and stands on the empty space closest to the said counter.

- **Heuristic H1:** Seeks the nearest food in the clockwise direction, picks it up, and continues to move clockwise to the appropriate food processing counter, where it processes the food.
- **Heuristic H2:** Seeks the nearest food in the anti-clockwise direction, picks it up, and continues to move anti-clockwise to the appropriate food processing counter, where it processes the food.
- **Heuristic H3:** Takes the shortest path to the nearest food item, picks it up, and continues to take the shortest path to the appropriate food processing counter, where it processes the food.
- **Heuristic H4:** Seeks the furthest away food in the clockwise direction, picks it up, and continues to move clockwise to the appropriate food processing counter, where it processes the food.
- **Heuristic H5:** Seeks the furthest away food in the anti-clockwise direction, picks it up, and continues to move anti-clockwise to the appropriate food processing counter, where it processes the food.
- **Heuristic H6:** Same as Heuristic H3, except 25% of the time, the agent takes a uniform random action.
- **Heuristic H7:** This heuristic seeks the nearest processed food in the clockwise direction. It then picks up the processed food and checks whether the plate is on one of the counter or not. If the plate is on one of the counters, the agent moves clockwise to the plate in order to put the processed food. Otherwise, the agent goes towards the serving counter to place the food. Once there are no processed food to move, this agent moves clockwise to stand in front of an outer counter without any items on top.
- **Heuristic H8:** This heuristic is similar to H7 except that agents under this heuristic always move in an anti-clockwise direction.
- **Heuristic H9:** This heuristic is similar to heuristics H7 and H8 except that agents under this heuristic always decide its clockwise or anti-clockwise movement based on the shortest distance between its target object or location.
- **Heuristic 10:** This heuristic is similar to heuristics H7 except that agents under this heuristic will immediately put the processed food on the serving counter.
- **Heuristic H11:** This heuristic is similar to heuristics H8 except that agents under this heuristic always put the retrieved processed food on the service counter.
- **Heuristic H12:** This heuristic is similar to heuristics H9 except that agents under this heuristic will immediately put retrieved processed food on the service counter.

C Experiment Hyperparameters

This section provides details of the hyperparameters and neural network architectures used in our teammate generation experiments.

- When optimising BRDiv, we run 32 parallel threads to collect self-play experiences during training. Meanwhile, the remaining methods use 160 parallel threads to gather self-play experiences used during their teammate generation process.

- Aside from the threads used to gather self-play experiences, we use 128 parallel environments to collect cross-play experiences when optimising BRDiv.
- All evaluated methods have their actor and critic networks updated every 8 timesteps.
- γ is set to 0.99.
- The generated actor networks alongside the critic network are trained using Adam optimiser (Kingma & Ba, 2014) with a learning rate of 10^{-4}.
- We clip the gradients of the model so that it always lies between -1 and 1.
- Each actor network corresponding to policies in the generated Π^{train} and $\text{BR}(\Pi^{\text{train}})$ are implemented as multilayer perceptrons. The size of these networks for each environment is detailed below:
  - **Cooperative Reaching.** The model comprises of four hidden layers with 128, 256, 256, and 128 neurons respectively.
  - **LBF.** The model comprises of two hidden layers, each consisting of 128 neurons.
  - **Simple Cooking.** Our network for this environment has two hidden layers with each layer having 256 neurons.
- We also associated different weights to the optimised loss functions when generating Π^{train} using our proposed method, TrajeDi, Any-Play and the independent baseline. The weights of each loss function optimised by these methods are detailed below:
  - For all methods, the critic loss function for SP data is also set to 1.0. Meanwhile, BRDiv assigns a weight of 1.0 to the loss function that minimizes the critic loss function following cross-play interaction data.
  - For BRDiv, the weights of the losses optimised for training the actor networks is set to 25.
  - The Jensen-Shannon Divergence term maximised by TrajeDi is given a weight of 10^{-3}. We arrive at this value after finding the largest possible weight from $\{10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}\}$ that still ensures every policy in Π^{train} to achieve optimal performances in the environment when collaborating with its associated best response policy.
  - The weights of Any-Play's intrinsic reward to maximise diversity between populations is tuned in the same way as how we tuned the Jensen-Shannon Divergence weights for TrajeDi. This results in the intrinsic reward weights of 10^{-2}, 10^{-3}, and 10^{-3} for Cooperative Reaching, LBF, and Simple Cooking.
  - The classifier Any-Play uses to compute the intrinsic rewards uses the same architecture of other methods' critic networks. The term associated with the supervised learning loss utilised to train this classifier is also set to 1.
  - For TrajeDi, Any-Play, and the independent baseline, the weights associated with the term that maximises the self-play performance between a policy in Π^{train} and their associated best response policies is set to 1.