Meta-Black-Box-Optimization through Offline Q-function Learning

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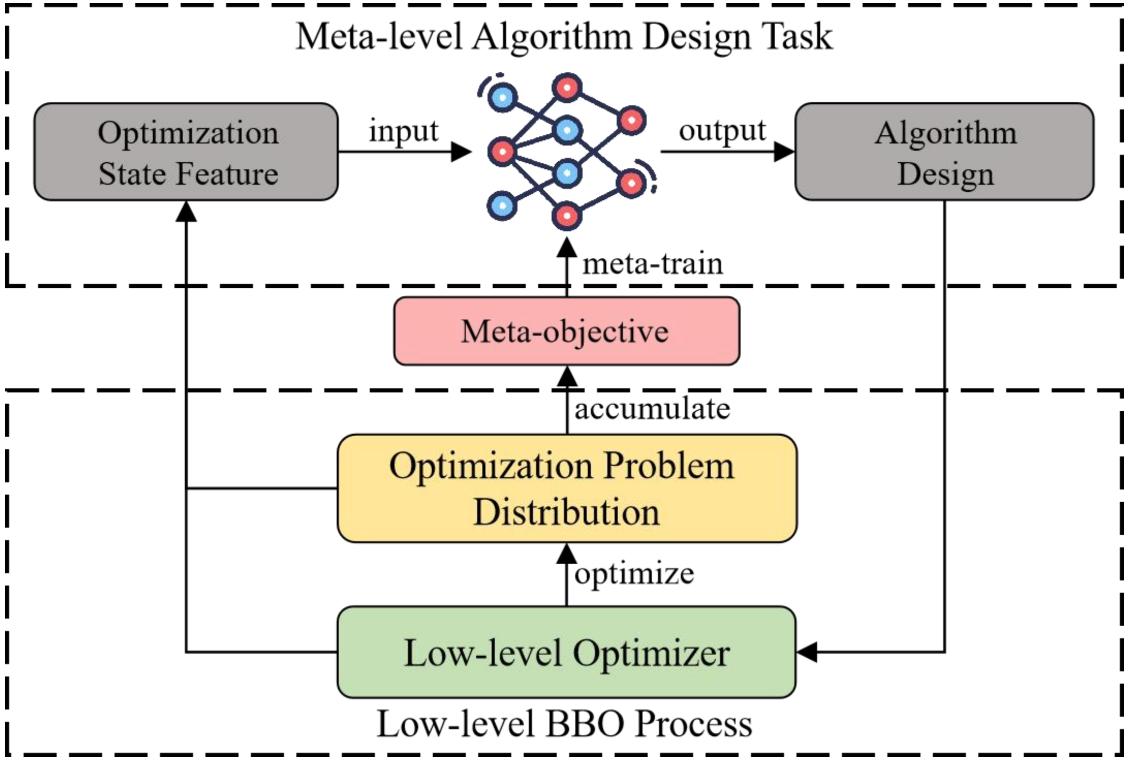
Part I: What is Meta-Black-Box-Optimization (MetaBBO)?



MetaBBO leverages the generalization strength of Meta-learning to enhance the optimization performance of BBO algorithms in the minimal expertise cost [1] [2].

Bi-level Paradigm:

$$\mathbb{J}(\theta) = \frac{1}{N}\sum_{i=1}^{N}\sum_{t=1}^{H} Perf(A, c_i^t, p_i)$$

$$c_i^t = \pi_\theta(s_i^t), \quad s_i^t = \mathrm{sf}(A, p_i, t)$$

Meta-level Algorithm Design Task:
The policy π_θ is trained to dictates desired algorithm design c by conditioning the optimization state feature s.

Low-level Optimization Task:
The algorithm A adopts the dictated design to optimize a distribution of problems $\mathcal{I}$, providing meta-performence $Perf(\cdot)$ for training the policy.

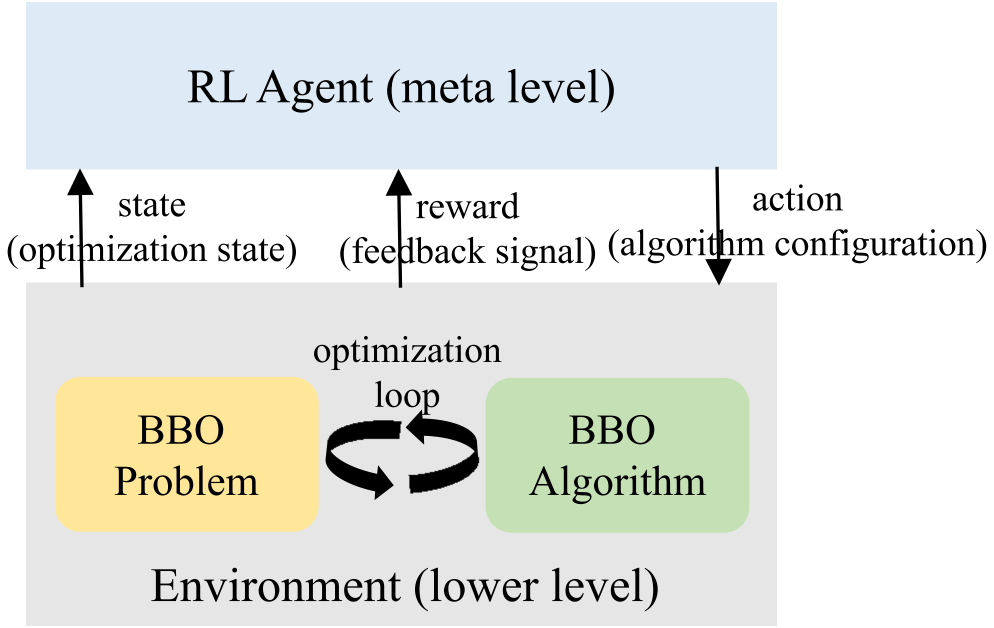
[1] Ma Zeyuan, et al. MetaBox: A Benchmark Platform for Meta-Black-Box Optimization with Reinforcement Learning. NeurIPS 2023.
[2] Ma, Zeyuan, et al. "Toward automated algorithm design: A survey and practical guide to meta-black-box-optimization." IEEE TEVC (2025).

Part I: What is Meta-Black-Box-Optimization?

In this work, we focus on a particular MetaBBO algorithm design task: Dynamic Algorithm Configuration

Meanwhile, we focus on a particular learning methodology: Reinforcement Learning

A general workflow of using RL for DAC can be instantiated from MetaBBO as below [1] [2]:



[1] Xue K et al. Multi-Agent Dynamic Algorithm Configuration. NeurIPS 2022.

[2] Ma Z et al. Auto-Configuring Exploration-Exploitation Tradeoff in Evolutionary Computation via Deep Reinforcement Learning. GECCO 2024.

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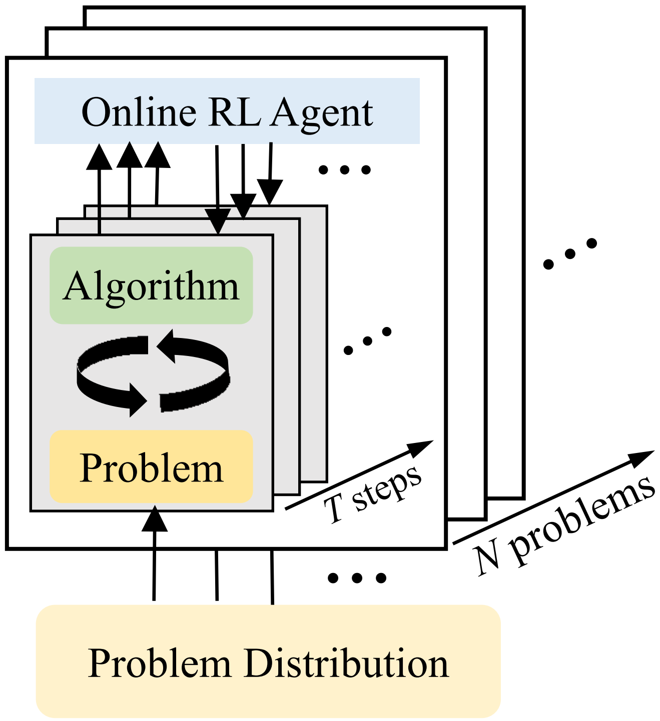
Part II: Motivation?

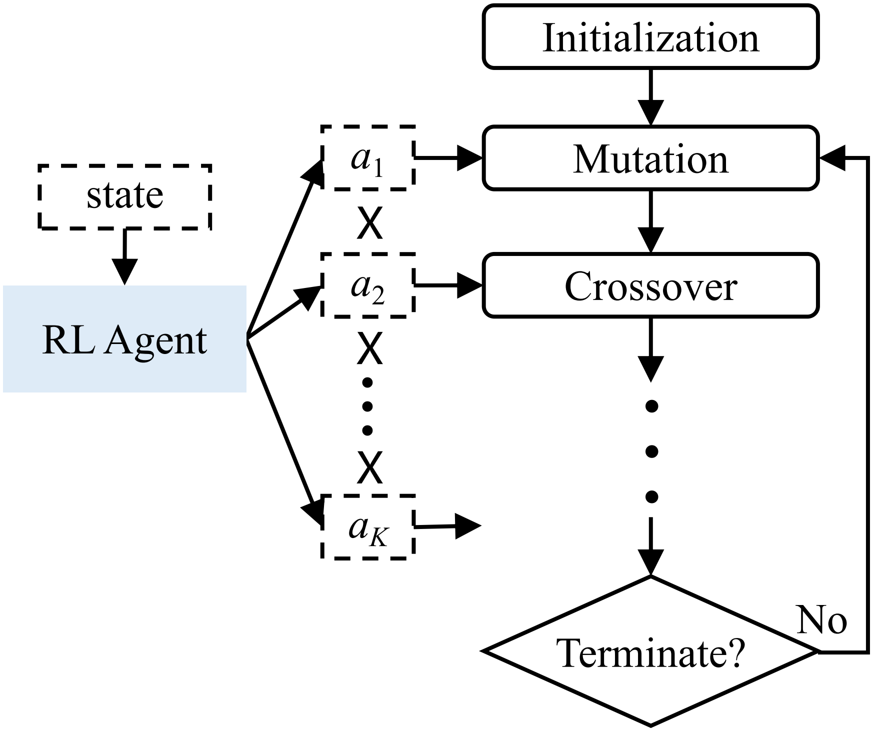
➢ Problematic Efficiency

In BBO scenarios, the collection of trajectories is expensive or time-consuming, making the efficiency of the online learning paradigms in existing MetaBBO works problematic.



➢ Massive Configuration Space

Existing BBO Algorithms usually contain many controllable hyper-parameters, making it difficult to search for the optimal algorithm configuration policy and slowing down the training.



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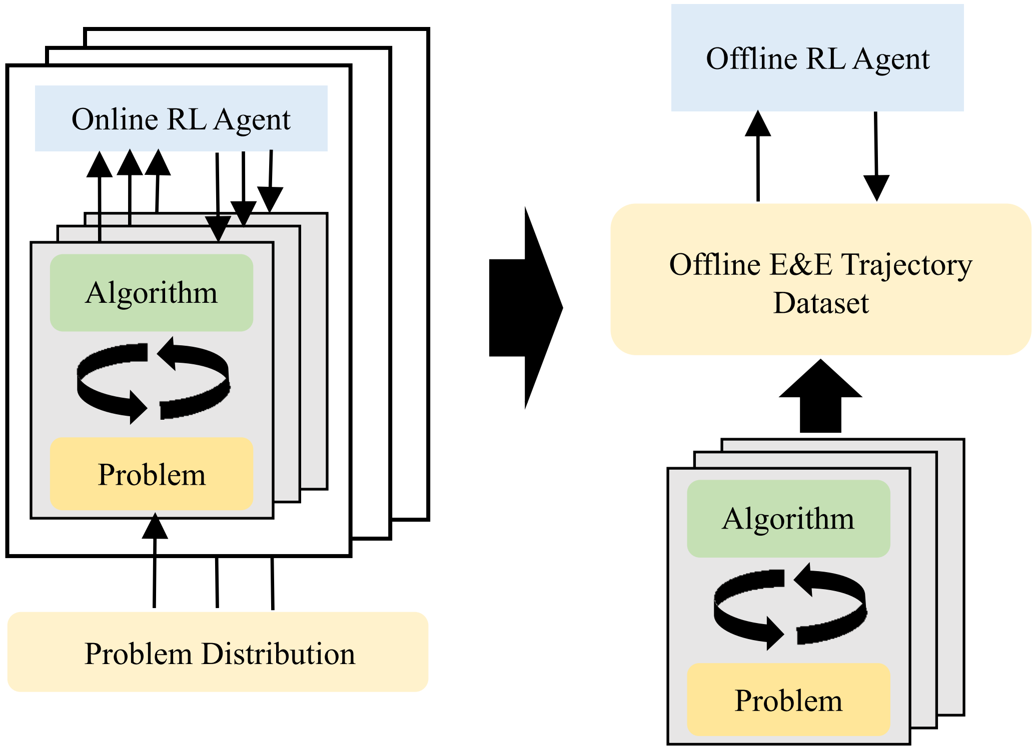
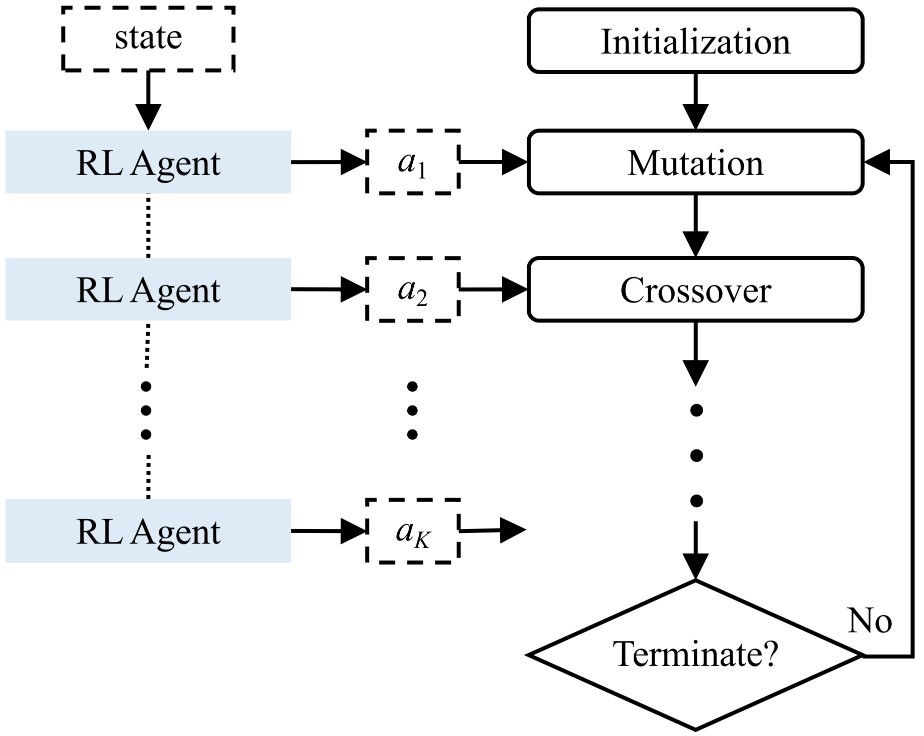
Part II: Motivation?

➢ Problematic Efficiency



We collect offline DAC experience trajectories from both strong MetaBBO baselines and a random policy to provide exploitation and exploration data used for robust training.

➢ Massive Configuration Space



We transform DAC task into a long-sequence decision process and introduce a Q-function decomposition scheme to represent each hyper-parameter as a single action step.

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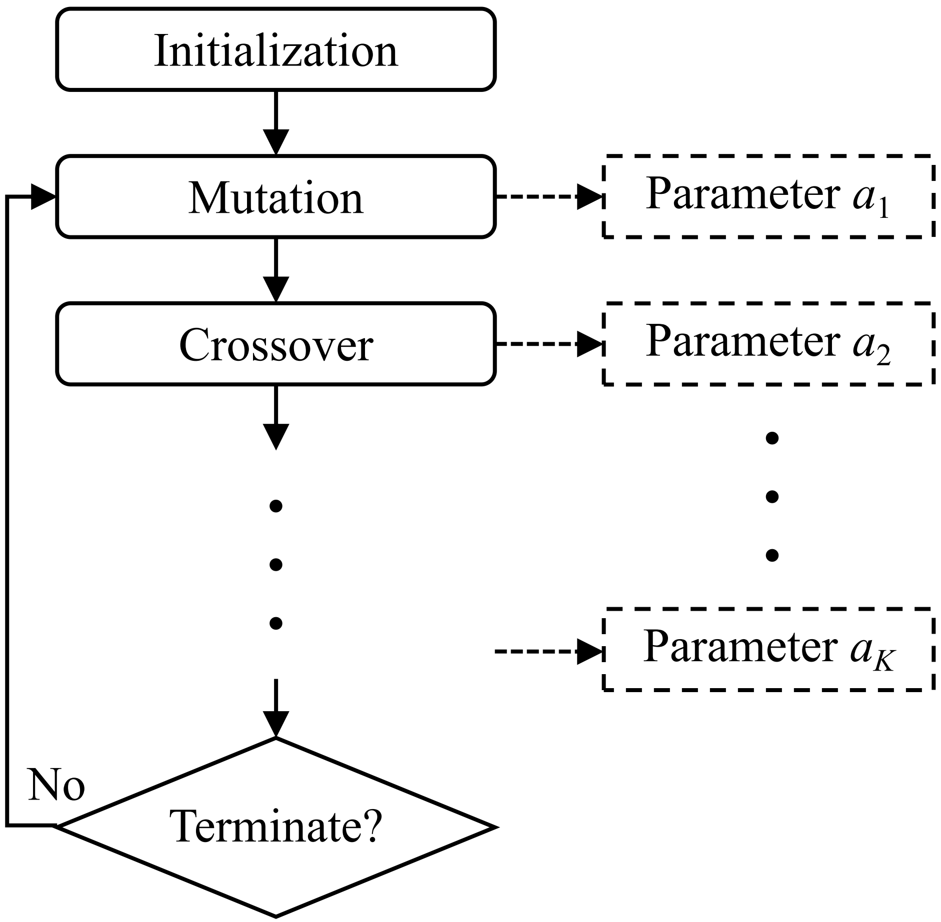
Part III: Problem Formulation



- Transform dynamic algorithm configuration (DAC) task into a long-sequence decision process and introduce a Q-function decomposition scheme to represent each hyper-parameter as a single action step.

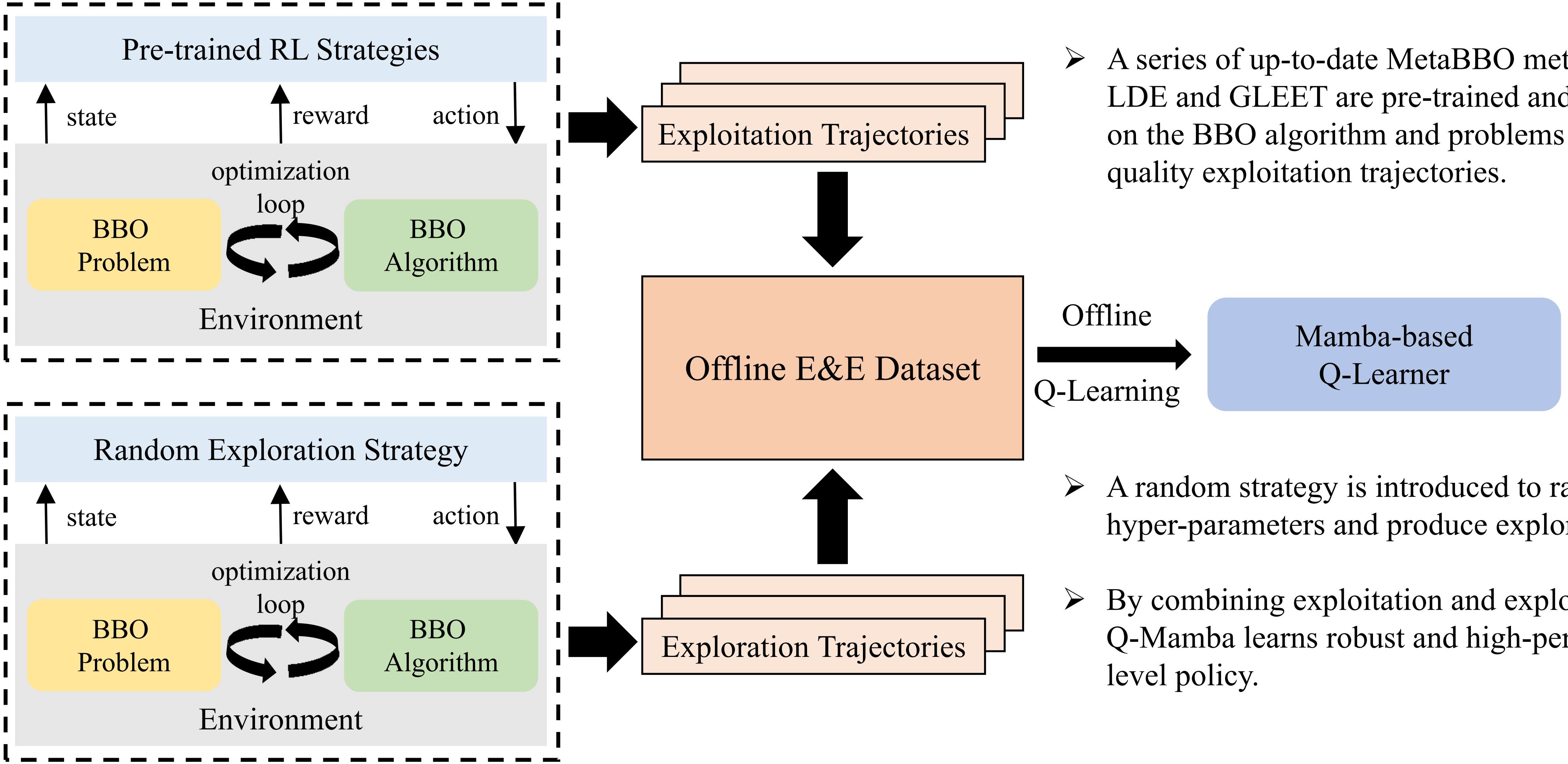
$$Q(a_{1:K}^t|s^t) \leftarrow R(s^t, a_{1:K}^t) + \gamma \max_{a_{1:K}^{t+1}} Q(a_{1:K}^{t+1}|s^{t+1})$$

$$Q(a_i^t|s^t) \leftarrow \begin{cases} \max_{a_{i+1}^t} Q(a_{i+1}^t|s^t, a_{1:i}^t), & if \quad i < K \\ R(s^t, a_{1:K}^t) + \gamma \max_{a_1^{t+1}} Q(a_1^{t+1}|s^{t+1}). & \\ & if \quad i = K \end{cases}$$

- The meta-objective of MetaBBO is to search the optimal policy $\pi_{\theta*}$ that maximizes the expectation of accumulated performance improvement over all problem instances in the training set:

$$\theta^* = \arg\max_\theta \frac{1}{N} \sum_{j=1}^{N} \sum_{t=1}^{T} R(s^t, a_{1:K}^t|\pi_\theta)$$

Part IV: Offline E&E Dataset Collection



- A series of up-to-date MetaBBO methods: RLPSO, LDE and GLEET are pre-trained and then rollouted on the BBO algorithm and problems to collect high quality exploitation trajectories.

- A random strategy is introduced to randomly control the hyper-parameters and produce exploration trajectories.

- By combining exploitation and exploration experience, Q-Mamba learns robust and high-performance meta-level policy.

Part V: Conservative Q-learning Loss

We represent each hyper-parameter as a single action step in the decision process and learn the decomposed sequential Q-function through offline RL to improve the training efficiency of MetaBBO. A compositional Q-loss which enhances the offline learning by removing distributional shift is proposed.

$$J(\tau|\theta) = \sum_{t=1}^{T}\sum_{i=1}^{K}\sum_{j=1}^{M} J(Q^t_{i,j}|\theta) = \begin{cases} \frac{1}{2}(Q^t_{i,j} - \max\limits_{j} Q^t_{i+1,j})^2, & if \quad i < K, j = a^t_i \\ \frac{\beta}{2}\left[Q^t_{i,j} - (r^t + \gamma \max\limits_{j} Q^{t+1}_{1,j})\right]^2, & \\ & if \quad i = K, j = a^t_i \\ \frac{\lambda}{2}(Q^t_{i,j} - 0)^2, & if \quad j \neq a^t_i \end{cases}$$

- The first two branches are TD errors following the Bellman backup for decomposed Q-function, with weight β=10 on the last action dimension to reinforce the learning on this dimension.
- The conservative regularization introduced in offline RL method CQL, which is used to relieve the over-estimation due to the distribution shift. We set λ=1 in this paper to strike a good balance.

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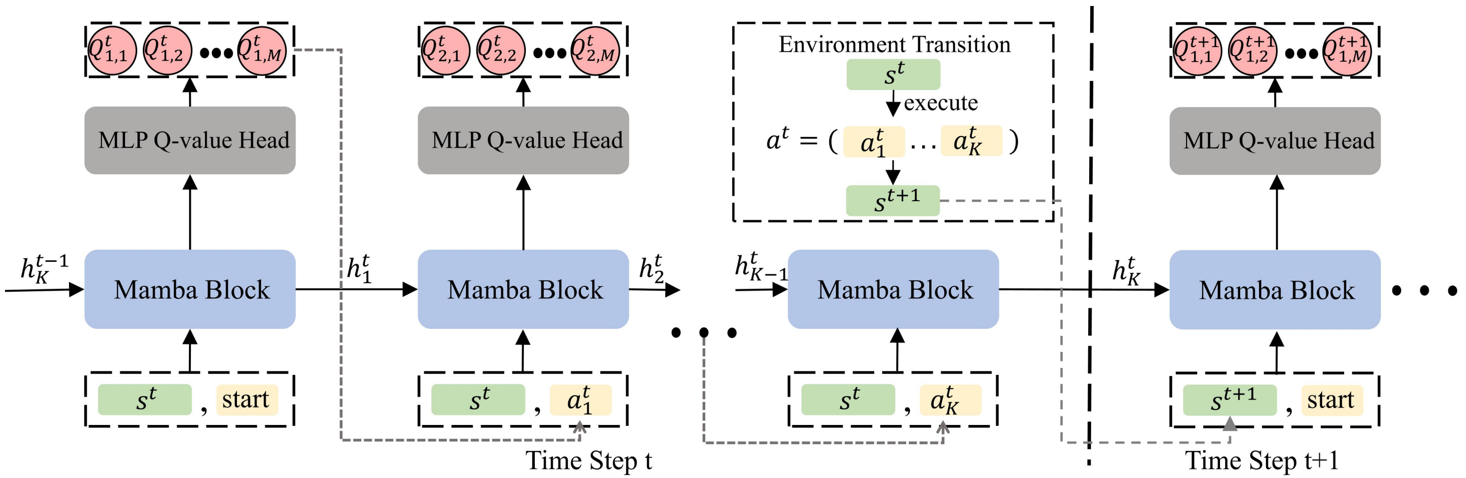
Part VI: Mamba-based Q-Learner



- MetaBBO task features long-sequence process that involves thousands of decision steps since there are hundreds of optimization steps and K hyper-parameters to be decided per optimization step. Mamba is adopted since it parameterizes the dynamic parameters as functions of input state token, which facilitate flexible learning of long-term and short-term dependencies from historical state sequence.

- Mamba equips itself with hardware-aware I/O computation and a fast parallel scan algorithm: PrefixSum, which allows Mamba has the same memory efficiency as highly optimized FlashAttention

Part VII: Some Empirical Obervation

- **Experiment Setup**:

Training dataset: Three low-level BBO algorithms with 3, 10 and 16 hyper-parameters sampled from the algorithm space in ConfigX. The problem distribution includes 16 problems (5D-50D) from CoCo BBOB Testsuites which contains 24 synthetic functions.

In-Dsitribution Test Set: The three low-level BBO algorithms on the 8 problems (5D-50D) from CoCo BBOB Testsuites which have not been used for training.

Out-Of-Distribution Test Sets: A continuous control neuroevolution task on a 2-layer MLP policy for Mujoco.

Training Settings: Decomposed Offline Q-function Learning, 300 epoch, learning rate 5e-3.

Baselines:

- **Online**: **RLPSO** that uses simple MLP , **LDE** that facilitates LSTM and **GLEET** that uses Transformer architecture.
- **Offline**: **DT**, **DeMa**, **QDT** and **QT** that apply conditional imitation learning on the E&E dataset, and **Q-Transformer** that uses similar Q-value decomposition scheme as Q-Mamba, while the neural network architecture is Transformer.

Part VII: Some Empirical Obervation

- **<u>In-distribution Generalization</u>**:

Table 1. Performance comparison between Q-Mamba and other online/offline baselines. All baselines are tested on unseen problem instances within the training distribution P_{bbob}. We additionally present the averaged training/inferring time of all baselines in the last row.

	Online			Offline					
	RLPSO (MLP)	LDE (LSTM)	GLEET (Transformer)	DT	DeMa	QDT	QT	Q-Transformer	Q-Mamba
$Alg0$ $K=3$	9.855E-01 ±9.038E-03	9.563E-01 ±1.830E-02	9.616E-01 ±3.110E-03	9.325E-01 ±2.680E-02	9.492E-01 ±2.467E-02	9.683E-01 ±2.131E-02	9.729E-01 ±1.934E-02	9.666E-01 ±1.975E-02	**9.889E-01 ±7.779E-03**
$Alg1$ $K=10$	9.953E-01 ±3.322E-03	9.877E-01 ±1.118E-02	9.938E-01 ±2.834E-03	6.764E-01 ±1.193E-01	9.015E-01 ±1.688E-02	9.917E-01 ±5.454E-03	9.955E-01 ±3.115E-03	9.951E-01 ±3.487E-03	**9.973E-01 ±2.441E-03**
$Alg2$ $K=16$	9.914E-01 ±4.497E-03	9.904E-01 ±6.306E-03	9.910E-01 ±5.846E-03	8.706E-01 ±3.951E-02	9.159E-01 ±2.015E-02	9.919E-01 ±7.456E-03	9.926E-01 ±6.874E-03	9.895E-01 ±6.754E-03	**9.950E-01 ±9.981E-03**
Avg Time	28h / 11s	28h / 12s	25h / 13s	13h / 10s	12h / 10s	20h / 12s	20h / 12s	16h / 11s	13h / 10s

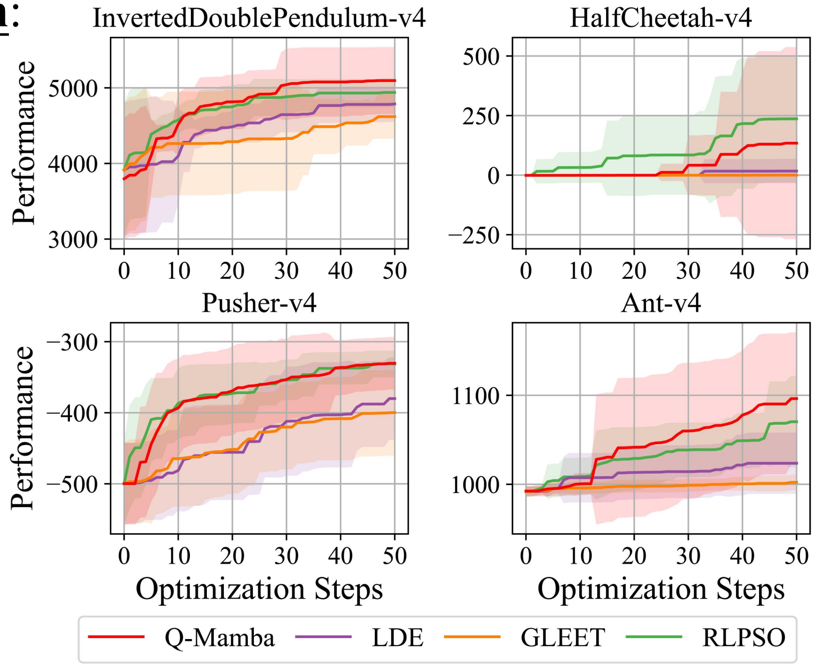
- Q-Mamba effectively achieves competitive or even superior optimization performance to prior online/offline baselines.

- Q-Mamba v.s. Online MetaBBO: By learning from the offline E&E dataset, Q-Mamba reduces the training budget which is especially appealing for BBO scenarios where the simulation is expensive or time-consuming.

- Q-Mamba v.s. Offline MetaBBO: The weighted Q-loss function accelerates the learning of the TD error and the Mamba architecture allows selectively remember or forget historical states which avoids the linear time invariance of Transformer.

Part VII: Some Empirical Obervation

- **Out-of-distribution Generalization**:



- While only trained on low-dimensional synthetic problems, Q-Mamba is capable of optimizing the MLP polices which hold thousands of parameters in neuroevolution tasks.

- Compared to online baselines, Q-Mamba is capable of learning effective policy with comparable generalization performance, with only consuming less than half training resources.

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