Self-adaptive PSRO: Towards an Automatic Population-based Game Solver

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Abstract
Policy-Space Response Oracles (PSRO) as a general algorithmic framework has achieved state-of-the-art performance in learning equilibrium policies of two-player zero-sum games. However, the hand-crafted hyperparameter value selection in most of the existing works requires extensive domain knowledge, forming the main barrier to applying PSRO to different games. In this work, we make the first attempt to investigate the possibility of self-adaptively determining the optimal hyperparameter values in the PSRO framework. Our contributions are three-fold: (1) Using several hyperparameters, we propose a parametric PSRO that unifies the gradient descent ascent (GDA) and different PSRO variants. (2) We propose the self-adaptive PSRO (SPSRO) by casting the hyperparameter value selection of the parametric PSRO as a hyperparameter optimization (HPO) problem where our objective is to learn an HPO policy that can self-adaptively determine the optimal hyperparameter values during the running of the parametric PSRO. (3) To overcome the poor performance of online HPO methods, we propose a novel offline HPO approach to optimize the HPO policy based on the Transformer architecture. Experiments on various two-player zero-sum games demonstrate the superiority of SPSRO over different baselines.

1 Introduction
Policy-Space Response Oracles (PSRO) [Lanctot et al., 2017] since proposed has been the mainstream algorithmic framework for solving two-player zero-sum games. At each epoch, PSRO constructs a meta-game by simulating outcomes of all match-ups of policies of all players and computes the meta-strategies for all players via a meta-solver. It then trains new policies for each player against the opponent’s meta-strategy through an oracle and appends the new policies to the player’s policy space. The two components – meta-solver and oracle – determine the nature of PSRO and various PSRO variants have been proposed [Balduzzi et al., 2019; Muller et al., 2020; Marris et al., 2021]. Despite the advancements, determining the hyperparameter values in PSRO is non-trivial [Smith et al., 2021] and typically involves extensive domain knowledge, which impedes it from broader real-world applications.

Precisely, one needs to determine the meta-solver and the best response (BR) oracle when instantiating PSRO. On one hand, existing works have suggested various meta-solvers such as uniform [Heinrich and Silver, 2016], Nash equilibrium [Lanctot et al., 2017], α-Rank [Muller et al., 2020], and correlated equilibrium [Marris et al., 2021]. However, we observe that none of the meta-solvers can consistently beat all the others in terms of learning performance during game solving. On the other hand, the BR policies of a player are typically obtained via a deep reinforcement learning (RL) oracle, e.g., DQN [Mnih et al., 2015], which involves the initialization and the number of updates of the BR policies. Unfortunately, the determination of these hyperparameter values in most of the existing works is often domain-specific (e.g., poker, soccer). Therefore, an important question is: Can we automatically determine the optimal hyperparameter values in PSRO?

In this work, we make the first attempt to answer this question. Specifically, we first propose a parametric PSRO (PPSRO) by introducing two types of hyperparameters: i) game-free hyperparameters are the weights of different meta-solvers considered during game solving, and ii) game-based hyperparameters are the initialization and the number of updates of a player’s BR policies. PPSRO provides a general framework to unify the gradient descent ascent (GDA) [Fiez and Ratliff, 2021] and various PSRO variants [Ho et al., 1998; Balduzzi et al., 2019; Muller et al., 2020; Marris et al., 2021]. Then, a natural problem is how to determine the hyperparameter values of PPSRO. To solve this problem, we propose a novel framework, self-adaptive PSRO (SPSRO), by casting the hyperparameter value selection of PPSRO as a hyperparameter optimization (HPO) problem where our objective is to learn an HPO policy that can self-adaptively select the optimal hyperparameter values of PPSRO during game solving. A straightforward method to optimize the HPO policy is to use online approaches such as Optuna [Akiba et al., 2019]. Unfortunately, online HPO methods only use online generated data (past epochs of SPSRO), typically constraining the training objectives to be cheaply computable [Chen et al., 2022] and the performance could be poor. To overcome these limitations, we
propose an offline HPO approach to optimize the HPO policy based on the Transformer architecture [Vaswani et al., 2017; Chen et al., 2021]. Specifically, we formulate the HPO policy optimization as a sequence modeling problem where a Transformer model is trained by using an offline dataset and then used to predict the hyperparameter values conditioned on past epochs of SPSRO. Intuitively, a well-trained HPO policy has the potential to transfer to different games, reducing the effort needed for researchers to conduct the costly hyperparameter tuning when applying PSRO to various games.

In summary, the contributions of this work are three-fold: (1) By introducing several hyperparameters, we propose a parametric version of PSRO (PPSRO) which unifies GDA and various PSRO variants. (2) We propose a novel framework, self-adaptive PSRO (SPSRO), by formulating an optimization problem where our objective is to learn an HPO policy that can self-adaptively determine the optimal hyperparameter values of PPSRO. (3) To overcome the poor performance of classic online HPO methods, we propose an offline HPO approach to optimize the HPO policy based on the Transformer architecture. We evaluate the effectiveness of our approach through extensive experiments on a set of two-player zero-sum games, and the results demonstrate that SPSRO with Transformer performs significantly better than different baselines.

2 Related Works

PSRO [Lanctot et al., 2017] generalizes the double oracle algorithm [McMahan et al., 2003] and unifies various multi-agent learning methods including the fictitious play (FP) [Robinson, 1951; Brown, 1951], neural fictitious self-play (NFSP) [Heinrich and Silver, 2016] (an extension of FP in the context of deep RL), iterated best response (IBR) [Ho et al., 1998], and independent reinforcement learning (InRL) [Matignon et al., 2012]. Recently, many works have been done toward improving PSRO, including the scalability [McAleer et al., 2020; Smith et al., 2021], diversity of BRs [Perez-Nieves et al., 2021; Liu et al., 2021], the introduction of novel meta-solvers, e.g., α-Rank [Muller et al., 2020], correlated equilibrium [Marris et al., 2021], and neural meta-solver [Feng et al., 2021], and application to mean-field games [Muller et al., 2022]. Moreover, the challenging strategy exploration problem has also been extensively investigated [Wellman, 2006; Schwartzman and Wellman, 2009a; Schwartzman and Wellman, 2009b; Jordan et al., 2010; Wang et al., 2022]. Despite the advancements, a critical observation we obtained is that given a set of meta-solvers, none of them can consistently beat (dominate) all the others in terms of learning performance during game solving (in the sense that we just evaluate PSRO as an online algorithm). On the other hand, the BRs of a player are typically obtained via a deep RL oracle such as DQN [Mnih et al., 2015], where the hyperparameters (e.g., the initialization and the number of updates) are often domain-specific (e.g., poker, soccer) and most of the existing works manually select the hyperparameter values based on domain knowledge. In this work, we develop a novel framework to self-adaptively determine the optimal hyperparameter values in PSRO, which can be transferred to different games without fine-tuning.

Another line of related work is hyperparameter optimization (HPO). Existing works on HPO can be roughly categorized into online and offline HPO. The classic online HPO methods include Bayesian optimization [Snoek et al., 2012] and its variants [Krause and Ong, 2011; Bardenet et al., 2013; Swersky et al., 2013; Feurer et al., 2015; Volpp et al., 2019; Wistuba and Grabocka, 2020; Rothfuss et al., 2021], and recurrent neural networks (RNNs) [Duan et al., 2016; Wang et al., 2016; Chen et al., 2017]. However, online HPO methods only use online generated data, typically constraining the training objectives to be cheaply computable and the performance could be poor. Our work is closely related to [Chen et al., 2022] which proposes the first offline Transformer-based HPO method. Nevertheless, it is non-trivial to optimize the HPO policy as it involves several critical challenges such as how to generate an offline dataset for training. To our knowledge, this work is the first attempt to explore and develop a self-adaptive hyperparameter value selector in game theory.

3 Preliminaries

In this section, we first present the game definition and then the procedure of the PSRO algorithm.

3.1 Games

Consider a two-player zero-sum game represented by a tuple \( G = (N, S, A, p, \{r^i\}_{i \in N}, T) \), where players are indexed by \( N = \{1, 2\} \). Let \( N = |N| = 2 \), and \( A \) denote the players’ state and action spaces, respectively. \( T = \{0, 1, \ldots, T\} \) is time index set. At \( t \in T \), player \( i \) in state \( s_i^t \in S \) takes an action \( a_i^t \in A_i \) and then changes to new state \( s_i^{t+1} \sim p(\cdot|s_i^t, a_i^t) \) and receives a reward \( r_i^t(s_i^t, a_i^t) \), where \( s_i^0 = s_i^t \in \mathbb{N} \) and \( a_i^t = (a_i^t)^{i \in N} \) are respectively joint state and joint action of all players, \( p : S^N \times A^N \to \Delta(S)^i \) is the transition function and \( r^t : S^N \times A^N \to \mathbb{R} \) is the reward function with \( \sum_{i \in N} r^t(s_i, a_i) = 0 \). Let \( \pi_i : S \to \Delta(A_i) \) denote the player \( i \)’s policy (strategy)\(^1\) with \( \pi_i \in \Pi_i ^\ast \) where \( \Pi_i \) is the policy space. Given the joint policy of all players \( \pi = (\pi_i)^i_{i \in N} \in \Pi = \times_{i \in N} \Pi_i \), each player \( i \) aims to maximize its own value function \( V_i(\pi; s_0) = \mathbb{E} \sum_{t=0}^{\infty} r_i^t(s_i, a_i) | a_i \sim \pi, s_{t+1} \sim p \) where \( s_0 \) is the players’ initial states.

A mixed strategy \( \sigma^i \in \Delta(\Pi_i) \) is called a meta-strategy which is the probability distribution over the player \( i \)’s policy space \( \Pi_i \). More precisely, suppose that there are \( c \geq 1 \) policies in player \( i \)’s policy space, then the meta-strategy of \( i \) is \( \sigma^i = (\sigma^{i,1}, \ldots, \sigma^{i,c}) \) with \( \sigma^{i,j} \geq 0 \) and \( \sum_j \sigma^{i,j} = 1 \).

Accordingly, \( \sigma = (\sigma^i)^i_{i \in N} \in \Delta(\Pi) \) is the joint meta-strategy of all players. Given the joint meta-strategy of all players except \( i \), \( \sigma^{-i} \), the expected payoff to player \( i \)’s policy \( \pi_i \in \Pi_i ^\ast \) is given by \( R_i^\pi(\sigma^{-i}) = \sum_{\pi^{-i} \in \Pi^{-i}} (\pi^{-i}) V_i^\pi(\pi^{-i}) \) and the set of best responses (BRs) of player \( i \) is defined as \( BR_i(\sigma^{-i}) = \arg \max_{\pi^{-i} \in \Pi^{-i}} R_i^\pi(\sigma^{-i}) \). The quality of \( \sigma \) can be measured by the NashConv [Lanctot et al., 2017]. For player \( i \in N \), the NashConv is defined as \( R_i^\pi(\sigma) = \Delta(\mathcal{X}) \) denotes the probability distribution over the space \( \mathcal{X} \).

\(^1\)We interchangeably use policy and strategy in this work.

\(^2\)In principle \( \Pi_i ^\ast \) could be an infinite set. However, \( \Pi_i ^\ast \) is typically iteratively expanded by learning algorithms such as PSRO and hence, is considered finite in this work.
For the three meta-solvers, none of them can consistently beat (dominate) all the others in terms of NashConv during the PSRO procedure. For instance, at the early stage of the PSRO procedure, Uniform performs better than the other two meta-solvers in terms of NashConv. However, it only converges to a high NashConv value, which is also observed in previous works [Muller et al., 2020]. (2) By switching from one meta-solver to another during the PSRO procedure, we can achieve better learning performance in terms of NashConv. Moreover, the comparison between the two cases: “α-Rank → PRD” and “PRD → α-Rank”, again verifies the previously observed fact that none of the meta-solvers can consistently beat all the others in terms of NashConv during the PSRO procedure.

The above observations motivate us to think about a natural question: How to determine the meta-solvers during the PSRO procedure such that we can obtain better learning performance? Note that the examples in Figure 1 are NFGs. For extensive-form games (EFGs), in addition to the meta-solver, the hyperparameters also include the initialization of a BR policy \( \pi^1_{BR} \) and the number of updates \( K \) for training the BR policy. Most of the existing works determine the values of these hyperparameters by hand-crafted tuning, which typically requires extensive domain knowledge.

Thus, a critical problem to be addressed is: how to automatically determine the optimal hyperparameter values during the PSRO running? Specifically, at each epoch, we need to i) choose one or multiple meta-solver(s), ii) determine how to initialize the new BR policies, e.g., random initialization, copy from one of the previous BRs, or mix, and iii) determine the number of updates \( K \) of the new BR policy of each player. In this work, we make the first attempt to develop a novel framework that can self-adaptively determine the optimal hyperparameter values during the PSRO running.

4 Motivating Example

In this section, we provide some examples to better illustrate the motivation of this work. Consider a two-player zero-sum normal-form game (NFG) of size \(|A_1| \times |A_2|\). Let \( \mathcal{M} \) denote the set of meta-solvers of interest. In this example (as well as this work), we consider the three most commonly used meta-solvers: Uniform [Heinrich and Silver, 2016], \( \alpha \)-Rank [Muller et al., 2020], and PRD [Lanctot et al., 2017]. We conduct two types of experiments: i) consistently using a single meta-solver during the PSRO procedure, and ii) switching the meta-solver from one to another at some intermediate iteration of the PSRO. The results are shown in Figure 1.

![Figure 1: NashConv of different PSRO runs.](image)

From the results, we can obtain the following observations. (1) For the three meta-solvers, none of them can consistently

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1Note that throughout this work, \( e \) always represents the index of PSRO epoch, neither the power of \( e \) nor the Euler’s number.

5 Self-adaptive PSRO

In this section, we establish the Self-adaptive PSRO (SPSRO) through two steps: (1) We parameterize the PSRO algorithm (PPSRO) by introducing several hyperparameters. (2) We cast the hyperparameter value selection of PPSRO as a hyperparameter optimization (HPO) problem where our objective is to learn an HPO policy that will self-adaptively determine the optimal hyperparameter values of PPSRO.

5.1 Parametric PSRO

First, inspired by the observations in the previous section, in this work, instead of considering a single meta-solver as most of the existing works, we use the meta-solver set \( \mathcal{M}^\alpha \) with \( m \) different meta-solvers and associate it with a vector \( \alpha = (\alpha_1, \ldots, \alpha_m) \) specifying the weight of each meta-solver. Intuitively, by combining multiple meta-solvers, we could obtain better performance. As \( \alpha \) is only dependent on

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1These observations are different from [Wang et al., 2022] which regards the strategy exploration and its evaluation as two orthogonal components. For example, one can use PRD to guide the BR policies computation but use \( \alpha \)-Rank to compute the meta-distribution for decision-making after the new BR policies of players are added to their respective policy spaces. However, it is worth noting that our observations do not cause inconsistency with [Wang et al., 2022] as we just evaluate PSRO as an online algorithm.
the meta-game payoff tensor $M$ regardless of the underlying games (normal-form or extensive-form games), we refer to the weights in it as game-free hyperparameters.

Second, we introduce a parametric BR oracle $O^i(\sigma; \beta, K)$ where the hyperparameters include$: (1)$ the initialization parameter $\beta \in [0, 1]$ which determines the initialization of the new BR policy of player $i$ by mixing the BR policy obtained in the last epoch with a randomly initialized policy $\pi_{1, \text{random}}$, and $(2)$ the number $K$ which determines the number of updates needed for training the new BR policy. Formally, at each epoch $e$, we initialize player $i$’s BR policy as $\pi_{1, \text{BR}, e} = \beta \pi_{1, \text{BR}, e-1} + (1 - \beta) \pi_{1, \text{random}}$, and then update this BR policy $\pi_{1, \text{BR}, e}$ for $K$ steps. After that, the trained BR policy $\pi_{1, \text{BR}, e}$ is added to player $i$’s policy space $\Pi^i$. As $\beta$ and $K$ are highly dependent on the underlying games (e.g., poker, soccer), we refer to them as game-based hyperparameters.

By specifying $\alpha$, $\beta$ and $K$, we can obtain GDA and various PSRO variants (Table 1). For example, GDA can be instantiated as follows. Suppose that $M_b$ is the meta-solver “Last-One”, then we set $\sigma_0 = 1$ and $\alpha_{i \neq b} = 0$, which implies that the meta-strategy of player $i$ is $\sigma_b = (\sigma_b^1 = 0, \ldots, \sigma_b^{|K| - 1} = 1)$ at epoch $e$. Then, player $i$ initializes the BR policy $\pi_{1, \text{BR}, e}$ with $\beta = 1$ and trains $\pi_{1, \text{BR}, e}$ with $K = 1$ update.

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>$\mathcal{M}^\alpha$</th>
<th>$O^i(\sigma; \beta, K)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>GDA</td>
<td>Last-One</td>
<td>$\beta = 1 \land K = 1$</td>
</tr>
<tr>
<td>InRL</td>
<td>Last-One</td>
<td>$\beta = 1 \land K = \bar{K}$</td>
</tr>
<tr>
<td>PSROP</td>
<td>Penultimate</td>
<td>$\beta \in [0, 1] \land K = \bar{K}$</td>
</tr>
<tr>
<td>PSROU</td>
<td>Uniform</td>
<td>$\beta \in [0, 1] \land K = \bar{K}$</td>
</tr>
<tr>
<td>PSRON</td>
<td>Nash</td>
<td>$\beta \in [0, 1] \land K = \bar{K}$</td>
</tr>
<tr>
<td>PSRON</td>
<td>Rectified Nash</td>
<td>$\beta \in [0, 1] \land K = \bar{K}$</td>
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<tr>
<td>PSRO$_{\alpha}$-Rank</td>
<td>$\alpha$-Rank</td>
<td>$\beta \in [0, 1] \land K = \bar{K}$</td>
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<td>PSRO$_{\alpha}$-Centered Rank</td>
<td>$\alpha$-Rank</td>
<td>$\beta \in [0, 1] \land K = \bar{K}$</td>
</tr>
</tbody>
</table>

Table 1: Specifications of PSRO variants. $\bar{K}$ is the number of updates needed to obtain a converged BR policy. The references for these methods: GDA [Fiez and Ratliff, 2021], InRL [Matignon et al., 2012], PSROP [Ho et al., 1998], PSROU [Heinrich and Silver, 2016], PSRON [Lanctot et al., 2017], PSRO$_{\alpha}$-Rank [Balduzzi et al., 2019], PSRO$_{\alpha}$-Centered Rank [Muller et al., 2020], PSRO$_{\alpha}$-Centered Rank [Marris et al., 2021].

5.2 HPO Policy Optimization

With the PPSRO introduced in the previous section, a natural problem is how to determine the values of $\alpha$, $\beta$, and $K$ in PPSRO. To address this problem, we propose a novel algorithmic framework, Self-adaptive PSRO (SPSRO), which is shown in Figure 2 and Algorithm 1. In the following, we first present the overall procedure of SPSRO, then define the performance metric of a given selection of hyperparameter values, and finally formalize the hyperparameter optimization (HPO) problem where our objective is to learn an HPO policy that will self-adaptively select the optimal hyperparameter values of PPSRO during game solving.

Let $\tau \in \Gamma$ denote an HPO policy where $\Gamma$ is the policy space. Let $u^e = (\alpha^e, \beta^e, K^e) \in \mathcal{U}$ denote the hyperparameter values selected according to the HPO policy $\tau$ at each epoch $e \geq 1$ of SPSRO, where $\mathcal{U}$ is the admissible set of the hyperparameter values. That is, we have $u^e \sim \tau$. We run one epoch of SPSRO as follows. (1) Compute the payoff tensor $M$ through game simulation (Line 3). (2) Compute the final joint meta-strategy $\sigma^e$ (Line 4). (3) Expand each player’s policy space (Line 5). Specifically, for each player $i$, we initialize the BR policy as $\pi_{1, \text{BR}, e} = \beta \pi_{1, \text{BR}, e-1} + (1 - \beta) \pi_{1, \text{random}}$, and then train the BR policy $\pi_{1, \text{BR}, e}$ for $K^e$ updates and add it to player $i$’s policy space $\Pi^i = \Pi^i \cup \{\pi_{1, \text{BR}, e}\}$. (4) Compute the performance metric $y^e(u^e)$ of the current selection (Line 6). (5) Select new hyperparameter values $u^{e+1}$ according to $\tau$ (Line 7).

![Figure 2: Illustration of Self-adaptive Policy-Space Response Ora-cles (SPSRO). PSRO and PPSRO are two special cases of SPSRO. Illustration inspired by [Muller et al., 2020].](image)

Algorithm 1 SPSRO

1. Initialize $\Pi^i$ with random policies, $\forall i \in \mathcal{N}, e \leftarrow 1$, select initial hyperparameter values $u^1 = (\alpha^1, \beta^1, K^1), \tau \in \Gamma$.
2. for epoch $e \in \{1, 2, 3, \ldots\}$ do
3. Update payoff tensor $M$ via game simulation
4. Compute $\sigma^e$ using $\mathcal{M}$ and $\alpha^e$: $\sigma^e = \sum_{b=1}^{m} \alpha_b \sigma_b^e$
5. Expand policy spaces $O^e: \Pi^i \leftarrow \Pi^i \cup O^e(\sigma^e; \beta^e, K^e)$
6. Compute the performance metric $y^e(u^e)$
7. Select new hyperparameter values $u^{e+1} \sim \tau$
8. end for

Given a selection of the hyperparameter values $u^e$, we define its performance metric as $y^e(u^e) = \frac{R(\sigma^e)}{R(\tau)} + h\|e\|_\tau$, where $h\|e\|$ is the run-time of BR training at the $e$-th epoch. Roughly speaking, it consists of two parts: the NashConv of all players and the BR training effort, which implies that using larger $K^e$ could obtain lower NashConv $R(\sigma^e)$ from the long-run standpoint but at the cost of longer BR training time $h\|e\|$, and using smaller $K^e$ could shorten the BR training time while at the cost of higher NashConv $R(\sigma^e)$.

Given the performance metric, our objective is to learn an HPO policy $\tau$ by solving the following HPO problem: $\forall e \geq 1,\arg\min_{\tau \in \Gamma} y^e(u^e \sim \tau)$.

(1)
6 A Novel Offline HPO Algorithm

The most straightforward method to optimize the HPO policy is to employ the classic HPO methods such as Bayesian optimization [Snoek et al., 2012]. However, most HPO methods typically predict hyperparameter values based on online generated data (history of past epochs in our work), which could be less efficient in exploring the space of the hyperparameter values, and thus, the performance could be poor. To overcome the limitations of online HPO, we propose a novel offline HPO method to optimize the HPO policy, which possesses the potential to transfer to different games without fine-tuning.

6.1 HPO as Sequence Modeling

As presented in Algorithm 1, selecting the hyperparameter values in SPSRO can be naturally regarded as a sequence modeling problem where we model the probability of the next token \( x^e \) conditioned on all prior tokens: \( P_\theta(x^e|x^{<e}) \), similar to the decoder-only sequence models [Zhao et al., 2023; Touvron et al., 2023]. Specifically, we consider the sequence of hyperparameter values up to \( e \)-th epoch:

\[
\mathcal{H}^e = (\cdots, \alpha_1^e, \cdots, \alpha_m^e, \beta^e, K^e, y^e)
\]  

(2)

Figure 3 presents the overview of the architecture.

\[
\begin{align*}
&\alpha_1^e \quad \alpha_2^e \quad \cdots \quad \beta^e \quad K^e \quad y^e \\
&\bar{u^e} \\
&\alpha_1^e \quad \cdots \quad \alpha_m^e \quad \beta^e \quad K^e
\end{align*}
\]

Figure 3: HPO based on Transformer. At each epoch, the Transformer model predicts parameter values in an autoregressive manner using a causal self-attention mask, i.e., each predicted parameter value will be fed into the model to generate the next parameter value.

6.2 Tokenization

We convert each element in Eq. (2) into a single token. The idea is to normalize and discretize each element such that it falls into one of \( Q \) bins each with size 1. \( Q \) is referred to as the quantization level. Specifically, we have:

\[
\bar{x}^e = \text{int}[x^e_{\text{norm}} \cdot Q],
\]

where \( x^e_{\text{norm}} = (x^e - x_{\text{min}})/(x_{\text{max}} - x_{\text{min}}) \). \( x_{\text{min}} \) and \( x_{\text{max}} \) are determined by the space \( \mathcal{U} \) and the range of \( y^e \) is determined by observed values in the offline dataset (introduced in the next subsection) or the underlying games (e.g., normal-form and extensive-form). After tokenization, we have:

\[
\bar{\mathcal{H}}^e = (\cdots, \bar{\alpha}_1^e, \cdots, \bar{\alpha}_m^e, \bar{\beta}^e, \bar{K}^e, \bar{y}^e).
\]  

(4)

6.3 Training Dataset

To train the Transformer model \( \theta \), one of the critical steps is to generate the offline dataset, which is non-trivial due to the computational complexity of running SPSRO. Specifically, to generate a dataset \( \mathcal{D} \) consisting of \( |\mathcal{D}| \) sequences of Eq. (2) or Eq. (4), we need to run the SPSRO for \( |\mathcal{D}| \) times. However, it is well-known that running PSRO can be computationally difficult in complex games. One of the main difficulties is that solving the meta-game using \( \alpha \)-Rank could be NP-hard [Yang et al., 2020] and as it requires enumerating all the joint strategies to construct the response graph [Omidshafiei et al., 2019], it is time-consuming as the progress of the PSRO procedure. To more efficiently generate the dataset, we use a simple pruning technique to constrain the size of the support set of the meta-strategy when using \( \alpha \)-Rank to solve the meta-game.

Let \( C \) denote the maximum size of the support set of the meta-strategy. At the first \( C \) epochs, we follow the standard PSRO_{\alpha-Rank}. After that, at each epoch \( e > C \), we construct the meta-game of size \((C + 1) \times (C + 1)\) where a new BR is obtained by deep RL algorithms. Next, we compute the meta-distribution by solving the meta-game via \( \alpha \)-Rank. Let \( \pi_{\text{min}} \) denote the policy with the minimum probability in the meta-distribution. Then, we get the final meta-strategy by setting \( \pi(\pi_{\text{min}}) = 0 \) and normalizing the resulting distribution.

During the dataset generation, we employ the widely used tool, Optuna [Akiba et al., 2019] (not the target HPO policy \( \tau \)), to determine the value of \( u^e \). Using the terminology of offline RL [Levine et al., 2020; Chen et al., 2021], Optuna is a behavior policy to generate the offline training dataset (see Appendix B for the code of Optuna showing how to generate the dataset). Furthermore, we distinguish between normal-form games (NFGs) and extensive-form games (EFGs) when generating the dataset. The primary reason is that the parameters of interest are different. In EFGs, in addition to the weights of different meta-solvers \( \alpha \), Eq. (2) also includes the parameters related to the BR oracle, \( \beta \) and \( K \). Therefore, the transformer model trained on the NFG dataset cannot be directly applied to EFGs. In addition, generating the NFG dataset is relatively easier as the computational difficulty mainly resulted from the meta-game solving using \( \alpha \)-Rank, which can be effectively addressed by the previously proposed pruning technique. For the EFG dataset, obtaining the BR policies requires extra computational overhead as the BR policies are typically approximated via deep RL algorithms such as DQN [Mnih et al., 2015].

6.4 Loss Function and Inference

Given the dataset \( \mathcal{D} \), we train the Transformer model \( \theta \) by maximizing the log-likelihood for each sequence \( \bar{\mathcal{H}}^e \sim \mathcal{D} \):

\[
\mathcal{L}(\theta; \bar{\mathcal{H}}^e) = \sum_{n=1}^{\bar{\epsilon}(m+3)} \log P_\theta(\bar{\mathcal{H}}^n|\bar{\mathcal{H}}^{1:n-1}),
\]

where \( \bar{\epsilon} \) is the maximum number of epochs, \( \bar{\mathcal{H}}^n \) is the \( n \)-th token in Eq. (4), and \( \bar{\mathcal{H}}^{1:n-1} \) is all tokens up to the \((n-1)\)-th token in Eq. (4). After training, we can apply the Transformer \( \theta \) to a given game to predict the value of \( u^e \). Specifically, we reverse the tokenization to obtain the token distribution:

\[
p_\theta(x^e|\bar{x}) = \frac{Q \cdot P_\theta(\bar{x})}{(x_{\text{max}} - x_{\text{min}})}.
\]

(6)

Then, we can sample \( u^e \) from the model’s prior distribution and thus, define the HPO policy as follows:

\[
\tau(u^e|\mathcal{H}^{e-1}) = \prod_{b=1}^{m} p_\theta(\alpha_b^e|\mathcal{H}^{e-1}, \alpha_1^e, \cdots, \alpha_{b-1}^e) \\
\times p_\theta(\beta^e|\mathcal{H}^{e-1}, \{\alpha_b^e\}_{1 \leq b \leq m}) \\
\times p_\theta(K^e|\mathcal{H}^{e-1}, \{\alpha_b^e\}_{1 \leq b \leq m}, \beta^e).
\]

(7)
That is, at epoch \( e \), \( \tau \) predicts each parameter value in \( u_e \) conditioned on: i) the sequence of past epochs \( \mathcal{H}^{e-1} \), and ii) the values of the preceding predicted parameters.

7 Experiments
In this section, we evaluate the effectiveness of SPSRO.

7.1 Experimental Setup
All experiments are performed on a machine with a 24-core 3.2GHz Intel i9-12900K CPU and an NVIDIA RTX 3060 GPU, and the results are averaged over 30 independent runs.

Games. We consider the following games. (1) Normal-form games (NFGs) of size \(|A_1| \times |A_2|\). The payoff matrices are randomly sampled from the range \([-1, 1]\). The set of size is \(\{150 \times 150, 200 \times 200, 250 \times 250, 100 \times 200, 150 \times 300\}\). (2) Extensive-form games (EFGs): Leduc, Goofspiel, Liar’s Dice, Negotiation, and Tic-Tac-Toe, which are implemented in OpenSpiel [Lanctot et al., 2019].

Methods. (1) GDA [Fiez and Ratliff, 2021]. At each epoch, a player only best responds to the opponent’s newest BR action (NFGs) or policy (EFGs). (2) Uniform [Heinrich and Silver, 2016]. The meta-distribution is the uniform distribution. (3) PRD [Lanctot et al., 2017; Muller et al., 2020], an approximation of Nash equilibrium. We choose PRD instead of an exact Nash solver as it has been widely adopted in PSRO-related research. (4) \( \alpha \)-Rank [Muller et al., 2020]. (5) Optuna [Akiba et al., 2019]. (6) Transformer. Among these methods, (2) to (4) are classic PSRO methods, while (5) and (6) are SPSRO methods involving multiple meta-solvers and different HPO policies. Note that, although our work is related to NAC [Feng et al., 2021], directly comparing NAC with our method is not suitable as NAC does not serve as a base component in our mixing method due to extra computational cost for training the neural meta-solver.

Training and Testing. We generate the training datasets for NFGs and EFGs separately. For NFGs, we generate the dataset on the game of size \(|A_1| \times |A_2| = 200 \times 200\). For EFGs, we generate the dataset on the Leduc Poker. During testing, in addition to the games used to generate the dataset, we directly apply the trained Transformer model to the other games to verify the zero-shot generalization ability of the model.

7.2 Results
The results are summarized in Figure 4. From the results, we can draw several conclusions as follows.

By combining multiple meta-solvers, we could obtain better performance than using a single meta-solver. In all the NFGs, the final NashConvs of Optuna and Transformer are lower than that of the classic PSRO baselines considering a single meta-solver (Uniform, PRD, or \( \alpha \)-Rank). For EFGs, in Negotiation and Tic-Tac-Toe, the final NashConvs of Transformer are lower than the classic PSRO baselines. The results clearly verify the necessity of synergistically integrating multiple meta-solvers during game solving.

Transformer-based HPO could achieve better performance. Transformer-based HPO can learn a better prior distribution of hyperparameter values from offline data, providing a better scheme for weighting multiple meta-solvers, and therefore, achieving better performance than Optuna which is an online method and only relies on past epochs to obtain the prior distribution of hyperparameter values. In addition, in EFGs, we found that the NashConv of Optuna decreases quickly, but converges to a high value (also shown in Figure 5). In contrast, the Transformer can converge to a lower NashConv, though it needs a longer time in terms of BR training.

Transformer has the potential to provide a universal and plug-and-play hyperparameter value selector. As shown in Figure 4, the trained Transformer model can be applied to the games that are different from the training dataset: for NFGs, it can be applied to games with different sizes of action (strategy) spaces, and for EFGs, it can be applied to different games even with different reward scale (e.g., the maximum reward in Goofspiel is 1 while in Negotiation it is 10). This corresponds to the desiderata of a universal and plug-and-play hyperparameter value selector as mentioned in Section 6.

Given a set of meta-solvers, none of them can consistently beat (dominate) all the others during game solving (the observation in Section 4). This can be derived by comparing the performance of the three single-solver-based PSRO base-
lines: Uniform, PRD, and $\alpha$-Rank. For example, consider the NFG of size $200 \times 200$. In the early stage of PSRO, the NashConv of Uniform is lower than PRD and $\alpha$-Rank. In the middle stage, $\alpha$-Rank quickly surpasses Uniform and PRD, but Uniform still performs better than PRD. However, in the final stage, Uniform is beaten by PRD and $\alpha$-Rank. Moreover, we note that in the final stage, PRD could also perform better than $\alpha$-Rank, as shown in the NFG of size $100 \times 200$. Similar results are observed in EFGs, further verifying the conclusion.

For EFGs, in Figure 4, at first glance, one may come to the conclusion that Optuna is a better option than Transformer. However, we note that the x-axis in Figure 4 is the BR running time (which is appropriate as in our experiments only one BR policy is added to each player’s policy space). To avoid this misleading conclusion, we plot the NashConv versus epoch in Figure 5. The results clearly show that instead of terminating too early, Optuna cannot further decrease the NashConv even if it is given more epochs (10 epochs more than Transformer). The primary reason we hypothesize is that, as the SPSRO progresses, it is a struggle for Optuna to balance the two parts (NashConv and BR training time) in the performance metric $y^\nu$. Specifically, at the latter stage of SPSRO, the second term in $y^\nu$ would dominate the first term, even though they have been normalized by using the values obtained at the first epoch, making Optuna suggest a smaller number of updates for the BR policies (see Figure 7 in Section 7.3), which on the contrary cannot further decrease the NashConv because the quality of the BR policies would be low without providing enough training amount. The results demonstrate that Transformer is more effective in handling such a dilemma.

### 7.3 More Discussion

In this section and Appendix C, we provide more discussion to further deepen our understanding of our approach.

Figure 6 shows the weights of three meta-solvers (Uniform, PRD, and $\alpha$-Rank) determined by Optuna and Transformer during SPSRO running. We can see that the weights determined by Optuna vary dramatically throughout SPSRO running, while Transformer’s predictions are more stable (around $1/3$ for each solver). We hypothesize that such a relatively stable weighting scheme for multiple meta-solvers is necessary to obtain better performance. In addition, an interesting observation is that the weights of Uniform and PRD change almost in a mirror form. More results can be found in Appendix C.

In Figure 7, we found that Optuna and Transformer follow very different patterns to select the computing amount used for training the BR policy at each epoch. For Optuna, the number of episodes suddenly decreases to a very low value after about 10 epochs. Intuitively, when $K$ is much smaller than $\bar{K}$ (the maximum number of episodes to obtain a converged BR policy), the policy obtained through the BR oracle may be far away from the true BR policy, resulting in poor performance. This is also reflected in Figure 5 where Optuna cannot obtain a lower NashConv even if it is given more epochs. In contrast, by offline learning, Transformer could better trade-off between the NashConv and BR training time and hence, performs better than Optuna. More results can be found in Appendix C.

### 8 Conclusions

In this work, we first attempt to explore the possibility of self-adaptively determining the optimal hyperparameter values in the PSRO framework and provide three contributions: (1) the parametric PSRO (PPSRO) which unifies GDA and various PSRO variants; (2) the self-adaptive PSRO (SPSRO) where we aim to learn a self-adaptive HPO policy; (3) a novel offline HPO approach to optimize the HPO policy based on the Transformer architecture. The well-trained Transformer-based HPO policy has the potential of transferring to different games without fine-tuning. Experiments on different games demonstrate the superiority of our approach over different baselines.
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Contribution Statement

Shuxin Li and Chang Yang make equal contributions to this work. Xinrun Wang is the corresponding author of this work.

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