

Auto-configuring Exploration-Exploitation Tradeoff in Evolutionary Computation via Deep Reinforcement Learning

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ABSTRACT

Evolutionary computation (EC) algorithms, renowned as powerful black-box optimizers, leverage a group of individuals to cooperatively search for the optimum. The exploration-exploitation tradeoff (EET) plays a crucial role in EC, which, however, has traditionally been governed by manually designed rules. In this paper, we propose a deep reinforcement learning-based framework that autonomously configures and adapts the EET throughout the EC search process. The framework allows different individuals of the population to selectively attend to the global and local exemplars based on the current search state, maximizing the cooperative search outcome. Our proposed framework is characterized by its simplicity, effectiveness, and generalizability, with the potential to enhance numerous existing EC algorithms. To validate its capabilities, we apply our framework to several representative EC algorithms and conduct extensive experiments on the augmented CEC2021 benchmark. The results demonstrate significant improvements in the performance of the backbone algorithms, as well as favorable generalization across diverse problem classes, dimensions, and population sizes. Additionally, we provide an in-depth analysis of the EET issue by interpreting the learned behaviors of EC.

CCS CONCEPTS

- Computing methodologies → Bio-inspired approaches; Reinforcement learning.

KEYWORDS

Automatic configuration, differential evolution, particle swarm optimization, reinforcement learning, meta-black-box optimization

1 INTRODUCTION

Using Evolutionary Computation (EC) algorithms as black-box optimizers has received significant attention in the last few decades [8, 34]. Typically, the EC algorithms deploy a population of individuals that work cooperatively to undertake both *exploration* (that discovers new knowledge) and *exploitation* (that advances existing knowledge), so as to make the black-box optimization problem “white” [5]. Targeting global convergence to the global optimum,

the *exploration-exploitation tradeoff* (EET) is the most fundamental issue in the development of EC algorithms.

Among the extensive literature focusing on the EET issues in EC algorithms, hyper-parameters tuning is one of the most promising way. In the vanilla EC [13, 36], the EET-related hyper-parameters such as cognitive coefficient and social coefficient in Particle Swarm Optimization (PSO) are set as static values throughout the search, necessitating laborious tuning for different problem instances. The adaptive EC algorithms [17, 41], which introduce manually designed rules to dynamically adjust EET hyper-parameters according to optimization states, soon became flexible and powerful optimizers that dominate performance comparisons. However, they rely heavily on human knowledge to turn raw features of the search into decisions on EET control, which are hence labour-intensive [23].

In the recent “learning to optimize” paradigm, deep reinforcement learning (DRL)-based approaches have been found successful to complement or well replace conventional rule-based optimizers [22, 24]. When it comes to the hyper-parameters tuning, several early attempts have already been made to control the EET hyper-parameters through DRL automatically [39, 51]. Though these works have demonstrated effectiveness in automating the EET strategy design process in an end-to-end manner, they still suffer from several major limitations.

The first issue is the generalization of the learnt model. Some of the existing works stipulated DRL to be conducted online, where they trained and tested the model directly on the target problem instance, that is, their methods require (re-)training for every single problem, such as DRL-PSO [46], DE-DDQN [31], DE-DQN [39] and RLHPSDE [40]. Such design, in our view, may prevent DRL from learning generalizable patterns and result in overfitting. To this end, we present a Generalizable Learning-based Exploration-Exploitation Tradeoff framework, called **GLEET**, that could explicitly control the EET hyper-parameters of a given EC algorithm to solve a class of problems via reinforcement learning. GLEET performs training only once on a class of black-box problems of interest, after which it uses the learned model to directly boost the backbone algorithm for other problems within (and even beyond) the same class. The overview of GLEET is illustrated in Fig. 1. To fulfill the purpose, we formulate it as a more comprehensive Markov Decision Process (MDP) than those in the existing works, with specially designed state, action, and reward function to facilitate efficient learning.

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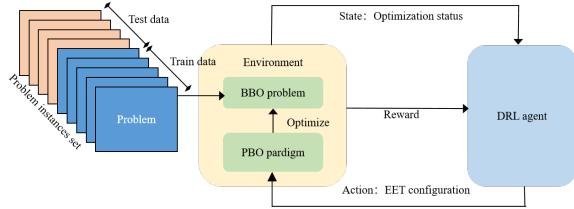


Figure 1: The overview of GLEET as an MDP.

The second issue arises from the oversimplified state representation and network architecture (i.e., a multilayer perceptron), which fail to effectively extract and process the features of the EET and problem knowledge. In this paper, we design a Transformer-styled [44] network architecture that consists of a *feature embedding* module for feature extraction, a *fully informed encoder* for information processing amongst individuals, and an *exploration-exploitation decoder* for adjusting EET parameters. On the one hand, the transformer architecture achieves invariance in the ordering of population members, making it generalizable across problem dimension, population size and problem class. On the other hand, the proposed model allows different individuals to adaptively and dynamically attend to the knowledge of others via the self-attention mechanism, so as to decide the EET behavior in a joint manner.

Lastly, we conduct extensive experiments to verify GLEET. Different from existing works, our augmented dataset from the CEC2021 benchmark [25] is larger and more comprehensive. We evaluate GLEET by applying it to several representative EC algorithms, i.e., vanilla PSO [13], DMSPSO [18] and vanilla DE [36], though we note that GLEET has the potential to boost many other EC algorithms. In this paper, we focus on the application of PSO algorithms and include the contents about GLEET-DE in the Appendix due to paper length limitations. Experimental results show that GLEET could significantly ameliorate the backbone algorithms, making them surpass adaptive methods and existing learning-based methods. Meanwhile, GLEET exhibits promising generalization capabilities across different problem classes. We visualize the knowledge GLEET learnt and interpret how it learns different EET strategies for different problems, which further provides insights to the area.

The rest of this paper is organized as follows: Section 2 reviews how the EET issue has been addressed in traditional EC algorithms and recently proposed RL-based frameworks. Section 3 introduces the preliminary concepts and notations. In Section 4, we present the technical details, including the problem definition, network design and training process. The experimental results are presented in Section 5, followed by a conclusion in Section 6.

2 RELATED WORKS

2.1 Traditional EET Methods

The vanilla EC algorithms address the EET issue in a static manner. For example, each individual in the vanilla Particle Swarm Optimization (PSO) [13] controls the EET by paying equal attention to the global best experience (for exploitation) and its personal best experience (for exploration). Another example is vanilla Differential Evolution (DE) [36], where the EET hyper-parameters F

(exploitation by learning from the best history) and CR (exploration by perturbation or so called crossover) is pre-defined by expert knowledge to balance the EET. However, static EET parameters are problem agnostic hence require a tedious tuning process for each new problem, and may also limit the overall search performance.

Several adaptive EC variants that dynamically adjust the EET-related hyper-parameters along the optimization process were then proposed to address this issue. For PSO, several early attempts focused on adaptively tuning its inertia weight (IW) hyper-parameter, such as [1, 33, 42], which were then surpassed by methods of considering tuning the acceleration coefficient (AC) hyper-parameter using adaptive rules based on constriction function [7], time-varying nonlinear function [6, 27], fuzzy logic [26], or multi-role parameter design [47]. GLPSO [9] self-adapts the EET by genetic evolution. In sDMSPSO [17], the tuning of IW and ACs are considered together into a well-known multi-swarm optimizer DMSPSO [18] to efficiently adjust EET, achieving superior performance. Generally, most of the above methods rely heavily on human knowledge and are hence labour-intensive and vulnerable to inefficiencies.

2.2 Learning-based EET Methods

The EET issue was also tackled via (deep) reinforcement learning automatically. In the following, We sort out some representative works and further highlight the motivation of this study.

Samma et al. [28] firstly explored to control the ACs in PSO by Q-learning, which inspired many followers to use deep Q-learning for topology structure selection in PSO [48] or parameter control in multi-objective EC algorithms [20]. In RLEPSO [51], the authors proposed to improve EPSO [21] by tuning its EET hyper-parameters based on the optimization schedule feature and policy gradient method. In another recent work [46], the DRL-PSO optimizer was presented to control the random variables in the PSO velocity update equations to address EET, where DRL-PSO outperformed the advanced adaptive method sDMSPSO on a small test dataset.

However, all the above works neglected the generalization ability of the learned model as established in the introduction. We note that in a related field of neural combinatorial optimization, researchers developed several generalizable solvers to solve a class of similar problems based on DRL [14, 22], however, their underlying MDPs and networks were specially designed for discrete optimization, making them not suitable for the hyper-parameter tuning task studied in this paper. Furthermore, their experiments are limited to small datasets (with only a dozen problem instances), which makes their performance comparison inconclusive. For example, when we train and test DRL-PSO on much larger datasets in our experiments, it could not outperform sDMSPSO. Finally, the simple network architecture and input features in most existing methods largely limit their performance, especially when compared to the advanced adaptive EC variants. Two recent works Meta-ES[16] and Meta-GA[15] may share the same ambition with GLEET. They provide a brand new paradigms to meta-learn an NN parameterized optimizer by Neural Evolution. Other works such as Symbol [4], RL-DAS [10] and EvoTF [43] also note the importance of EET. They are pre-trained on a set of synthetic problems with different landscape properties and directly applied to unseen tasks.

3 PRELIMINARY AND NOTATIONS

3.1 Deep Reinforcement Learning

DRL methods specialize in solving MDP by learning a deep network model as its decision policy [38]. Given an MDP formalized as $\mathcal{M} := \langle \mathcal{S}, \mathcal{A}, \mathcal{T}, \mathcal{R} \rangle$, the agent obtains a state representation $s \in \mathcal{S}$ and then decides an action $a \in \mathcal{A}$ which turns state s into next state s' according to the dynamic of environment $\mathcal{T}(s'|s, a)$ and then gets a reward $\mathcal{R}(s, a)$. The goal of DRL is to find a policy $\pi_\theta(a|s)$ (parameterized by the deep model θ) so as to optimize a discounted expected return $\mathbb{E}_{\pi_\theta}[\sum_{t=1}^T \gamma^{t-1} \mathcal{R}(s_t, a_t)]$.

3.2 Attention Mechanism

In the Transformer model [44], the attention is computed by

$$\text{Attn}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V \quad (1)$$

where Q, K, V are the vectors of queries, keys and values respectively, and d_k is the dimension of queries which plays a role as a normalizer. The Transformer consists of multiple encoders with self-Attention and decoders, which both use Multi-Head Attention to map vectors into different sub-spaces for a better representation:

$$\begin{aligned} H &= \text{MHA}(Q, K, V) = \text{Concat}(H_1, H_2, \dots, H_h)W^O \\ H_i &= \text{Attn}(QW_i^Q, KW_i^K, VW_i^V) \end{aligned} \quad (2)$$

where h denotes the number of heads, $W^O \in \mathbb{R}^{hd_v \times d_s}$, $W_i^Q \in \mathbb{R}^{d_s \times d_k}$, $W_i^K \in \mathbb{R}^{d_s \times d_k}$ and $W_i^V \in \mathbb{R}^{d_s \times d_v}$. For self-attention, Q, K, V can be derived from one input source, whereas for general attention, Q can be from a different source other than that of K and V .

3.3 Particle Swarm Optimization

This algorithm deploys a population of particles (individuals) as candidate solutions, in iteration t it improves each particle x_i as

$$\begin{aligned} x_i^{(t)} &= x_i^{(t-1)} + v_i^{(t)}, \\ v_i^{(t)} &= w \times v_i^{(t-1)} + c_1 \times \text{rnd} \times (pBest_i^{(t-1)} - x_i^{(t-1)}) \\ &\quad + c_2 \times \text{rnd} \times (gBest^{(t-1)} - x_i^{(t-1)}) \end{aligned} \quad (3)$$

where v_i is the velocity; $pBest_i$ and $gBest$ are the personal and global best positions found so far respectively; w is an inertia weight; rnd returns a random number from $[0, 1]$; and c_1 and c_2 induce the EET where a large c_1 encourages the particle to explore different regions based on its own beliefs and a large c_2 forces all particles to exploit the global best one. In the vanilla PSO [13], $c_1 = c_2$ for equal attention on exploitation and exploration.

4 METHODOLOGY OF GLEET

4.1 MDP Formulation

Given a population P with N individuals, an EC algorithm Λ , and a problem set D , we formulate the dynamic tuning as an MDP:

$$\mathcal{M} := \langle \mathcal{S} = \{s_i\}_{i=1}^N, \mathcal{A} = \{a_i\}_{i=1}^N, \mathcal{T}, \mathcal{R} \rangle \quad (4)$$

where state \mathcal{S} and action \mathcal{A} take all individuals in the Population P into account. Each $a_i \in \mathbb{R}^M$ denotes the choice of hyper-parameters for the i -th individual in Λ , where M denotes the number

of hyper-parameters to be controlled. For example, in DE/current-to-pbest/1 [53], the hyper-parameters F_1 , F_2 and Cr need to be determined. The transition function $\mathcal{T} : \mathcal{A} \times \Lambda \times P \rightarrow P$ denotes evolution of population P through algorithm Λ with hyper-parameters \mathcal{A} . The reward function $\mathcal{R} : \mathcal{S} \times \mathcal{A} \times D \rightarrow \mathbb{R}^+$ measures the improvement in a step brought by hyper-parameter settings.

While optimizing the hyper-parameters of Λ on a single problem instance may yield satisfactory results, it can limit the generalization performance on unseen problems. To address this, we construct a problem set D comprising F problems (detailed in Appendix A.2) to facilitate generalization. Correspondingly, the DRL agent targets at the optimal policy π_{θ^*} that controls the dynamic hyper-parameters for Λ to maximize the expected accumulated reward over all the problems $D_k \in D$ as

$$\theta^* := \arg \max_{\theta \in \Theta} \frac{1}{F} \sum_{k=1}^F \sum_{t=1}^T \gamma^{t-1} \mathcal{R}(S^{(t)}, A^{(t)} | D_k). \quad (5)$$

This approach ensures robust performance across a diverse range of problem instances and promotes generalization capabilities.

4.1.1 State. We provide four principles for the GLEET state space design: a) it should describe the state of every individual in the population; b) it should be able to characterize the optimization progress and the EET behavior of the current population; c) it should be compatible across different kinds of EC algorithms and achieve generalization requirement; and d) it should be convenient to obtain in each optimization step of the EC process.

Following these four principles, we use a K -dimensional vector to define the state s_i for each individual in EC algorithm at time step t . The information required to calculate this state vector includes the global best individual $gBest$ in the population, each individual's historical best information $pBest_i$ and current position x_i , as well as their evaluation values $f(gBest)$, $f(pBest_i)$ and $f(x_i)$. For most of EC algorithms, information above is compatible and easy to obtain, which makes GLEET a generic paradigm for boosting many kinds of EC algorithms. Computational detail is shown in Eq. (6), $K = 9$ where we compute: $s_{i,\{1,2\}}$ as the search progress w.r.t. the $gBest$ value and the currently consumed number of fitness evaluations (FE); $s_{i,\{3,4\}}$ as the stagnation status w.r.t. the number of rounds $z(\cdot)$ for which the algorithm failed to find a better $gBest$ or $pBest_i$, normalized by the total rounds T_{\max} ; $s_{i,\{5,6\}}$ as the difference in evaluation values between individuals and $gBest$ or $pBest_i$, normalized by the initial best value; $s_{i,\{7,8\}}$ as the Euclidean distance between particles and $gBest$ or $pBest_i$, normalized by the diameter of the search space; $s_{i,\{9\}}$ as the cosine function value of the angle formed by the current particle to the $gBest$ and $pBest_i$.

$$\begin{aligned} s_{i,\{1,2\}} &= \left\{ \frac{f(gBest)}{f(gBest^{(0)})}, \frac{FE_{\max} - FE}{FE_{\max}} \right\}, \\ s_{i,\{3,4\}} &= \left\{ \frac{z(gBest)}{T_{\max}}, \frac{z(pBest_i)}{T_{\max}} \right\}, \\ s_{i,\{5,6\}} &= \left\{ \frac{f(x_i) - f(gBest)}{f(gBest^{(0)})}, \frac{f(x_i) - f(pBest_i)}{f(pBest_i^{(0)})} \right\}, \\ s_{i,\{7,8\}} &= \left\{ \frac{\|x_i - gBest\|}{\text{diameter}}, \frac{\|x_i - pBest_i\|}{\text{diameter}} \right\}, \\ s_{i,\{9\}} &= \{\cos(\angle(gBest - x_i, pBest_i - x_i))\}, \end{aligned} \quad (6)$$

Note that we also calculate the above K features for the global best position and N personal best positions to learn embeddings for them (will be used in the decoder). We name the $N \times K$ state features of $\{x_i\}_{i=1}^N$ as the *population features*, the $1 \times K$ state features of $gBest$ as the *exploitation features*, and the $N \times K$ state features of $\{pBest_i\}_{i=1}^N$ as the *exploration features*, respectively. These three parts together composite the state. We again emphasize that this state design is generic across different EC algorithms which makes GLEET generalizable for a large body of EC algorithms.

4.1.2 Action. Since the hyper-parameters in most EC algorithms are continuous, and discretizing the action space may damage the action structure or cause the curse of dimensionality issue [19], GLEET prefers continuous action space that jointly controls all N individuals' choices of hyper-parameters $(a_1^{(t)}, a_2^{(t)}, \dots, a_N^{(t)})$, where $a_i^{(t)}$ denotes M hyper-parameters for individual i at time step t . Concretely, the action probability $\text{Pr}(a)$ is a multiplication of normal distributions as follows,

$$\text{Pr}(a) = \prod_{i=1}^N \prod_{m=1}^M p(a_i^m), \quad a_i^m \sim \mathcal{N}(\mu_i^m, \sigma_i^m) \quad (7)$$

where μ_i^m and σ_i^m are controlled by DRL agent. Generally, our policy network outputs $N \times M$ pairs of (μ_i^m, σ_i^m) , where each (μ_i^m, σ_i^m) is used to sample a parameter to control the EET of each individual.

4.1.3 Reward. We consider the reward function as follows,

$$r^{(t)} = \frac{f(gBest^{(t-1)}) - f(gBest^{(t)})}{f(gBest^{(0)})} \quad (8)$$

where the reward is positive if and only if a better solution is found. It is worth mentioning that there are several practical reward functions proposed previously. Yin et al. [51] rewards an improvement of solution 1 otherwise -1 . Sun et al. [37] calculates a relative improvement between steps as reward function. Wu et al. [46] has a similar form with our reward function but permits negative reward. We conduct comparison experiments on these reward functions, it turns out in our experiment setting, reward function proposed in Eq. (8) stands out. Results can be found in Appendix B.7.

4.2 Network Design

As depicted in Fig. 2, fed with the state features, our actor π_θ first generates a set of population embeddings (based on population features) and a set of EET embeddings (based on exploitation and exploration features). The former is further improved by the fully informed encoders. These embeddings are then fed into the designed decoder to specify an action. We also consider a critic v_ϕ to assist the training of the actor.

4.2.1 Feature embedding. We linearly project raw state features from Section 4.1 into three groups of 128-dimensional embeddings, i.e., exploration embeddings (EREs) $\{h_i\}_{i=1}^N$, exploitation embedding (EIE) $\{g\}$, and population embeddings (PEs) $\{e_i\}_{i=1}^N$. Then we concatenate each ERE with the EIE to form 256-dimensional vectors $\{h_i||g\}_{i=1}^N$ which are then processed by an MLP with structure $(256 \times 256 \times 128)$, ReLU is used by default) to obtain the EET embeddings (EETs) $\{EE_i\}_{i=1}^N$ that summarize the current EET status.

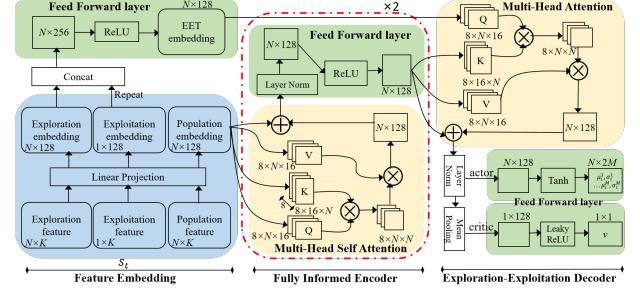


Figure 2: Illustration of our network. The network firstly embeds the state feature into two components: the EET embedding and the population embedding. Next, a Fully Informed Encoder is employed to attend the population embedding to the individual level. Finally, the individual's EET configuration is determined by decoding the information from the EET embedding using the Exploration-Exploitation Decoder.

4.2.2 Fully informed encoder. The encoders mainly follow the design of the original Transformer, except that the positional encoding is removed and layer normalization [2] is used instead of batch normalization [12]. There are three main factors that lead us to favor full attention over sparse attention [52]: a) the number of embeddings (i.e., population size) in our task is relatively small compared with the number of word embeddings in language processing, negating the need for sparse attention; and b) it gives the network maximum flexibility without any predefined restrictions on sparsity and hence via the attention scores, the network could automatically adjust the topology between individuals. Specifically, our encoders update the population embeddings by

$$\begin{aligned} \hat{e} &= \text{LN}(e^{(l-1)} + \text{MHA}^{(l)}(Q^{(l)}, K^{(l)}, V^{(l)})), \\ e^{(l)} &= \text{LN}(\hat{e} + \text{FF}^{(l)}(\hat{e})) \end{aligned} \quad (9)$$

where $Q^{(l)}$, $K^{(l)}$ and $V^{(l)}$ are transformed from population embeddings $e^{(l-1)}$ and $l = \{1, 2\}$ is the layer index (we stack 2 encoders). The initial condition $e^{(0)}$ is the population embeddings embedded from the population features as shown in Fig. 2. The Feed Forward (FF) layer is an MLP with structure $(128 \times 256 \times 128)$. The final output is the fully informed population embeddings (FIPes) $\{e_i^{(2)}\}_{i=1}^N$.

4.2.3 Exploration-exploitation decoder. Given the EETs and FIPes, the exploration-exploitation decoder outputs the joint distribution of hyper-parameter settings for each individual. The EET control logits $H(\{H_i\}_{i=0}^N)$ are calculated as:

$$\begin{aligned} \hat{H} &= \text{LN}(e^{(2)} + \text{MHA}^d(Q^d, K^d, V^d)), \\ H &= \text{ReLU}(\text{FF}^{\text{logit}}(\text{LN}(\hat{H}) + \text{FF}^d(\hat{H}))) \end{aligned} \quad (10)$$

where we let Q^d from EETs, and K^d, V^d from FIPes (different from the self-attention in the encoders); FF^d is with structure $(128 \times 256 \times 128)$; and FF^{logit} is with structure (128×128) . We then linearly transform each $\{H_i\}_{i=1}^N$ from 128 to $2M$ scalars which are then passed through the Tanh function and scaled to range $[\mu_{\min}^m, \mu_{\max}^m]$ and $[\sigma_{\min}^m, \sigma_{\max}^m]$, respectively, to obtain the $a_i^m = \mathcal{N}(\mu_i^m, \sigma_i^m)$ for each individual. We set all $[\mu_{\min}, \mu_{\max}] = [0, 1]$ and all $[\sigma_{\min}, \sigma_{\max}] =$

[0.01, 0.7]. To be specific, for PSO algorithms, we let $M = 1$ and take the sampled value a_i as the $c_{1,i}$ in Eq. (3) for each particle i (leaving $c_{2,i} = 4 - c_{1,i}$ by the suggestion of [45]).

4.2.4 Critic network. The critic v_ϕ shares the EET control logits H from the actor and has its own output layers. Specifically, it performs a mean pooling for the logits $\bar{H} = \sum_{i=1}^N H_i$, and then processes it using an MLP with structure (128 × 64 × 32 × 1 and LeakyReLU activation) to obtain the value estimation.

4.3 Training

Our GLEET agent can be trained via any off-the-shelf reinforcement learning algorithm, and we use the T -step PPO [30] in this paper. A training dataset containing a class of similar black-box problem instances is generated before training (details in Appendix A.2), from which a small batch of problem instances is randomly sampled on the fly during training (which is different from previous works that only leverages one single instance). Given the batch, we initialize a population of individuals according to the backbone EC algorithm for each problem instance and then let the on-policy PPO algorithm gather trajectories while updating the parameters of the actor and the critic networks defined in Section 4.2. We alternate between sampling trajectory \mathcal{T} by T time steps and update κ times of the network parameters. The learned model will be directly used to infer the EET control for other unseen problem instances.

5 EXPERIMENTS

Our experiments research the following questions:

- RQ1: How good is the control performance of GLEET against the previous static, adaptive tuning and DRL-tuning methods, and whether GLEET can be broadly used for enhancing different EC algorithms?
- RQ2: Does GLEET possess the generalization ability on the unseen problems instances?
- RQ3: Can the learned behavior of GLEET be interpreted and recognized by human experts?
- RQ4: How crucial are the EET embeddings and the attention modules in our GLEET implementation?

To investigate RQ1 to RQ4, we firstly instantiate GLEET to PSO and compare its optimization performance with several competitors such as PSO’s original version, adaptive variants and reinforcement learning-based versions, see Section 5.2. We then test the zero-shot generalization ability of GLEET by directly applying the trained agent to unseen settings, see Section 5.3. Next, we visualize the controlled EET patterns of GLEET and the decision layer of GLEET’s network to interpret the learned knowledge, see Section 5.4. At last, for answering RQ4, we conduct ablation study on the EET embeddings and the attention modules, see Section 5.5.

5.1 Experimental Setup

As established, existing studies control the EET in static, adaptive, and learning-based manners. We choose competitors for GLEET on PSO and GLEET on DE from these three categories. For PSO, we choose the vanilla PSO [32] as static baseline, the PSO variants DMSPSO [18], sDMSPSO [17], GLPSO [9] as adaptive baselines,

and DRL-PSO [46] and RLEPSO [51] as the learning-based competitors. We instantiate GLEET to the vanilla PSO and DMSPSO for comparison, denoted as GLEET-PSO and GLEET-DMSPSO. Baseline GLPSO is tested based on the original source code provided by the original authors. For the other baselines (including DMSPSO, sDMSPSO, DRL-PSO and RLEPSO) that do not have open-source code available, we implement them strictly following the pseudocodes in their original manuscripts. For all baselines, we have followed their recommended hyper-parameter settings and ensured that the code and settings we used could achieve similar performance on the benchmark they used in their original paper. The learning-based competitors are trained on the same training sets as GLEET methods. The parameter settings of GLEET is shown in Appendix A.1.

All algorithms are trained and tested on the augmented CEC 2021 numerical optimization test suite [25] which consists of ten challenging black-box optimization problems (f_1 – f_{10}). The f_1 to f_4 are single problems which are not any problems’ hybridization or composition. The f_5 to f_7 hybridize some basic functions, resulting more difficult problem because of solution space coupling. The f_8 to f_{10} are linear compositions of some single problems, resulting more difficult problem because of fitness space coupling. We augmented each problem class to a problem set D (the augmentation details can be found in Appendix A.2). We train one GLEET agent per problem class and also investigate the performance of GLEET if trained on a mixed dataset containing all the problem classes, denoted as f_{mix} .

5.2 Comparison Analysis

In this paper we conduct the comparison analysis on different PSO and DE algorithms over the 10D and 30D problems. In this section we only present the results and the ranks obtained by PSO algorithms over the 10D problems in Table 1. The remaining results and analysis can be found in Appendix B.1 and B.2. In Table 1 we also present the average performance improvement of GLEET compared with its backbone algorithm (e.g., GLEET-PSO improves PSO with a 35% performance gap), which lies on the right of the rank of the GLEET-PSO/GLEET-DMSPSO. It can be observed that the performance of the proposed GLEET-DMSPSO generally and consistently dominates the competitors. Both GLEET-PSO and GLEET-DMSPSO significantly improve their backbones, i.e., PSO and DMSPSO, respectively, which validates the effectiveness of our GLEET in learning generalizable knowledge to control the exploration and exploitation behavior for the algorithms under a given problem class. The superiority of GLEET over the traditional adaptive algorithms sDMSPSO and GLPSO further shows the powerfulness of using a learning-based agent to derive policies instead of manually designed heuristic.

Our GLEET achieves the state-of-the-art performance among learning-based competitors on all test cases when considering the comparison among GLEET-PSO, DRL-PSO and RLEPSO. The three algorithms are all based on DRL, amongst GLEET-PSO and DRL-PSO adopt the same backbone and the RLEPSO improves the EPSO algorithm. Different from the three peer algorithms, we explicitly embed EET information into the state representation to make it more expressive and design an attention-based architecture to make the individuals in population *fully informed* and *exploration-exploitation aware*. With the increasing of dimensions, difficulty of

Table 1: Numerical comparison results for PSO algorithms on 10D problems, where the mean, standard deviations and performance ranks are reported (with the best mean value on each problem highlighted in bold).

Algorithm	Type	Static PSO		Adaptive				DRL									
	Metrics	Mean (Std)	Rank	DMSPSO		sDMSPSO		GLPSO		DRL-PSO		RLEPSO		GLEET-PSO		GLEET-DMSPSO	
				Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank
f_1	7.071E+06 (1.104E+07)	7	5.903E+04 (8.036E+04)	4	6.408E+03 (1.670E+04)	2	1.646E+04 (1.652E+04)	3	1.296E+07 (1.513E+07)	8	5.418E+06 (7.420E+06)	6	2.748E+06 (4.205E+06)	5	2.471E+02 (7.676E+02)	1	
	8.428E+02 (2.716E+02)	8	3.376E+02 (1.549E+02)	2	5.232E+02 (1.722E+02)	5	3.750E+02 (2.264E+02)	3	6.253E+02 (2.166E+02)	6	7.188E+02 (2.405E+02)	7	5.105E+02 (1.776E+02)	4	2.440E+02 (1.396E+02)	1	
f_2	2.934E+01 (7.850E+00)	7	1.563E+01 (2.546E+00)	2	2.678E+01 (6.625E+00)	6	1.781E+01 (3.677E+00)	3	2.174E+01 (5.245E+00)	5	3.022E+01 (7.809E+00)	8	2.120E+01 (4.705E+00)	4	1.498E+01 (2.357E+00)	1	
	2.099E+00 (1.235E+00)	6	1.375E+00 (7.083E-01)	4	5.948E-01 (2.471E-01)	2	8.750E-01 (4.023E-01)	3	9.398E+00 (1.980E+00)	8	3.519E+00 (7.776E-01)	7	1.422E+00 (5.210E-01)	5	5.816E-01 (2.210E-01)	1	
f_3	3.395E+03 (5.793E+03)	6	4.282E+02 (2.221E+02)	3	3.714E+02 (2.183E+02)	1	2.223E+03 (1.614E+03)	6	1.048E+04 (2.057E+04)	8	2.119E+03 (2.912E+03)	5	1.847E+03 (2.552E+03)	4	3.716E+02 (1.866E+02)	2	
	8.443E+01 (5.844E+01)	8	2.870E+01 (2.146E+01)	4	1.981E+01 (1.704E+01)	2	2.768E+01 (2.560E+01)	3	6.379E+01 (4.684E+01)	6	8.270E+01 (5.471E+01)	7	4.449E+01 (3.381E+01)	5	1.300E+01 (1.020E+01)	1	
f_4	1.722E+03 (3.667E+03)	5	2.134E+02 (1.462E+02)	3	1.709E+02 (1.277E+02)	2	8.152E+02 (5.051E+02)	5	1.431E+03 (1.850E+03)	7	1.151E+03 (9.557E+02)	6	4.977E+02 (3.549E+02)	4	1.302E+02 (8.489E+01)	1	
	3.376E+02 (2.902E+02)	8	9.572E+01 (3.891E+01)	2	1.495E+02 (8.792E+01)	5	1.441E+02 (9.497E+01)	4	2.120E+02 (1.744E+02)	7	1.686E+02 (1.219E+02)	6	1.096E+02 (3.924E+01)	3	7.216E+01 (3.555E+01)	1	
f_5	2.370E+02 (5.916E+01)	8	1.690E+02 (4.759E+01)	4	1.392E+02 (5.788E+01)	2	1.953E+02 (2.989E+01)	6	2.010E+02 (6.135E+01)	7	1.862E+02 (6.679E+01)	5	1.665E+02 (6.137E+01)	3	1.202E+02 (2.016E+01)	1	
	2.227E+02 (3.946E+01)	8	2.035E+02 (2.030E+01)	4	1.955E+02 (2.287E+01)	3	2.166E+02 (2.221E+01)	5	2.201E+02 (3.665E+01)	7	2.199E+02 (3.300E+01)	6	1.882E+02 (4.127E+01)	2	1.682E+02 (1.648E+01)	1	
f_{mix}	8.445E+05 (1.090E+06)	7	1.612E+02 (7.617E+01)	2	5.105E+02 (9.813E+02)	4	4.747E+02 (3.273E+02)	3	3.184E+05 (5.086E+05)	6	1.156E+06 (1.380E+06)	8	4.225E+04 (2.068E+04)	5	1.364E+02 (5.839E+01)	1	
Avg Rank		7.45	3.09	3.09	4.00				6.82	6.45	4.00 ($\uparrow 48\%$)		1.09 ($\uparrow 35\%$)				

searching surges due to the exponential growth of search space. Facing that difficulty, DRL-PSO and RLEPSO suffer from sharp performance decline, which may be caused by the oversimplified network or the defect of EET information in state representation. Adaptive PSO variants sDMSPSO and GLPSO still have stable performance on high-dimensional problems, which proves that manually designed adaptive EC are still competing. Manual adaptive variants sDMSPSO can not improve the backbone DMSPSO on some functions (i.e., f_2 and f_3). However, on some specific functions (i.e., f_5), sDMSPSO dominates others. This may reveal that adaptive control of EET by manual design has poor generalization. GLEET dominates the optimization performance on composition problem sets (f_8 , f_9 and f_{10}) under 10D setting, which indicates that GLEET may perform more stable on complex problem, which is favorable.

Besides the conclusions above, we propose an especially challenging task to further examine the control of EET in each algorithm, where we mix all ten problem sets up for training and testing (f_{mix}). We trained GLEET-PSO and GLEET-DMSPSO on f_{mix} . The line f_{mix} in Table 1 shows the optimization results in such a mixed dataset of the GLEET and those competitors, which further verifies that GLEET can not only learn well among similar problems but also learns well among different problem classes.

5.3 Generalization Analysis

In the above experiments, the agents are trained on a set of problem instances and tested on another set of unseen ones within the same problem class, which in some ways showed the desired generalization ability of our GLEET. We now continue to evaluate the zero-shot generalization of GLEET under more critical conditions. Specifically, we will test GLEET's generalization across different CEC problem classes and Protein-Docking application problems in the following subsections. Additionally, we will analyze the impact of various factors such as problem dimensions, population sizes, optimization horizons, and training set sizes. These details can be found in Appendix B.3 to B.5.

Table 2: Generalization experiment results for different problem classes. The “Gap” column shows the difference in optimization performance compared to the original agent (with negative values indicating improvement).

		Ag- f_2	Ag- f_3	Ag- f_4	Ag- f_{mix}	PSO
		Mean (Std)				
		Gap	Gap	Gap	Gap	Gap
Simple	f_2	5.105E+02 (1.776E+02)	5.164E+02 (1.812E+02)	5.195E+02 (1.880E+02)	5.179E+02 (1.871E+02)	5.179E+02 (2.716E+02)
	f_3	2.213E+01 (5.090E+00)	2.120E+01 (4.705E+00)	2.179E+01 (4.786E+00)	2.175E+01 (4.805E+00)	2.934E+01 (7.850E+00)
	f_4	1.546E+00 (9.959E-01)	1.412E+00 (8.379E-01)	1.422E+00 (7.776E-01)	1.451E+00 (8.399E-01)	2.099E+00 (1.235E-01)
	f_5	1.928E+03 (2.374E+03)	1.592E+03 (1.980E+03)	1.514E+03 (1.600E+03)	1.709E+03 (2.126E+03)	3.395E+03 (5.793E+03)
Complex	f_8	4.356E+02 (2.492E+01)	-13.793% 2.596%	-18.043% 1.194%	-7.482% 0.400%	83.812% 208.029%

5.3.1 Generalization across problems. GLEET is generalizable across problem classes. We train four GLEET-PSO agents, denoted as Ag- f_2 , Ag- f_3 , Ag- f_4 , Ag- f_{mix} , on the following four problem sets: the Schwefel (f_2) class, the biRastrigin (f_3) class, the Griegrosen (f_4) class and the mixture problems of the above three (f_{mix}), and then test their performance on unseen problem classes including more complex problem f_5 and f_8 . Table 2 presents the averaged performance on ten runs and the performance “Gap” between each of the above agent and the original agent trained on the designated problem class. PSO is taken as a baseline and the “Gap” measures its performance difference with GLEET-PSO trained on the designated problem class. The “Gap” is calculated as $\frac{f' - f}{f}$, where f' is the performance of the agent trained on another problem class, and f is performance of the the original agent trained on the designated problem class.“Gap” indicates how much better (less than 0)

Table 3: Numerical comparison results on 12D Protein-Docking problems, where the mean, standard deviations, runtime and performance ranks (according to the mean costs) are reported (with the best mean value highlighted in bold).

Type Algorithm	Static PSO	Adaptive PSO		
	PSO	DMSPSO	sDMSPSO	GLPSO
Metrics	Mean (Std)	Mean (Std)	Mean (Std)	Mean (Std)
Protein Docking	5.153E+02 (2.151E+01)	4.771E+02 (3.345E+01)	5.101E+02 (3.155E+01)	5.061E+02 (3.700E+01)
Runtime(s)	0.539	1.156	1.137	1.103
Rank	7	2	6	5

Type Algorithm	DRL-based PSO			
	DRL-PSO	RLEPSO	GLEET-PSO	GLEET-DMSPSO
Metrics	Mean (Std)	Mean (Std)	Mean (Std)	Mean (Std)
Protein Docking	5.180E+02 (4.940E+01)	4.895E+02 (4.129E+01)	4.832E+02 (3.865E+01)	4.681E+02 (3.650E+01)
Runtime(s)	14.341	1.307	2.134	2.515
Rank	8	4	3	1

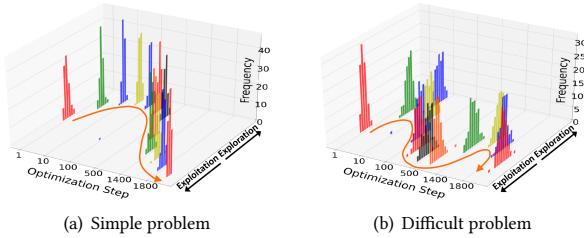


Figure 3: Visualization of action distribution changes as the optimization process advances.

or worse (greater than 0) when applying a model trained on another problem class. For example, Ag- f_2 is trained on f_2 , when we zero-shot it directly to f_5 , it achieves a slightly lower performance than the f_5 's original agent by 4.356%, which is acceptable. Generally speaking, it can be observed from the table that the agents exhibit promising and even better performance on those different problem classes, which validates the good generalization of the trained policies on unseen problem classes.

5.3.2 Generalization to protein-docking application. The generalization analysis in above experiments is conducted within CEC problems. To further evaluate the generalization of GLEET, we introduce a realistic continuous optimization benchmark, Protein-Docking [11]. The benchmark contains 280 instances of different protein-protein complexes. These problems are characterized by rugged objective landscapes and are computationally expensive to evaluate. The distribution of Protein-Docking problems is significantly different from the CEC problems, we zero-shot the models agents trained on 10D f_{mix} problems to the Protein-Docking benchmark to evaluate the generalization of GLEET. All algorithms optimize 1000 $\max FEs$ on each problem instances. We collect their mean values, standard deviations and average runtime for runs in Table 3. Results show that GLEET-DMSPSO outperforms the comparison algorithms. The performance indicates that GLEET achieve remarkable generalization performance on different problems.

5.4 Interpretability

In this section, we take GLEET-PSO as an example to show GLEET's interpretability since the exploration and exploitation tradeoff (EET) is explicitly represented by the “ c_1 ” and “ c_2 ” in PSO's update formula, which facilitates easy interpretation and analysis. Fig. 3 illustrates how the distribution of EET hyper-parameter $c_{1,i}$ ¹ changes along the optimization process for two different problems: a relatively simple problem, the Schwefel (f_2) and a difficult one, the Hybrid (f_6). Here we let X-axis represent the optimization steps, Y-axis represent the distribution of the output actions, and Z-axis represent the current distribution of $c_{1,i}$ for all particles under the control of GLEET. It can be observed that our GLEET automatically controls the EET hyper-parameters throughout the search, with the patterns displayed first in exploration and then in exploitation till the conclusion of the iteration. Meanwhile, it is worth noting that GLEET favors a more complex EET control pattern for difficult problems such as the one shown in Fig. 3(b), where two rounds of exploration and exploitation emerge.

In Fig. 4, we further visualize how the attention among the population (in GLEET-PSO's decoder) affects the moving of particles to perform exploration or exploitation on a 2D toy problem. We highlight an exploration example and an exploitation example in the convergence curve shown in Fig. 4(a). Pertaining to the first case, we observe that the particle made a big improvement after taking the action. In Fig. 4(b), we can see that the particle is located near the centre of the search space, while the majority of the other particles are scattered to the right. The $pBest$ and $gBest$ particles are in two opposite directions. Note that in this case the most attended particle is a negative sample with a very worse fitness value, the current particle learns to strengthen the utilization of the exemplar located on a much different direction from this negative sample, which hence learns from the $pBest$ direction and achieves a great improvement. Pertaining to the second case in Fig. 4(c), the particle attends to the $gBest$ and decides to perform exploitation around it. This interpretable behavior verifies our analysis of choosing full attention in Section 4.2.

5.5 Ablation study

In this section we conduct ablation studies to verify the effectiveness of our network designs (Section 4.2) in the instantiation of GLEET to PSO. We also perform the ablation study on the GLEET's own EET embeddings and the reward function we have designed in Eq. (8) to examine their effectiveness in Appendix B.6 and B.7, respectively.

For the network designs ablation, specifically, we compare GLEET-PSO with its degraded versions “GLEET w/o EETs”, “GLEET w/o MHA”, and “GLEET w/o both”. Here, the first version removes the exploration and exploitation features in the states and thus the decoder could only perform self-attention based on FIPEs given that EETs are no longer available; the second variant removes all the MHA in the en/decoders; and the third variant removes both the first and the second designs. The results presented in Table 4 demonstrate the critical importance of both EETs and MHA in GLEET. The inclusion of EETs allows for explicit incorporation of exploration and exploitation information from the optimization

¹ $c_{1,i}$ is the individual impact coefficient in Eq. (3) but differs for different particles, while the social impact coefficient is $c_{2,i} = 4 - c_{1,i}$.

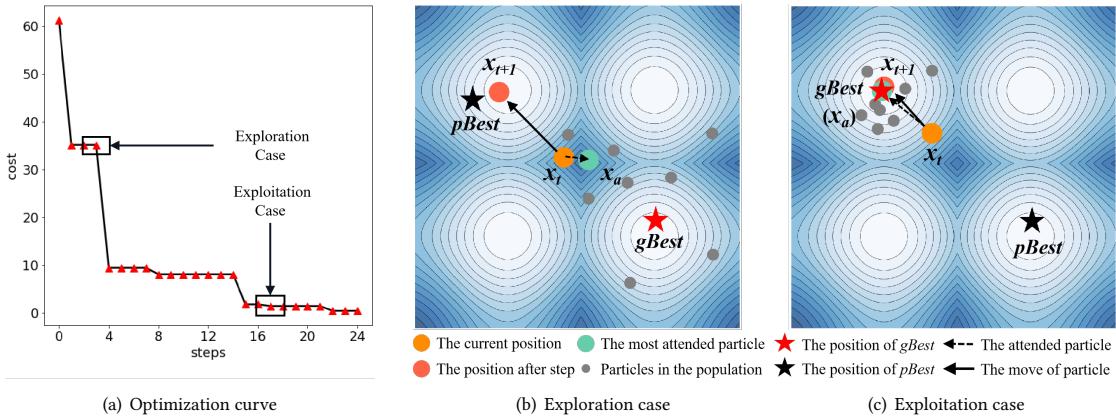


Figure 4: Visualization of the attention patterns and the moving of particles during exploration and exploitation controlled by GLEET. In Exploration case, GLEET leans to make the particle as far as possible from the most attended neighbour to get max exploration ability. In Exploitation case, GLEET leans to make the particle as close as possible to the most attended neighbour to reach the global optimum.

Table 4: Ablation studies on the the EET embeddings and the attention modules of GLEET, where the mean and standard deviations of ten runs on the test set are reported (with the best mean value on each problem highlighted in bold).

	Metric	f_1	f_2	f_3	f_4	f_5	f_6	f_7	f_8	f_9	f_{10}
w/o both	Mean	3.734E+06	6.055E+02	2.302E+01	1.849E+00	2.202E+03	9.543E+01	7.542E+02	3.633E+02	2.975E+02	2.222E+02
	(Std)	(7.314E+06)	(2.713E+02)	(6.237E+00)	(1.010E+00)	(3.284E+03)	(5.366E+01)	(7.417E+02)	(2.251E+02)	(6.088E+01)	(4.119E+01)
w/o EETs	Mean	3.345E+06	5.723E+02	2.252E+01	1.804E+00	2.050E+03	7.939E+01	7.034E+02	3.348E+02	2.351E+02	2.201E+02
	(Std)	(6.453E+06)	(2.018E+02)	(6.092E+00)	(1.003E+00)	(2.377E+03)	(6.198E+01)	(7.314E+02)	(2.507E+02)	(6.014E+02)	(3.414E+01)
w/o MHA	Mean	3.124E+06	5.066E+02	2.029E+01	1.710E+00	2.145E+03	8.159E+01	6.777E+02	3.132E+02	2.263E+02	2.180E+02
	(Std)	(5.269E+06)	(1.767E+02)	(4.273E+00)	(1.046E+00)	(2.540E+03)	(5.959E+01)	(6.397E+02)	(2.588E+02)	(6.031E+01)	(3.635E+01)
GLEET	Mean	2.748E+06	5.105E+02	2.120E+01	1.422E+00	1.847E+03	4.449E+01	4.977E+02	1.096E+02	1.665E+02	1.882E+02
	(Std)	(4.205E+06)	(1.776E+02)	(4.705E+00)	(7.776E-01)	(2.552E+03)	(3.381E+01)	(3.549E+02)	(3.924E+01)	(6.137E+01)	(4.127E+01)

process into the decoders. The fully-informed MHA plays a crucial role in facilitating the learning of more useful features through the interaction between individual embeddings of the population. This finding partly justifies the oversimplification of the network architectures used in existing learning-based approaches.

6 CONCLUSION

This paper proposed a generalizable GLEET framework for dynamic hyper-parameters tuning of the EET issue in EC algorithms. A novel MDP was formulated to support training on a class of problems, and then inference on the other unseen ones. We instantiated the GLEET to well-known EC algorithms by specially designing an attention-based network architecture that consists of a feature embedding module, a fully informed encoder, and an exploration-exploitation decoder. Experimental results verified that GLEET not only improves the backbone algorithms significantly, but also exhibits favorable generalization ability across different problem classes, dimensions, etc. However, there are still some limitations in this study. Although GLEET has shown the state-of-the-art generalization performance among the RL-based methods, the handcrafted population features and EET features based on the Fitness Landscape Analysis may still show vulnerability to high-dimensional scenario. Moreover, the population size of the backbone optimizer cannot change dynamically, since it will alter the action space of the MDP which makes the training meaningless. Future work includes

but is not limited to addressing the above limitations, in order to further boost the performance of learning-based EC algorithms.

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REFERENCES

- [1] Mohammad Javad Amoshay, Mousa Shamsi, and Mohammad Hossein Sedaaghi. 2016. A novel flexible inertia weight particle swarm optimization algorithm. *PLoS one* 11, 8 (2016), e0161558.
- [2] Jimmy Lei Ba, Jamie Ryan Kiros, and Geoffrey E Hinton. 2016. Layer normalization. In *Proceedings of the 30th Conference on Neural Information Processing Systems*.
- [3] Subhodip Biswas, Debanjan Saha, Shuvodeep De, Adam D Cobb, Swagatam Das, and Brian A Jalaiar. 2021. Improving differential evolution through Bayesian hyperparameter optimization. In *Proceedings of the 2021 IEEE Congress on Evolutionary Computation*. 832–840.
- [4] Jiacheng Chen, Zeyuan Ma, Hongshu Guo, Yining Ma, Jie Zhang, and Yue-jiao Gong. 2024. Symbol: Generating Flexible Black-Box Optimizers through Symbolic Equation Learning. In *The Twelfth International Conference on Learning Representations*.
- [5] Jie Chen, Bin Xin, Zihong Peng, Lihua Dou, and Juan Zhang. 2009. Optimal contraction theorem for exploration-exploitation tradeoff in search and optimization. *IEEE Transactions on Systems, Man, and Cybernetics* 39, 3 (2009), 680–691.

- [6] Ke Chen, Fengyu Zhou, Lei Yin, Shuqian Wang, Yugang Wang, and Fang Wan. 2018. A hybrid particle swarm optimizer with sine cosine acceleration coefficients. *Information Sciences* 422, - (2018), 218–241.
- [7] Maurice Clerc and James Kennedy. 2002. The particle swarm-explosion, stability, and convergence in a multidimensional complex space. *IEEE Transactions on Evolutionary Computation* 6, 1 (2002), 58–73.
- [8] Daniel Golovin, Benjamin Solnik, Subhodeep Moitra, Greg Kochanski, John Karro, and David Sculley. 2017. Google vizier: A service for black-box optimization. In *Proceedings of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*. 1487–1495.
- [9] Yue-Jiao Gong, Jing-Jing Li, Yicong Zhou, Yun Li, Henry Shu-Hung Chung, Yu-Hui Shi, and Jun Zhang. 2016. Genetic learning particle swarm optimization. *IEEE Transactions on Cybernetics* 46, 10 (2016), 2277–2290.
- [10] Hongshu Guo, Yining Ma, Zeyuan Ma, Jiacheng Chen, Xinglin Zhang, Zhiguang Cao, Jun Zhang, and Yue-Jiao Gong. 2024. Deep Reinforcement Learning for Dynamic Algorithm Selection: A Proof-of-Principle Study on Differential Evolution. *IEEE Transactions on Systems, Man, and Cybernetics: Systems*. to be published (2024), to be published.
- [11] Howook Hwang, Thom Vreven, Joël Janin, and Zhiping Weng. 2010. Protein-protein docking benchmark version 4.0. *Proteins: Structure, Function, and Bioinformatics* 78, 15 (2010), 3111–3114.
- [12] Sergey Ioffe and Christian Szegedy. 2015. Batch normalization: Accelerating deep network training by reducing internal covariate shift. In *Proceedings of the 32nd International conference on machine learning*. 448–456.
- [13] James Kennedy and Russell Eberhart. 1995. Particle swarm optimization. In *Proceedings of the International Conference on Neural Networks*. 1942–1948.
- [14] Yeong-Dae Kwon, Jinho Choo, Byoungjip Kim, Iljoo Yoon, Youngjune Gwon, and Seungjai Min. 2020. Pomo: Policy optimization with multiple optima for reinforcement learning. *Advances in Neural Information Processing Systems* 33, - (2020), 21188–21198.
- [15] Robert Lange, Tom Schaul, Yutian Chen, Chris Lu, Tom Zahavy, Valentin Dalibard, and Sebastian Flennerhag. 2023. Discovering Attention-Based Genetic Algorithms via Meta-Black-Box Optimization. In *Proceedings of the Genetic and Evolutionary Computation Conference*.
- [16] Robert Tjarko Lange, Tom Schaul, Yutian Chen, Tom Zahavy, Valentin Dalibard, Chris Lu, Satinder Singh, and Sebastian Flennerhag. 2022. Discovering Evolution Strategies via Meta-Black-Box Optimization. In *Proceedings of the 11th International Conference on Learning Representations*.
- [17] Jing J Liang, L Guo, R Liu, and Bo-Yang Qu. 2015. A self-adaptive dynamic particle swarm optimizer. In *Proceedings of the 2015 IEEE Congress on Evolutionary Computation*. 3206–3213.
- [18] Jane-Jing Liang and Ponnuthurai Nagaratnam Suganthan. 2005. Dynamic multi-swarm particle swarm optimizer. In *Proceedings of 2005 IEEE Swarm Intelligence Symposium*. 124–129.
- [19] Timothy P Lillicrap, Jonathan J Hunt, Alexander Pritzel, Nicolas Heess, Tom Erez, Yuval Tassa, David Silver, and Daan Wierstra. 2015. Continuous control with deep reinforcement learning. *arXiv preprint arXiv:1509.02971* (2015).
- [20] Yaxian Liu, Hui Lu, Shi Cheng, and Yuhui Shi. 2019. An adaptive online parameter control algorithm for particle swarm optimization based on reinforcement learning. In *Proceedings of the 2019 IEEE Congress on Evolutionary Computation*. 815–822.
- [21] Nandar Lynn and Ponnuthurai Nagaratnam Suganthan. 2017. Ensemble particle swarm optimizer. *Applied Soft Computing* 55, 3 (2017), 533–548.
- [22] Yining Ma, Jingwen Li, Zhiguang Cao, Wen Song, Hongliang Guo, Yuejiao Gong, and Yeow Meng Chee. 2022. Efficient Neural Neighborhood Search for Pickup and Delivery Problems. In *Proceedings of the 31st International Joint Conference on Artificial Intelligence*. 4776–4784.
- [23] Zeyuan Ma, Hongshu Guo, Jiacheng Chen, Zhenrui Li, Guojun Peng, Yue-Jiao Gong, Yining Ma, and Zhiguang Cao. 2023. MetaBox: A Benchmark Platform for Meta-Black-Box Optimization with Reinforcement Learning. *Advances in Neural Information Processing Systems* 36 (2023).
- [24] Florian Mischek and Nysret Musliu. 2022. Reinforcement Learning for Cross-Domain Hyper-Heuristics. In *Proceedings of the 31st International Joint Conference on Artificial Intelligence*. 4793–4799.
- [25] Ali Wagdy Mohamed, Anas A Hadi, Ali Khater Mohamed, Prachi Agrawal, Abhishek Kumar, and P. N. Suganthan. 2021. Problem definitions and evaluation criteria for the cec 2021 on Single Objective Bound Constrained Numerical Optimization. In *Proceedings of the 2021 IEEE Congress on Evolutionary Computation*.
- [26] Marco S Nobile, Paolo Cazzaniga, Daniela Besozzi, Riccardo Colombo, Giancarlo Mauri, and Gabriella Pasi. 2018. Fuzzy Self-Tuning PSO: A settings-free algorithm for global optimization. *Swarm and Evolutionary Computation* 39, - (2018), 70–85.
- [27] Asanga Ratnaweera, Saman K Halgamuge, and Harry C Watson. 2004. Self-organizing hierarchical particle swarm optimizer with time-varying acceleration coefficients. *IEEE Transactions on Evolutionary Computation* 8, 3 (2004), 240–255.
- [28] Hussein Samma, Chee Peng Lim, and Junita Mohamad Saleh. 2016. A new reinforcement learning-based memetic particle swarm optimizer. *Applied Soft Computing* 43, 3 (2016), 276–297.
- [29] Erhard Schmidt. 1907. Zur Theorie der linearen und nichtlinearen Integralgleichungen. *Math. Ann.* 63, 4 (1907), 433–476.
- [30] John Schulman, Filip Wolski, Prafulla Dhariwal, Alec Radford, and Oleg Klimov. 2017. Proximal policy optimization algorithms. *arXiv preprint arXiv:1707.06347* (2017).
- [31] Mudita Sharma, Alexandros Komninos, Manuel López-Ibáñez, and Dimitar Kazakov. 2019. Deep reinforcement learning based parameter control in differential evolution. In *Proceedings of the Genetic and Evolutionary Computation Conference*. 709–717.
- [32] Yuhui Shi and Russell Eberhart. 1998. A modified particle swarm optimizer. In *Proceedings of the IEEE World Congress on Computational Intelligence*. 69–73.
- [33] Yuhui Shi and Russell C Eberhart. 1999. Empirical study of particle swarm optimization. In *Proceedings of the 1999 Congress on Evolutionary Computation*. 1945–1950.
- [34] Adam Slowik and Halina Kwasnicka. 2020. Evolutionary algorithms and their applications to engineering problems. *Neural Computing and Applications* 32, 16 (2020), 12363–12379.
- [35] Vladimir Stanovov, Shakhnaz Akhmedova, and Eugene Semenkin. 2022. NL-SHADE-LBC algorithm with linear parameter adaptation bias change for CEC 2022 Numerical Optimization. In *Proceedings of the 2022 IEEE Congress on Evolutionary Computation*. 01–08.
- [36] Rainer Storn and Kenneth Price. 1997. Differential evolution—a simple and efficient heuristic for global optimization over continuous spaces. *Journal of Global Optimization* 11, 4 (1997), 341–359.
- [37] Jianyong Sun, Xin Liu, Thomas Bäck, and Zongben Xu. 2021. Learning adaptive differential evolution algorithm from optimization experiences by policy gradient. *IEEE Transactions on Evolutionary Computation* 25, 4 (2021), 666–680.
- [38] Richard S Sutton and Andrew G Barto. 2018. *Reinforcement learning: An introduction*. MIT press.
- [39] Zhiping Tan and Kangshun Li. 2021. Differential evolution with mixed mutation strategy based on deep reinforcement learning. *Applied Soft Computing* 111, - (2021), 107678.
- [40] Zhiping Tan, Yu Tang, Kangshun Li, Huasheng Huang, and Shaoming Luo. 2022. Differential evolution with hybrid parameters and mutation strategies based on reinforcement learning. *Swarm and Evolutionary Computation* 75, - (2022), 101194.
- [41] Ryoji Tanabe and Alex S Fukunaga. 2014. Improving the search performance of SHADE using linear population size reduction. In *Proceedings of the 2014 IEEE Congress on Evolutionary Computation*. 1658–1665.
- [42] Muhammad Rizwan Tanweer, Sundaram Suresh, and Narasimhan Sundararajan. 2015. Self regulating particle swarm optimization algorithm. *Information Sciences* 294, 10 (2015), 182–202.
- [43] Robert Tjarko Lange, Yingtao Tian, and Yujin Tang. 2024. Evolution Transformer: In-Context Evolutionary Optimization. *arXiv e-prints* (2024), arXiv-2403.
- [44] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. 2017. Attention is all you need. In *Proceedings of the 31st Conference on Neural Information Processing Systems*. 5998–6008.
- [45] Dongshu Wang, Dapei Tan, and Lei Liu. 2018. Particle swarm optimization algorithm: an overview. *Soft Computing* 22, 2 (2018), 387–408.
- [46] Di Wu and G Gary Wang. 2022. Employing reinforcement learning to enhance particle swarm optimization methods. *Engineering Optimization* 54, 2 (2022), 329–348.
- [47] Xuewen Xia, Ying Xing, Bo Wei, Yinglong Zhang, Xiong Li, Xianli Deng, and Ling Gui. 2019. A fitness-based multi-role particle swarm optimization. *Swarm and Evolutionary Computation* 44, - (2019), 349–364.
- [48] Yue Xu and Dechang Pi. 2020. A reinforcement learning-based communication topology in particle swarm optimization. *Neural Computing and Applications* 32, 14 (2020), 10007–10032.
- [49] Ke Xue, Jiacheng Xu, Lei Yuan, Miqing Li, Chao Qian, Zongzhang Zhang, and Yang Yu. 2022. Multi-agent Dynamic Algorithm Configuration. In *Proceedings of the 36th Conference on Neural Information Processing Systems*.
- [50] Qingyong Yang, Shu-Chuan Chu, Jeng-Shyang Pan, Jyh-Horng Chou, and Junzo Watada. 2023. Dynamic multi-strategy integrated differential evolution algorithm based on reinforcement learning for optimization problems. *Complex & Intelligent Systems* (2023), 1–33.
- [51] Shiyuan Yin, Yi Liu, GuoLiang Gong, Huaxiang Lu, and Wenchang Li. 2021. RLEPSO: Reinforcement learning based Ensemble particle swarm optimizer*. In *Proceedings of the 4th International Conference on Algorithms, Computing and Artificial Intelligence*. 1–6.
- [52] Manzil Zaheer, Guru Guruganesh, Kumar Avinava Dubey, Joshua Ainslie, Chris Alberti, Santiago Ontanon, Philip Pham, Anirudh Ravula, Qifan Wang, Li Yang, et al. 2020. Big bird: Transformers for longer sequences. In *Proceedings of the 33th Conference on Neural Information Processing Systems*. 17283–17297.
- [53] Jingqiao Zhang and Arthur C Sanderson. 2009. JADE: adaptive differential evolution with optional external archive. *IEEE Transactions on Evolutionary Computation* 13, 5 (2009), 945–958.

A EXPERIMENTAL SETTINGS

A.1 Parameter Settings

Following the suggestion of Ali et al. [25], the maximum number of function evaluations (*maxFEs*) for all algorithms in experiments is set to 2×10^5 for 10D and 10^6 for 30D problems. The search space of all problems is a real-parameter space $[o_{min}, o_{max}]^d$ with $o_{min} = -100$ and $o_{max} = 100$. We accelerate the learning and testing process through batching problem instances in the training set and testing set, with *batch_size* = 16. For the optimization of each instance, GLEET agent acquires states from the population with $N = 100$ and samples hyper-parameters. For every $T = 10$ steps of optimization, the agent updates its network for $\kappa = 3$ steps in an PPO algorithmic manner. The training runs *MaxEpoch* = 100 with the learning rates $lr = 4e-5$ and decays to $1e-5$ at the end for both policy net and critic net. We present the RL hyper-parameter analysis in Appendix B.8. For the fairness of comparison, all learning based algorithms update their model by equal steps. The rest configurations of comparison algorithms follow that proposed in corresponding original papers. Experiments are run on Intel i9-10980XE CPU, RTX 3090 GPU and 32GB RAM. When testing, each algorithm executes 10 independent runs and reports the statistical results.

A.2 Dataset augmentation

The CEC 2021 numerical optimization test suite by Ali et al. [25] consists of ten challenging black-box optimization problems. The f_1, f_2, f_3 and f_4 are single problems which are not any problems' hybridization or composition. For example, Bent Cigar function (f_1) has the form as $f(\mathbf{x}) = x_1^2 + 10^6 \sum_{i=2}^d x_i^2$, where d is the dimension of \mathbf{x} . The f_5, f_6 and f_7 hybridize some basic functions, resulting more difficult problem because of solution space coupling. The f_8, f_9 and f_{10} are linear compositions of some single problems, resulting more difficult problem because of fitness space coupling. Each problem has the form $F(\mathbf{x}) = f(M^T(\mathbf{x}-\mathbf{o}))$, where f is the objective function, \mathbf{o} is shift vector of the global optimum position, M is the rotation matrix of the entire problem space, and we have the optimal cost as 0 for all the cases. We then augment these ten problems to their problem sets by adding different shift and rotation. To be concrete, for a function f_i , we firstly generate a random shift with a range $[o_{min}, o_{max}]$ which assures that the optimum of the shifted problem instances will not escape from the present search space. Then we generate a random standard orthogonal matrix M [29] and then apply it to the shifted function instance. By repeatedly applying these two transformations above, we can get an augmented problem sets D . As one purpose of this study is to perform generalizable learning on a class of problems, we construct an augmented dataset D of a large number of benchmark problem instances. Specifically, for each problem class in the CEC 2021, a total number of 1152 instances are randomly generated and divided into training and testing sets with a partition of 128:1024 (note that we use small training but large testing sets to fully validate the generalization). We train one GLEET agent per problem class and also investigate the performance of GLEET if trained on a mixed dataset containing all the problem classes (all ten functions with different M and \mathbf{o} in a training set), denoted as f_{mix} .

B ADDITIONAL EXPERIMENTAL RESULTS

B.1 Comparison on the 30D problems

Table 5 shows the optimization results and the ranks obtained by different PSO algorithms over the ten problem classes on 30D spaces as a supplement to Table 1 in the paper. Both GLEET-PSO and GLEET-DMSPSO still significantly improve their backbones. Manual adaptive variants sDMSPSO can not improve the backbone DMSPSO on 30D problems (considering the average rank) but dominates others on some specific functions such as f_5 and f_7 . The advantage of GLEET on 30D spaces is more significant than that on 10D spaces in Table 1, which further verified the conclusion mentioned in Section 5.2 that GLEET may perform more stable on complex problem, which is favorable.

B.2 Comparison among the DE variants

In this section we extend the application of GLEET to DE algorithms which used mutation, crossover and selection to handle a population of solution vectors iteratively and search optimal solution using the difference among population individuals. At each iteration t , the mutation operator is applied on individuals to generate trial vectors. One of the classic mutation operators DE/current-to-pbest/1 on the individual x_i could be formulated as

$$v_i^{(t)} = x_i^{(t-1)} + F_{i,1}^{(t)} \cdot (x_{tpb}^{(t-1)} - x_i^{(t-1)}) + F_{i,2}^{(t)} \cdot (x_{r1}^{(t-1)} - x_{r2}^{(t-1)}) \quad (11)$$

where $F_{i,1}^{(t)}$ and $F_{i,2}^{(t)}$ are the step lengths controlling the variety of trials, $x_{tpb}^{(t-1)}$ is the random selected individual from the top- $p\%$ best cost individuals, $x_{r1}^{(t-1)}$ and $x_{r2}^{(t-1)}$ are two different random selected individuals. Then, the crossover is adopted to exchange values between the parent $x_i^{(t-1)}$ and the trial individual $v_i^{(t)}$ to produce an offspring $u_i^{(t)}$:

$$u_{i,j}^{(t)} = \begin{cases} v_{i,j}^{(t)} & \text{if } \text{rand}[0, 1] \leq Cr_i^{(t)} \text{ or } j = jrand \\ x_{i,j}^{(t-1)} & \text{otherwise} \end{cases} \quad (12)$$

where $u_{i,j}^{(t)}$ is the j -th value of the individual $u_i^{(t)}$ and so do the items for $x_i^{(t-1)}$ and $v_i^{(t)}$. The $Cr_i^{(t)}$ is the crossover rate and $jrand$ is an index to ensure the difference between $u_i^{(t)}$ and $x_i^{(t)}$. Finally, the selection method eliminates those individuals with worse fitness than their parents.

As mentioned in Section 4.2.3, we let $M = 1$ to control $c_{1,i}$ for each particle i in GLEET-PSO and GLEET-DMSPSO. Here for DE, we set $M = 3$ to control $F_{1,i}, F_{2,i}$ and Cr_i in Eq. (11) and Eq. (12).

For baselines, we choose the DE/current-to-pbest/1 [53] as static baseline, the DE variants MadDE [3], NL-SHADE-LBC [35] as adaptive baselines, and DE-DDQN [31], DEDQN [39], LDE [37], RLD-MDE [50], RLPSDE [40] as the learning-based competitors. We instantiate GLEET on DE/current-to-pbest/1 to join the comparison, denoted as GLEET-DE.

Table 6 and Table7 shows the optimization results and the ranks obtained by different DE algorithms over the eleven problem classes on 10D and 30D spaces respectively. A consistent conclusion can be deduced as the results above on PSO algorithms. Additionally, it can be noticed that, by taking DE as backbone, the GLEET-DE performs generally better than the GLEET-PSO algorithm.

Table 5: Numerical comparison results for PSO algorithms on 30D problems, where the mean, standard deviations and performance ranks are reported (with the best mean value on each problem highlighted in bold).

Type Algorithm	Static		Adaptive						DRL							
	PSO		DMSPSO		sDMSPSO		GLPSO		DRL-PSO		RLEPSO		GLEET-PSO		GLEET-DMSPSO	
	Metrics	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	
f_1	2.261E+08 (2.343E+08)	6	4.491E+07 (2.733E+07)	4	1.319E+06 (1.444E+06)	2	4.568E+05 (4.164E+05)	1	9.316E+08 (9.470E+08)	8	2.616E+08 (1.591E+08)	7	1.336E+08 (1.512E+08)	5	9.731E+06 (6.314E+06)	3
f_2	4.022E+03 (6.617E+02)	8	3.114E+03 (5.146E+02)	3	3.248E+03 (4.834E+02)	4	2.841E+03 (7.063E+02)	2	3.759E+03 (6.517E+02)	6	3.998E+03 (3.071E+02)	7	3.442E+03 (5.692E+02)	5	2.648E+03 (5.041E+02)	1
f_3	2.070E+02 (5.150E+01)	7	1.006E+02 (1.475E+01)	3	2.772E+02 (5.886E+01)	8	6.921E+01 (1.156E+01)	2	1.486E+02 (4.956E+01)	4	1.884E+02 (2.173E+01)	6	1.552E+02 (3.701E+01)	5	6.613E+01 (1.146E+01)	1
f_4	2.762E+01 (1.660E+01)	6	1.066E+01 (3.076E+00)	3	5.738E+01 (4.634E+01)	7	6.644E+00 (2.526E+00)	1	1.237E+03 (2.401E+03)	8	1.860E+01 (1.087E+01)	5	1.680E+01 (9.320E+00)	4	9.433E+00 (2.633E+00)	2
f_5	3.972E+05 (4.395E+05)	7	7.148E+04 (8.678E+04)	4	2.653E+03 (1.441E+032)	1	3.050E+04 (1.763E+04)	2	7.231E+05 (1.119E+06)	8	3.893E+05 (1.578E+05)	6	1.868E+05 (1.921E+05)	5	6.751E+04 (5.630E+04)	3
f_6	9.998E+02 (3.003E+02)	8	3.778E+02 (1.581E+02)	3	5.722E+02 (1.994E+02)	4	3.162E+02 (1.816E+02)	2	9.500E+02 (3.291E+02)	7	8.127E+02 (1.257E+02)	6	6.880E+02 (2.149E+02)	5	3.114E+02 (1.159E+02)	1
f_7	1.222E+05 (1.469E+05)	7	2.110E+04 (2.143E+04)	4	1.387E+03 (6.703E+02)	1	2.011E+04 (1.024E+04)	3	2.680E+05 (4.235E+05)	8	4.652E+04 (4.199E+04)	5	4.930E+04 (4.420E+04)	6	1.817E+04 (1.299E+04)	2
f_8	3.659E+03 (1.379E+03)	7	1.009E+03 (6.969E+02)	2	2.185E+03 (1.061E+031)	4	1.774E+03 (1.002E+03)	3	3.196E+03 (1.347E+03)	6	3.867E+03 (6.564E+02)	8	2.414E+03 (1.283E+03)	5	8.505E+02 (5.703E+02)	1
f_9	7.835E+02 (1.345E+02)	8	4.079E+02 (2.885E+01)	3	5.335E+02 (5.327E+01)	4	4.069E+02 (1.860E+01)	2	7.194E+02 (1.191E+02)	6	7.323E+02 (5.245E+01)	7	6.377E+02 (9.189E+01)	5	3.941E+02 (2.848E+01)	1
f_{10}	4.158E+02 (7.642E+01)	6	2.984E+02 (3.578E+01)	4	2.765E+02 (2.845E+01)	2	2.836E+02 (3.336E+01)	3	6.963E+02 (3.283E+02)	8	4.222E+02 (3.785E+01)	7	3.930E+02 (7.612E+01)	5	2.608E+02 (2.852E+01)	1
f_{mix}	2.218E+07 (3.048E+07)	7	5.774E+06 (3.103E+06)	4	6.366E+04 (6.227E+04)	3	5.313E+04 (4.039E+04)	2	1.948E+07 (3.566E+07)	6	4.438E+07 (3.849E+07)	8	7.452E+06 (6.845E+06)	5	4.894E+04 (4.098E+04)	1
Avg Rank	7.00	3.36	3.64	2.09				6.82	6.54	5.00 (↑ 35%)		1.55 (↑ 28%)				

Table 6: Numerical comparison results for DE algorithms on 10D problems, where the mean, standard deviations and performance ranks are reported (with the best mean value on each problem highlighted in bold).

Type Algorithm	Static		Adaptive						DRL						GLEET-DE			
	DE		MadDE		NL-SHADE-LBC		DE-DDQN		DE-DQN		LDE		RLPSDE		RLDMDE		GLEET-DE	
	Metrics	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	
f_1	6.423E+06 (6.523E+06)	9	7.951E-09 (1.447E-09)	3	6.545E-09 (1.017E-09)	2	5.631E+06 (4.565E+06)	6	5.723E+06 (5.065E+06)	7	3.855E+04 (6.856E+04)	4	6.453E+04 (1.142E+05)	5	6.333E+06 (6.246E+06)	8	1.136E-09 (1.789E-09)	1
f_2	7.699E+02 (2.037E+02)	9	3.911E+02 (1.108E+02)	2	3.843E+02 (1.198E-02)	1	7.534E+02 (1.867E-02)	7	6.811E+02 (2.134E+02)	6	5.999E+02 (1.190E+02)	4	6.358E+02 (1.842E+02)	5	7.593E+02 (2.753E+02)	8	4.522E+02 (1.403E+02)	3
f_3	2.099E+01 (2.393E+00)	6	1.793E+01 (2.489E+00)	2	1.821E+01 (2.430E+00)	3	3.052E+01 (2.355E+00)	8	3.242E+01 (3.564E+00)	9	1.903E+01 (1.675E+00)	4	2.101E+01 (1.716E+00)	7	1.971E+01 (2.123E+00)	5	1.746E+01 (2.419E+00)	1
f_4	1.329E+00 (3.606E-01)	9	5.161E-01 (1.722E-01)	2	5.234E-01 (1.587E-01)	3	1.265E+00 (3.545E-01)	7	1.054E+00 (3.455E-01)	6	6.172E-01 (2.464E-01)	4	7.886E-01 (2.646E-01)	5	1.311E+00 (3.297E-01)	8	4.990E-01 (1.629E-01)	1
f_5	1.747E+02 (9.863E+01)	7	1.789E+01 (2.175E+01)	2	1.711E+01 (2.543E+01)	1	1.652E+02 (9.665E+01)	6	1.795E+02 (1.005E+02)	8	3.719E+01 (3.878E+01)	4	3.831E+01 (3.857E+01)	5	3.573E+01 (9.993E+01)	9	3.274E+01 (3.274E+01)	3
f_6	1.303E+01 (6.778E+00)	6	5.160E+00 (3.277E+00)	3	3.735E+00 (2.178E+00)	2	1.132E+02 (9.545E+00)	7	1.359E+02 (9.426E+00)	8	6.269E+00 (5.417E+00)	4	6.569E+00 (5.851E+00)	5	1.366E+01 (6.179E+00)	9	6.671E-01 (1.448E+00)	1
f_7	4.726E+01 (4.073E+01)	9	9.162E+00 (9.163E+00)	3	8.424E+00 (8.127E+00)	2	3.656E+01 (3.212E+01)	6	4.598E+01 (3.532E+01)	7	1.278E+01 (1.552E+01)	4	1.953E+01 (2.354E+01)	5	4.612E+01 (3.831E+01)	8	8.226E+00 (1.497E+01)	1
f_8	6.803E+01 (1.136E+01)	4	5.757E+01 (1.659E+01)	3	5.014E+01 (1.451E+01)	2	6.956E+01 (1.215E+01)	5	7.083E+01 (1.125E+01)	6	8.867E+01 (1.832E+01)	9	8.241E+01 (1.687E+01)	8	7.800E+01 (1.448E+01)	7	5.349E+01 (1.627E+01)	1
f_9	1.765E+02 (2.277E+01)	9	8.424E+01 (3.828E+01)	1	8.765E+01 (3.934E+01)	2	1.533E+02 (2.545E+01)	5	1.456E+02 (1.916E+01)	4	1.612E+02 (3.313E+01)	7	1.655E+02 (3.438E+01)	8	1.588E+02 (1.732E+01)	6	1.249E+02 (5.208E+01)	3
f_{10}	2.370E+02 (1.769E+01)	9	1.865E+02 (1.008E+01)	1	1.894E+02 (1.132E+01)	2	2.342E+02 (1.615E+01)	8	2.245E+02 (1.531E+01)	7	1.994E+02 (1.284E+01)	4	2.124E+02 (1.142E+01)	5	2.166E+02 (1.697E+01)	6	1.937E+02 (1.211E+01)	3
f_{mix}	1.733E+02 (7.912E+01)	8	7.570E+01 (2.311E+01)	2	7.413E+01 (2.234E+01)	1	1.681E+02 (7.456E+01)	5	1.762E+02 (6.465E+01)	9	1.564E+02 (3.656E+01)	4	1.724E+02 (3.773E+01)	6	1.726E+02 (3.851E+01)	7	1.340E+02 (3.851E+01)	3
Avg Rank	7.73	2.18	1.91				6.36	7.00	4.72		5.82		7.36		1.91 (↑ 52%)			

B.3 Generalization across dimensions and population sizes

We train GLEET-PSO on 10D problem, denoted as GLEET-10D, and apply the model to optimize 30D problems. The performance of GLEET-10D is compared with the original PSO and the GLEET-30D model trained on 30D problems. Fig. 5 depicts the convergence curves on the 10D problems for illustration, where we also annotate the “Gap” to quantify the final generalization bias. Without any further tuning, GLEET-10D outperforms the original PSO and with a well acceptable gap to GLEET-30D on most of the problems, which further verifies that GLEET is generalizable between

different problem dimensions owing to our dimension-free state representation in Section 4.1. In Fig. 6, GLEET-500Pop is the model trained with population size 500 while GLEET-100Pop is trained on population size 100. They are both tested on the scenario of 500 population size. We show that GLEET-100Pop outperforms not only the original PSO but also the GLEET-500Pop on most of the problems. This indicates that, on the one hand, the proposed attention-based en/decoder supports the generalization to a different population size; and on the other hand, through good EET control, a population of 100 particles is sufficient to provide good optimization results.

Table 7: Numerical comparison results for DE algorithms on 30D problems, where the mean, standard deviations and performance ranks are reported (with the best mean value on each problem highlighted in bold).

Type	Static		Adaptive				DRL											
	DE		MadDE		NL-SHADE-LBC		DE-DDQN		DE-DQN		LDE		RLPSDE		RLDMDE		GLEET-DE	
Algorithm	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank	Mean (Std)	Rank
f_1	1.658E+09 (5.924E+08)	9	7.098E+03 (7.247E+03)	3	6.234E+03 (6.435E+03)	2	5.362E+08 (4.631E+07)	6	5.659E+08 (4.355E+07)	8	4.563E+04 (3.624E+03)	4	4.863E+04 (3.731E+03)	5	5.653E+08 (4.662E+07)	7	1.639E-01 (4.818E-01)	1
f_2	6.033E+03 (3.499E+02)	9	2.421E+03 (2.690E+02)	2	2.134E+03 (2.121E+02)	1	4.563E+03 (3.612E+02)	4	4.327E+03 (3.121E+02)	5	5.325E+03 (3.205E+02)	6	5.877E+03 (3.643E+02)	8	5.476E+03 (3.345E+02)	7	3.083E+03 (2.838E+02)	3
f_3	1.701E+02 (2.740E+01)	8	7.796E+01 (7.228E+00)	3	7.345E+01 (7.048E+00)	2	1.673E+02 (2.445E+01)	6	1.995E+02 (2.853E+01)	9	1.456E+02 (1.656E+01)	4	1.683E+02 (1.343E+01)	7	1.669E+02 (2.136E+01)	5	6.733E+01 (8.379E+00)	1
f_4	1.741E+01 (8.485E+00)	9	6.168E+00 (1.003E+00)	1	6.867E+00 (1.353E+00)	2	1.447E+01 (7.456E+00)	6	1.698E+01 (8.334E+00)	7	8.366E+00 (5.546E+00)	4	1.135E+01 (9.312E+00)	5	1.705E+01 (8.045E+00)	8	7.468E+00 (3.679E+00)	3
f_5	4.503E+04 (4.176E+04)	9	1.183E+03 (3.542E+02)	2	1.023E+03 (3.334E+02)	1	1.463E+04 (3.642E+03)	8	1.386E+04 (4.545E+03)	7	3.945E+03 (5.645E+02)	4	4.895E+03 (5.997E+02)	5	5.464E+03 (8.760E+02)	6	3.099E+03 (4.503E+02)	3
f_6	2.192E+02 (1.003E+02)	5	2.127E+02 (7.915E+01)	2	2.169E+02 (7.043E+01)	4	2.362E+02 (1.406E+02)	8	2.458E+02 (1.556E+02)	9	2.155E+02 (9.615E+01)	3	2.301E+02 (1.137E+02)	6	2.341E+02 (1.549E+02)	7	1.705E+02 (5.046E+01)	1
f_7	1.056E+04 (9.032E+03)	9	5.156E+02 (2.473E+02)	3	4.675E+02 (2.122E+02)	2	1.037E+03 (6.373E+02)	7	1.652E+03 (5.193E+02)	8	7.893E+02 (2.435E+02)	4	8.961E+02 (3.154E+02)	5	9.465E+02 (2.977E+02)	6	3.788E+02 (2.277E+02)	1
f_8	1.620E+03 (1.188E+03)	9	1.501E+02 (7.258E+01)	3	1.443E+02 (7.345E+01)	2	7.693E+02 (3.543E+02)	6	7.798E+02 (3.523E+02)	7	3.453E+02 (8.816E+01)	5	3.410E+02 (8.311E+01)	4	7.868E+02 (4.798E+02)	8	1.375E+02 (7.646E+01)	1
f_9	4.227E+02 (2.089E+01)	4	3.989E+02 (1.330E+01)	1	4.231E+02 (1.437E+01)	5	4.313E+02 (2.345E+02)	7	5.015E+02 (2.577E+02)	9	4.132E+02 (1.346E+02)	3	4.303E+02 (1.825E+02)	6	4.741E+02 (2.334E+01)	8	4.105E+02 (1.523E+02)	2
f_{10}	5.177E+02 (7.687E+01)	9	2.660E+02 (3.307E+00)	2	2.101E+02 (2.744E+00)	1	4.637E+02 (6.756E+01)	6	4.879E+02 (7.231E+01)	8	4.025E+02 (3.445E+01)	4	4.333E+02 (4.131E+01)	5	4.869E+02 (7.132E+01)	7	3.532E+02 (2.357E+01)	3
f_{mix}	7.324E+07 (7.104E+07)	9	7.193E+03 (2.803E+03)	3	6.831E+03 (2.435E+03)	2	4.337E+07 (5.156E+07)	6	5.237E+07 (3.460E+07)	7	4.354E+04 (3.641E+03)	4	5.610E+04 (3.451E+03)	5	5.379E+07 (3.974E+07)	8	6.356E+03 (4.325E+03)	1
Avg Rank	8.09	2.27	2.18		6.36	7.64	4.09		5.55		7.00		1.82	(↑ 64%)				

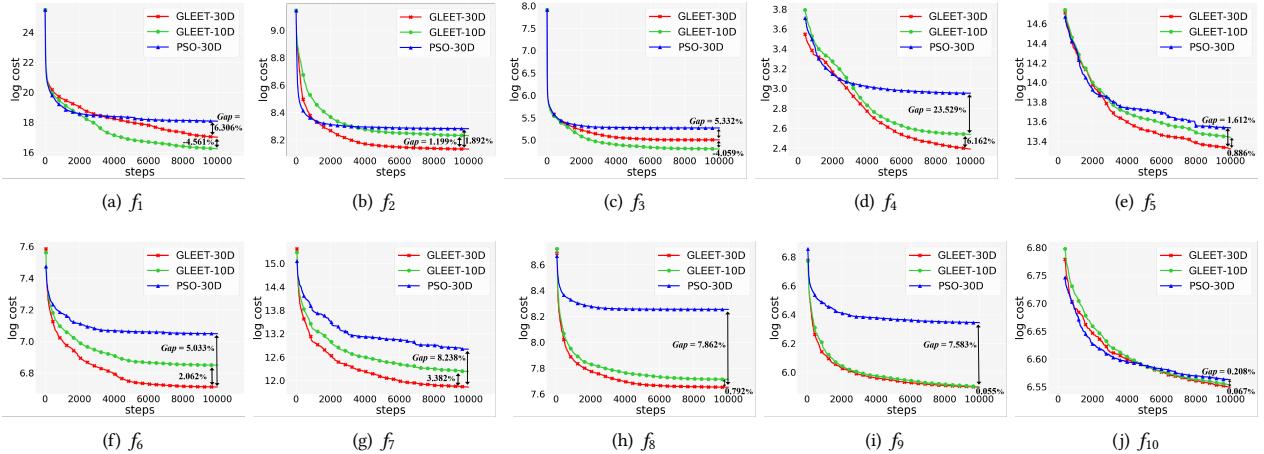


Figure 5: Generalization across different problem dimensions.

B.4 Generalization beyond optimization horizon

Running the agent for more generations than the training horizon is a well-known challenge for meta-learned optimizers. To reveal GLEET’s generalization ability across generations, we run GLEET-DMSPSO trained with $2e5$ maxFEs for more generations (up to $1e6$ maxFEs) and compare it with DMSPSO. Fig. 7 shows the generalization performance on 10D Schwefel (f_2) problems. It can be seen that comparing to the DMSPSO, GLEET-DMSPSO has a larger cost decrease alone the generations, indicating that GLEET agent has learned how to deal with a longer episode and improves the performance of the backbone DMSPSO.

B.5 Impact of Training set size

Existing RL-based optimizers were trained on a single or a few of problem instances. Although experiments in Section 5.2 have validated the effectiveness of GLEET, the relationship between the performance and the training set size remains to be explored. To showcase the benefits of training the policy on a distribution of problems, we train GLEET-DMSPSO with different training set sizes: 1, 16, 64, 256 and 1024. Taking 10D Schwefel (f_2) as a case, the performance of GLEET-DMSPSO is shown in Fig. 8. The results demonstrate that training agents on a set of problem instances may lead to a better performance than training on a single instance, which aligns with our motivations and conclusions. This may be because a larger training set allows the agent to capture full knowledge about the problem distribution and utilize the knowledge to adaptively control the

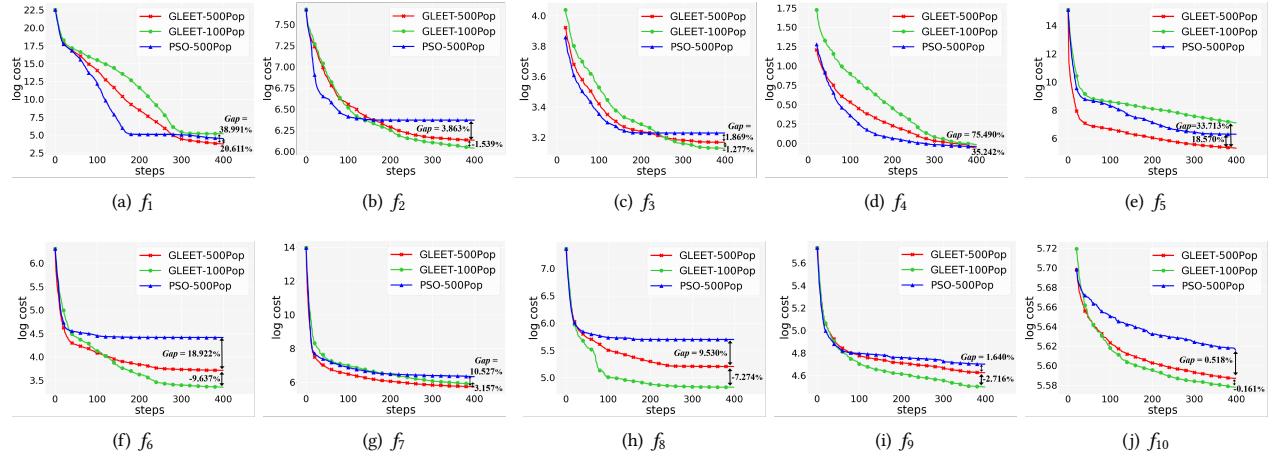


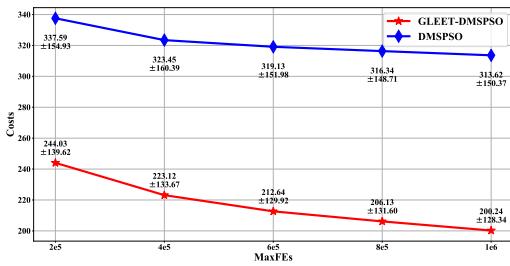
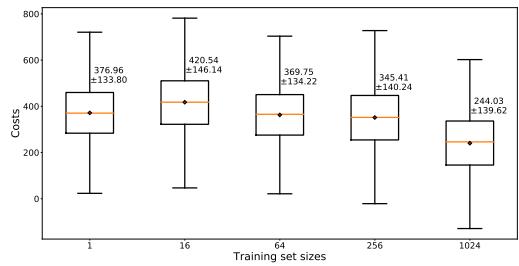
Figure 6: Generalization across different population sizes.

Table 8: Ablation studies on the state representation, where the mean and standard deviations of ten runs on the test set are reported (with the best mean value on each problem highlighted in bold).

	Metric	f_1	f_2	f_3	f_4	f_5	f_6	f_7	f_8	f_9	f_{10}
w/o $s_{1\sim 4}$	Mean	3.546E+06	6.672E+02	2.412E+01	1.745E+00	2.163E+03	7.329E+01	7.588E+02	5.971E+02	3.610E+02	2.876E+02
	(Std)	(6.675E+06)	(2.965E+02)	(6.153E+00)	(1.331E+00)	(2.974E+03)	(4.993E+01)	(7.464E+02)	(3.699E+02)	(6.631E+01)	(4.273E+01)
w/o $s_{5\sim 6}$	Mean	3.376E+06	6.034E+02	2.358E+01	1.773E+00	2.189E+03	6.912E+01	7.331E+02	2.062E+02	3.034E+02	2.766E+02
	(Std)	(5.975E+06)	(2.311E+02)	(6.274E+00)	(1.231E+00)	(2.112E+03)	(6.134E+01)	(7.762E+02)	(2.371E+02)	(6.237E+02)	(4.130E+01)
w/o $s_{7\sim 9}$	Mean	3.383E+06	5.977E+02	2.316E+01	1.786E+00	2.107E+03	6.812E+01	7.201E+02	4.691E+02	2.981E+02	2.537E+02
	(Std)	(5.668E+06)	(2.232E+02)	(5.985E+00)	(1.187E+00)	(2.313E+03)	(6.900E+01)	(6.861E+02)	(2.743E+02)	(6.217E+01)	(3.935E+01)
GLEET	Mean	2.748E+06	5.105E+02	2.120E+01	1.422E+00	1.847E+03	4.449E+01	4.977E+02	1.096E+02	1.665E+02	1.882E+02
	(Std)	(4.205E+06)	(1.776E+02)	(4.705E+00)	(7.776E-01)	(2.552E+03)	(3.381E+01)	(3.549E+02)	(3.924E+01)	(6.137E+01)	(4.127E+01)

Table 9: The comparison among different reward functions, where the mean and standard deviations of ten runs on the test set are reported (with the best mean value on each problem highlighted in bold).

	Metric	f_1	f_2	f_3	f_4	f_5	f_6	f_7	f_8	f_9	f_{10}	
Ours	Mean	2.471E+02	2.440E+02	1.498E+01	5.816E-01	3.716E+02	1.300E+01	1.302E+02	7.216E+01	1.202E+02	1.202E+02	1.682E+02
	(Std)	(7.676E+02)	(1.396E+02)	(2.357E+00)	(2.210E-01)	(1.866E+02)	(1.020E+01)	(8.489E+01)	(3.555E+01)	(2.016E+01)	(1.648E+01)	
r_1	Mean	5.846E+05	3.253E+02	1.559E+01	1.412E+00	4.515E+02	3.089E+01	2.254E+02	1.136E+02	1.742E+02	1.923E+02	
	(Std)	(5.353E+05)	(1.433E+02)	(6.938E+00)	(7.098E-01)	(2.043E+02)	(2.492E+01)	(1.577E+02)	(4.948E+01)	(6.542E+01)	(2.184E+01)	
r_2	Mean	1.461E+01	2.591E+02	1.490E+01	7.330E-01	4.052E+02	1.799E+01	1.715E+02	7.816E+01	1.345E+02	1.699E+02	
	(Std)	(4.200E+01)	(1.408E+02)	(2.272E+00)	(2.801E-01)	(2.156E+02)	(1.087E+01)	(1.257E+02)	(3.618E+01)	(6.539E+01)	(1.678E+01)	
r_3	Mean	4.752E+04	2.404E+02	1.510E+01	6.065E-01	3.645E+02	2.315E+01	2.056E+02	8.305E+01	1.311E+02	1.705E+02	
	(Std)	(9.845E+04)	(1.256E+02)	(2.283E+00)	(2.045E-01)	(1.721E+02)	(1.774E+01)	(2.043E+02)	(3.945E+01)	(6.742E+01)	(1.719E+01)	

Figure 7: The performance curve of GLEET-DMSPSO and DMSPSO on 10D Schwefel (f_2) problem along the maxFEs .Figure 8: The performance curve of GLEET-DMSPSO on 10D Schwefel (f_2) problem along the training set size.

exploration-exploitation tradeoff which promotes the optimization performance (as done in our GLEET), while training on single

instances may lead to overfitting and lose the generalization on

unseen instances even in the similar distribution (as done in most existing works).

B.6 Analysis on the state representation

In this section we conduct ablation studies on the features in state representation. As introduced in Section 4.1.1, there are nine features in the state which can be divided into three parts: the features about search progress ($s_{1\sim 4}$), the distribution of costs ($s_{5\sim 6}$) and about population distribution ($s_{7\sim 9}$). To evaluate their effect we ablate each of them from GLEET-PSO agent and train them on the 10D problems. Their performance is shown in Table 8 where GLEET is the baseline with full state features. Results indicates that firstly removing any one of the three parts features would significantly affect the learning effectiveness of GLEET. Besides, the optimization progress feature $s_1 \sim s_4$ contribute most to GLEET, which can be interpreted as a informative signal telling GLEET when and where to adjust the hyper-parameter values for better searching behaviour. A comprehensive state representation would help learning indeed.

B.7 Analysis on the reward design

Reward quality plays a crucial role in determining the final performance of the policy as it guides the policy update during the training process. In Table 9, we provide a comparison of various practical reward functions recently proposed, including our own approach. Specifically, we consider the reward function r_1 proposed by Yin et al. [51], which assigns a reward of 1 for improvement and -1 otherwise:

$$r_1^{(t)} = \begin{cases} 1 & \text{if } f(gBest^{(t)}) < f(gBest^{(t-1)}) \\ -1 & \text{otherwise} \end{cases} \quad (13)$$

Sun et al. [37] introduced another reward function, denoted as r_2 , which measures the relative improvement between consecutive steps as the reward:

$$r_2^{(t)} = \frac{f(Best^{(t-1)}) - f(Best^{(t)})}{f(Best^{(t-1)})} \quad (14)$$

where $Best^{(t)}$ is the best particle in the t time step population.

Furthermore, Xue et al. [49] identified the issue of premature convergence in EC algorithms and proposed a novel triangle-like reward function, denoted as r_3 , to address this concern:

$$r_3^{(t)} = (1/2) \cdot (p_{t+1}^2 - p_t^2), \quad (15)$$

$$p_{t+1} = \begin{cases} \frac{f(g^{(0)}) - f(g^{(t)})}{f(g^{(0)})} & \text{if } f(g^{(t)}) < f(g^{(t-1)}) \\ p_t & \text{otherwise} \end{cases} \quad (16)$$

where $g^{(t)}$ denotes $gBest^{(t)}$.

We train GLEET-PSO with these reward functions and compare their optimization results. It turns out that under the experiment setting in this paper, our reward function stands out. In comparison, r_1 presents poor performance on all problems, r_2 and r_3 are acceptable on simpler problems. Notably, our reward function demonstrated better performance on more complex problems. We recognize the importance of investigating this issue further in future work, with the aim of designing more compatible and effective reward functions.

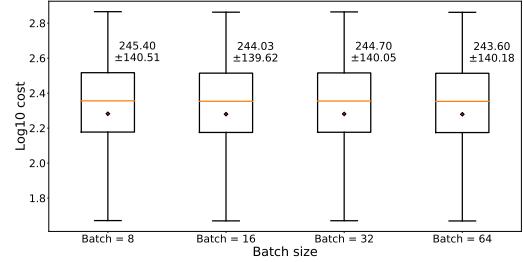


Figure 9: The boxplots of GLEET-DMSPSO on Schwefel (f_2) problem with different batch sizes.

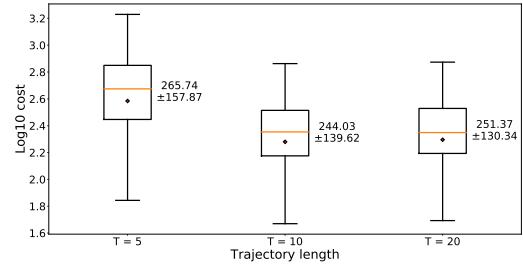


Figure 10: The boxplots of GLEET-DMSPSO on Schwefel (f_2) problem with different trajectory length T .

B.8 Analysis on the RL hyper-parameters

RL algorithms can be very sensitive to hyper-parameters, to make a deeper analysis on GLEET we explore the effect of batch size and trajectory length T . The batch size may not influence the training stability. In PPO, the length of trajectory segments could impact the reward accumulation and the later learning steps. For the batch size we compare the performance with 8, 16, 32 ad 64 batch sizes. For the trajectory length we adopt the values of 5, 10 and 20. The other hyper-parameters are frozen in the experiment. Taking GLEET-DMSPSO with 10D Schwefel (f_2) as a case, the results for batch sizes and trajectory lengths are shown in Fig. 9 and Fig. 10 respectively. The experimental results show that GLEET-DMSPSO with 8, 16, 32, and 64 batch sizes consistently exhibits good performance on 10D Schwefel (f_2) problems regardless of the numbers of the batch size, and the results of varying trajectory lengths reveal that a proper and moderate length may benefit the final performance since a shorter trajectory may increase the training variance and an overlong trajectory may reduce leaning steps in episodes (10 length trajectory has 200 K-epoch learning in a 2000 generation episode but the 20 length one only has 100) which may degrade the performance.