

Generalizable Meta-Heuristic based on Temporal Estimation of Rewards for Large Scale Blackbox Optimization

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Abstract

The generalization abilities of heuristic optimizers may deteriorate with the increment of the search space dimensionality. To achieve generalized performance across Large Scale Blackbox Optimization (LSBO) tasks, it is possible to ensemble several heuristics and devise a meta-heuristic to control their initiation. This paper first proposes a methodology of transforming LSBO problems into online decision processes to maximize efficiency of resource utilization. Then, using the perspective of multi-armed bandits with non-stationary reward distributions, we propose a meta-heuristic based on Temporal Estimation of Rewards (TER) to address such decision process. TER uses a window for temporal credit assignment and Boltzmann exploration to balance the exploration-exploitation tradeoff. The prior-free TER generalizes across LSBO tasks with flexibility for different types of limited computational resources (*e.g.* time, money, *etc.*) and is easy to be adapted to new tasks for its simplicity and easy interface for heuristic articulation. Tests on the benchmarks validate the problem formulation and suggest significant effectiveness: when TER is articulated with three heuristics, competitive performance is reported across different sets of benchmark problems with search dimensions up to 10000.

Introduction

Optimization problems with partial information, mappings too complex to capture are regarded as “black-box” optimization problems (Martinez-Cantin 2019). With minimal assumptions and no requirements for domain-specific knowledge, heuristic methods show promising performance in these problems (Ma et al. 2019; Ge et al. 2018; Lu et al. 2018; Cao et al. 2019). Large Scale Blackbox Optimization (LSBO) problems focus on optimizing deterministic scalar functions with high-dimensional search space, constrained by limited number of computational resources, *e.g.* the number of function evaluations, time and money, *etc.* Under this setting however, the performance of heuristics deteriorate as most of them are not scalable to higher dimen-

sional search spaces (Sun, Kirley, and Halgamuge 2018; Ge et al. 2017; Loshchilov, Glasmachers, and Beyer 2019).

Efforts have been put into devising heuristics with more scalable performance (Li et al. 2018; Al-Dujaili and Sundaram 2017). However, empirical evidence suggests that their unsatisfactory generalization abilities: their capabilities inevitably vary when applied on problems with different characteristics. In the LSBO setting, it is nearly impossible to understand the nature of a given problem without prior knowledge. This no-free-lunch phenomenon directs researchers to the field of meta-heuristics, which are higher-level procedures to initiate heuristics using the feedback during the optimization process. With meta-heuristics, users can focus on articulating powerful heuristics to obtain satisfactory performance.

However, the existing meta-heuristic methods are still with huge space for improvement for the following concerns: 1) Recognition of the objective: the LSBO problems can all be summarized as given limited number of computational resources (*e.g.* the number of evaluations for the blackbox objective functions), achieve the lowest possible error by searching the best solutions. The true objective of these tasks is the efficiency of resource utilization, which most of the existing methods fail to recognize. In the literature of existing methods for meta-heuristics, many surrogate objectives for resource utilization, *e.g.* number of individuals that gained better fitness during evolution, however there is no direct connection between these surrogates and the true objective of efficiency; 2) Overfitting: for better performance on benchmark functions, a large portion of existing meta-heuristics are designed with components specially effective for the corresponding test cases. The prior knowledge for designing “overfitting” meta-heuristics on those tasks is of no help for deeper investigation. The meta-heuristics of this kind are expected to lose their effectiveness once transferred to other tasks. For example, SHADE-ILS (Molina, La-Torre, and Herrera 2018), the current state-of-the-art method, calls a global search heuristic that is partic-

ularly effective for CEC'2013 benchmark problems in every iteration. It can outperform most of the existing methods on those tasks by a significant margin, yet only achieving intermediate performance when applied on CEC'2008 and CEC'2010 benchmark functions. Similarly, MTS (Tseng and Chen 2008), which was designed with the same methodology, achieves matchless performance on the CEC'2008 benchmark problems however performs badly on the later benchmark problems; 3) Generalization: Some meta-heuristics are with too many hyperparameters to tune for the tasks, making it hard to generalize and transfer.

The main contributions of this paper lie in:

- We transform the LSBO problem setting into a decision process, in which the actions are the initiations of heuristics and the rewards are the improvement of best known solution during the initiations. In this new setting, the objective of the LSBO problem is converted to maximizing the expected cumulative return. This principled framework is not only meaningful for theoretical purposes but also beneficial for application scenarios.
- We propose a simplified view of treating such decision process as multi-armed bandit problems and propose a simple algorithm of using a window for temporal credit assignment, which enables local estimation of the non-stationary reward distributions. With this, we use a Boltzmann exploration (softmax) method to balance exploration and exploitation.
- We analyze the complexity and the behavior of the proposed algorithm, and give principled guidelines for practical use.

Preliminaries

Most of the existing meta-heuristics suffer from the “overfitting” problem: the meta-heuristics are often proposed together with several specific articulated heuristics and it is either impossible or very costly to re-articulate the meta-heuristics with new heuristics. The difficulties are caused by the fact that researchers introduce strong prior knowledge and couplings into the designed systems. Meta-heuristic is however emerged with the expectation to automatically adapt to the differences in diverse objectives to optimize. For such goal, a prior-free meta-heuristic with easy interfaces for heuristic articulation is desired. To reach it, a principled framework that could capture the key features of optimization is needed. In the following parts of this section, we introduce a perspective to transform the optimization problem (with meta-heuristics) into a decision process and then discuss its characteristics.

Notations & Definitions

Before stating the ideas, some prerequisite notations and definitions are to be introduced:

Definition 1 (Best Fitness). *Given a scalar objective function f and some t that represents the amount of consumed computational resources, e.g. time elapsed or the number of*

*used function evaluation, the best known objective value (minimum for minimization or maximum for maximization) queried via function evaluation from the start of the optimization process until t is called **best fitness** until t .*

Definition 2 (Improvement & Efficiency). *Given f and t_1, t_2 of computational resource consumption, where $t_1 < t_2$, the difference between the best fitness y_2 until t_2 and the best fitness y_1 until t_1 is called the **improvement of global best fitness** (or **improvement**) during $(t_1, t_2]$. The **efficiency** during such period is defined as the fraction of improvement and the resource consumption, i.e. $(y_2 - y_1)/(t_2 - t_1)$.*

Definition 3 (Efficiency of Actions). *Given f , the fraction of the improvement (from y_1 to y_2) and the consumption of resources (from t_1 to t_2) after taking an action a is defined as the **efficiency of action a** (or **action efficiency**), denoted as $\mathcal{E}(y_1, y_2, t_1, t_2, a)$.*

The notions of best fitness and improvement are algorithm agnostic. By cutting the resource consumption into equal pieces, we can achieve a piece-wise approximation of the real-time efficiency along the optimization process.

Definition 4 (Expected Overall Improvement). *Given function f to be optimized, and an initial distribution d_0 of the global best fitness, the **expected overall improvement** $\mathbb{E}_{\mathcal{A}, y_0 \sim d_0} [\Delta_{0:T}]$ achieved by algorithm \mathcal{A} given all the computational resources T provided is defined as*

$$\mathbb{E}_{\mathcal{A}, y_0 \sim d_0} [\Delta_{0:T}] = \mathbb{E}_{\mathcal{A}, y_0 \sim d_0} [y^*(\mathcal{A}, y_0, T) - y_0]$$

where $y^*(\mathcal{A}, y_0, T)$ is the best fitness found by \mathcal{A} from initialization t_0 until $t = T$.

Definition 5 (Expected Overall Efficiency). *Given function f to be optimized, and a initial distribution d_0 of the global best fitness, the **expected overall efficiency** $\mathbb{E}_{\mathcal{A}, y_0 \sim d_0} [\mathcal{E}_{0:T}]$ achieved by algorithm \mathcal{A} given all the computational resources T provided is defined as*

$$\mathbb{E}_{\mathcal{A}, y_0 \sim d_0} [\mathcal{E}_{0:T}] = \mathbb{E}_{\mathcal{A}, y_0 \sim d_0} [y^*(\mathcal{A}, y_0, T) - y_0] / T$$

The notions of improvement and efficiency is translation invariant, i.e. they do not change if the search landscape is shifted up or down.

Proposition 1 (Efficiency Maximization is Optimization). *Given fixed initialization scheme and the same computational resources, maximizing expected overall improvement (efficiency) is equivalent to optimizing the objective function itself.*

Proof. Trivial. □

Formulation

Whether using meta-heuristics, the pursuit of resource-constrained optimization should be maximizing the expected overall efficiency, in a sense that with limited computational resources, we should improve the best fitness by the most. Such recognition gives us a perspective of building meta-heuristics: we can treat initiation of the articulated heuristics as actions and taking the actions will result in improvements of the

best fitness at the cost of some resources. The fraction of these two terms yields an “action efficiency” that is closely connected to the “efficiency” that we pursue ultimately, which is the improvement upon the initial objective value divided by the total number of computational resources given: the integral of the action efficiency yields the overall efficiency.

Using the definitions, the goal is formalized as:

Find a sequence $\{a^{(i)}\}, i \in \{1, \dots, n\}$, to maximize

$$\mathbb{E} \left[\sum_{i=1}^n (t_2^{(i)} - t_1^{(i)}) \mathcal{E}(f_1^{(i)}, f_2^{(i)}, t_1^{(i)}, t_2^{(i)}, a^{(i)}) \right], s.t. \sum_{i=1}^n (t_1^{(i)} - t_2^{(i)}) \leq T \quad (1)$$

where T is the total amount of given resources.

With this formulation, the meta-heuristic problem is transformed into online decision problems to maximize the overall efficiency of taking actions. We can fit the online decision process with the goal to maximize the expected cumulative rewards.

Devising meta-heuristics under this formulation requires the heuristics to be decoupled, *i.e.* each action does not affect the behavior of others. At the cost of potential information loss during consecutive initiations of heuristics, the decoupling gives lots of advantages by enabling the meta-heuristics to generalize to new tasks by granting them the flexibility of articulating any appropriate heuristics. The flexibility gives us the freedom to use the best configuration (*w.r.t.* resource allocation for each initiation) of the articulated heuristics, which is crucial of the effective heuristics are sensitive to the resource allocation. Moreover, the decoupling grants the decision process with semi-Markovian properties, which may be systematically investigated in the future research.

Unfortunately, because of the expensive nature of the problem, episodes of training is prohibited and thus the problem cannot be solved using most of the existing methods for semi-MDPs.

TER

The decision we seek is under arguably the most complex scenarios - partially observable semi-Markov decision processes. Also, for LSBO problems, we can only run for one episode as there is no training allowed. However, if we reasonably assume that the reward distribution of taking an action changes slowly with the transition of the states, *i.e.* the reward distribution of each action changes gradually overtime, we can approximate the decision problem with a multi-armed bandits setting (with non-stationary rewards). In such setting, we have to find an effective way to do temporal credit assignment *s.t.* the recent rewards can be used to well-approximate the rewards for the recent future.

With the reached formulation, in this section, we propose an algorithm to address the decision process.

Typical temporal credit assignment techniques in multi-armed bandits include exponential weighting,

change point detection, *etc.* In this paper, we turn to the simplest of its kind, a fixed-size window for lower variance behavior and better generalization. The decisions of actions only consider the pieces of performance of the recent initiations of heuristics inside the window, *i.e.* we use only the recent rewards to estimate the recent future.

To implement such idea, we have a memory queue (first-in-first-out) of size w to buffer all the efficiency records of the heuristic initiations. When an initiation of some heuristic is finished, we first linearly normalize the efficiency values into the interval $[0, 1]$ and use the mean of the normalized efficiency records of each action to approximate the mean of the reward distribution in the recent future. The normalization helps to regularize the behavior of the bandit algorithms and give us a bound of the greediness when used with soft decision methods.

Boltzmann Exploration with Strict Exploration

We use a modified Boltzmann exploration (softmax) method to handle the non-stationary multi-armed bandits problem: we softmax the mean of the normalized rewards for each action within the sliding window to obtain the probability distribution of selecting each action and sample the actions accordingly.

The greediness of softmax is controlled by a hyperparameter τ , with which we divide the energy values, *i.e.* the means, and take the exponential, as follows.

$$\text{softmax}(\mathbf{x}, \tau) \equiv \frac{e^{\mathbf{x}/\tau}}{\mathbf{1}^T e^{\mathbf{x}/\tau}}$$

The higher the value of τ , the less greedy the output distribution is *w.r.t.* the energy values in \mathbf{x} . τ can also be set to be time-variant or more complex. In this paper, we treat it as a fixed hyperparameter.

Boltzmann exploration alone is problematic for the case in which there are no records of an action within the window. Since softmax decision requires at least one mean value for each action. This can be fixed with a simple rule: we define the mean of an empty set to be infinite. This means if no record of an action is found, such action will be taken directly. This additional rule not only ensures exploration across the whole optimization process no matter how bad the hyperparameters are chosen but us also beneficial for exploration which must be guaranteed in such a non-stationary setting: if a heuristic behaved badly before, it may behave well now.

The elaboration of our proposed meta-heuristic framework TER is now complete. Its pseudocode is presented in Algorithm 1.

Analyses

Computational Complexity

For runtime complexity, the mean and softmax operate at the level $O(w|A|)$, which is trivial compared to those

Algorithm 1: TER-based LSBO

Input: f (blackbox function to be optimized), A (set of heuristics), T (total number of computational resources), τ (greediness for softmax), w (size of temporal window), \mathbf{x}_{best} (initial \mathbf{x}_{best}), y_{best} (function value of initial \mathbf{x}_{best})

Output: \mathbf{x}_{best} (best known solution), y_{best} (function value of \mathbf{x}_{best})

```
1  $Q \leftarrow \text{queue}();$  //initialize an empty queue
2  $t \leftarrow 0;$  //initialize counter for consumed resources
3 while  $t < T$  do
4   //normalize efficiency values in  $Q$  to  $[0, 1]$ 
5    $Q_{temp} \leftarrow \text{normalize}(Q, 0, 1);$ 
6   //sample action from distribution formed by softmax
7    $\mathbf{x} \leftarrow \mathbf{0}_{|A| \times 1}$ 
8   for  $i \in \{1, \dots, |A|\}$  do
9      $x_i \leftarrow \text{mean}(\text{records of } a_i \text{ in } Q_{temp});$  // $\infty$  if no existing records of  $a_i$ 
10   $a \sim \text{softmax}(\mathbf{x}, \tau);$  //sample action
11   $[\mathbf{x}_{best}, y_{best}, \Delta t] \leftarrow \text{apply\_on}(a, f, \mathbf{x}_{best}, y_{best});$ 
    //apply heuristic  $a$  on  $f$ , update  $\mathbf{x}_{best}, y_{best}$ , get the consumption  $\Delta t$ 
12   $Q.\text{add}(\langle \mathbf{x}_{best}, y_{best}, \Delta t \rangle);$  //add record into  $Q$ 
13  if  $|Q| > w$  then
14     $Q.\text{pop}();$  //only maintain  $Q$  with size  $w$ 
15   $t \leftarrow t + \Delta t;$ 
```

of the heuristics. For space complexity, since the historical records outside the credit assignment window can be safely discarded, a trivial one at most $O(w)$ can also be reached.

Probability Bounds for Behavior

TER has two hyperparameters, w (length of the temporal window) and τ (temperature coefficient for softmax). Suppose that there are $|A|$ actions, we have the following proposition for the behavior of TER:

Proposition 2 (Exploration Bounds for TER). *Suppose every action is corresponded with at least one efficiency record within the window of size w and τ is the softmax hyperparameter, the probability of taking an action with not-the-highest mean normalized record (exploration) in the fragment of length w satisfies the bounds*

$$p_{\text{explore}} \in \left[\frac{e^{1/\tau}}{|A| - 1 + e^{1/\tau}}, \frac{|A| - 1}{(|A| - 1) \cdot e^{1/\tau} + e^{\frac{w - |A|}{\tau(w - |A| + 1)}}} \right] \quad (2)$$

Proof. See Appendix. \square

The proposition gives a measurement of behavior for TER. We can use the bounds inversely to do efficient hyperparameter search, for which we offer details in the Appendix.

Related Works

There are different ideas of initiating the articulated heuristics. Some meta-heuristics initiate all the articulated heuristics in a certain order alternately. The primitive algorithms of this kind enable fixed resources for each heuristic (Boluf-Rohler, Fiol-Gonzalez, and Chen 2015). There are also ideas of modifying the resource allocation for each heuristic dynamically. In (Tseng and Chen 2008), the authors proposed to use some small amount of resources to test-run the articulated heuristics and run the best-performing one with large amount of resources. MOS (LaTorre, Muelas, and Pena 2012) runs each of its articulated heuristics within each iteration and dynamically adjusts the resources for each heuristic according to their performance. The adjustment of the resources, or more accurately the change of the configuration for the articulated heuristics, is problematic for the fact that heuristics often require sufficient iterations to show their full capacities for the current state of optimization (Hansen and Auger 2014). This kind of allocation strategy is likely to undermine the effectiveness of heuristics, which leads to the loss of many potentially useful heuristic articulation choices; Some meta-heuristics samples the initiation of articulated heuristics according to some distribution constructed by the historical performance. In (Ye et al. 2014), the authors proposed a greedy method, which simply switches from the two articulated heuristics when one of them has poor performance. Yet, the greedy exploitation of heuristic performance without in-time exploration may lead to premature convergence. In (Molina and Herrera 2015), the algorithm uses this idea for initiating some of the articulated heuristics. However, there are also some heuristic to be initiated in every main loop, which are specifically effective for the benchmark functions it was tested on. Also, since it does not use the efficiency as the evaluation criteria of temporal performance, the resources for initiating each heuristic is strictly fixed to be the same.

The second perspective is about the evaluation criteria for the performance of articulated heuristics. Most of the existing methods based on evolutionary strategies use the number of improved offsprings (which, after crossover and mutation, improved their fitness values) (Tseng and Chen 2008; LaTorre, Muelas, and Pena 2012). Some also take into consideration the magnitude of change. Efficiency, however, have hardly been investigated in the literature.

The third perspective focuses on the applicability on practical scenarios. Articulation of heuristics is constrained by how the meta-heuristic will be coupled with them. In existing literature of meta-heuristics, some heuristics are often chosen and fixed and their operations or structure are often exploited, *i.e.* the articulated heuristics are not treated as blackboxes, and such coupling makes it difficult for the meta-heuristics to be transferred to other tasks, when new heuristics needed to be articulated. Also, since algorithms are mostly tested on benchmark functions,

Table 1: Baseline Comparison Results

LSO13	BEK		TER		sim	RAN		sim	LS		sim	CC		sim	GS		sim
	mean	std	mean	std		mean	std		mean	std		mean	std		mean	std	
f_1	0.00e0	0.00e0	0.00e0	0.00e0	~	4.41e-10	1.36e-9	~	0.00e0	0.00e0	~	4.77e-4	1.32e-3	~	6.85e5	1.01e5	~
f_2	2.25e-2	1.02e-2	8.69e0	2.78e0	78.13%	2.44e2	3.83e1	31.56%	5.54e2	4.02e1	23.87%	2.40e0	1.50e0	92.25%	9.89e3	1.45e3	2.33%
f_3	4.85e-14	2.05e-14	9.83e-13	5.27e-14	69.13%	9.06e-13	6.55e-14	28.57%	1.04e-12	6.51e-14	71.43%	1.19e0	1.11e-1	31.43%	6.63e0	4.41e-1	0.00%
f_4	5.45e8	1.45e8	6.98e8	2.51e8	51.43%	1.23e9	3.90e8	16.47%	1.86e10	9.98e9	5.88%	1.22e11	6.65e10	12.25%	6.34e8	1.00e8	68.24%
f_5	9.54e5	4.32e5	2.68e6	4.38e5	30.34%	2.52e6	9.94e5	42.15%	1.23e7	2.93e6	11.05%	1.26e7	3.42e6	20.01%	2.20e6	6.93e5	65.98%
f_6	3.93e4	3.55e4	4.44e4	3.42e4	44.51%	5.99e4	3.35e4	46.58%	9.84e5	4.13e3	4.29%	9.82e5	4.62e3	2.17%	4.02e4	3.32e4	71.35%
f_7	8.07e4	9.25e3	1.58e5	3.68e4	44.25%	4.10e5	4.22e5	33.15%	3.10e8	4.81e8	19.77%	3.13e9	2.20e9	24.24%	1.06e6	1.00e5	33.37%
f_8	2.93e9	4.35e9	1.24e11	9.29e10	51.25%	1.45e12	1.42e12	44.42%	2.96e15	1.75e15	21.24%	4.93e16	3.12e16	9.13%	1.55e11	1.66e10	49.18%
f_9	1.43e8	2.25e7	2.36e8	2.61e7	26.14%	2.08e8	4.02e7	31.15%	1.01e9	1.91e8	12.31%	9.34e8	2.05e8	8.31%	2.63e8	4.35e7	26.75%
f_{10}	7.70e5	6.62e5	7.64e5	5.90e5	85.86%	9.33e5	5.28e5	42.00%	6.37e7	3.54e7	3.50%	6.46e7	3.40e7	6.87%	1.06e6	4.34e5	34.63%
f_{11}	1.35e7	2.21e6	3.33e7	1.08e7	71.54%	1.84e8	9.53e7	22.78%	1.07e11	1.19e11	3.15%	1.17e11	1.14e11	9.55%	1.34e7	2.60e6	83.36%
f_{12}	2.25e-4	2.25e1	6.27e2	2.11e2	32.57%	8.12e2	2.69e2	18.82%	6.14e2	2.65e2	31.10%	2.42e3	4.79e2	24.56%	2.33e3	1.77e2	3.87%
f_{13}	4.45e5	2.17e5	1.14e7	2.20e6	49.79%	9.28e7	1.05e8	22.53%	3.36e9	1.63e9	15.64%	5.34e9	1.90e9	19.35%	1.18e7	1.61e6	45.98%
f_{14}	5.99e5	1.01e5	4.35e7	6.85e6	31.95%	5.36e7	1.12e7	19.59%	1.25e11	1.41e11	11.25%	1.60e11	9.10e10	15.25%	5.04e7	5.73e6	28.65%
f_{15}	9.71e5	4.24e4	3.66e6	2.32e5	66.87%	8.78e6	2.82e6	31.66%	3.05e8	9.52e7	16.97%	2.15e9	2.77e9	22.65%	8.59e6	1.08e6	28.89%
F-rank	performance/sim		1.63		4.29	2.53		3.32	3.70		1.79	4.67		2.14	2.67		3.46
t-test	< / ≈ / >					9/5/1			13/2/0			14/0/1			8/5/2		

We cannot compute similarity scores for f_1 since the best decision sequence is not unique. For each test case, the greener the indicators, the better the performance.

For the Friedman tests on the errors, $p = 7.38 \times 10^{-6}$. The smaller the F-ranks, the better the performance. For the Friedman tests on the similarity scores, $p = 2.50 \times 10^{-3}$.

where the computational resources has only one form, *i.e.* the number of function evaluations, seldom investigations have been conducted on the incorporation of different kinds of resources. The flexibility of interface for costs or resources are well-pursued in Bayesian optimization methods (Shahriari et al. 2016; Martinez-Cantin 2019). The number of hyperparameters of the meta-heuristics also decides whether they are easy to be applied. The pursuit of simplicity however, is often neglected in the literature of LSBO. The method proposed in this paper is a generalized framework with heavy focus on this perspective and achieves satisfactory compatibility.

Experiments

Experimental Settings

To validate TER, we test it on two sets of LSBO benchmark functions. The CEC'2013 benchmark suite (LSO13) represents a wide range of real-world LSBO problems. With ill-conditioned complicated sub-components and irregularities (Li et al. 2013), serving to test the overall capabilities of TER. For the test cases in LSO13 suite, the resource for optimization is concretized as the total number of objective function evaluation $\max FEs = 3 \times 10^6$ and the problem dimensions are roughly 1000. The CEC'2008 benchmark problems (LSO08) are naturally scalable to higher dimensions, which serve as the test cases for scalabilityZ. For the test cases in LSO08, $\max FEs = 5 \times 10^3 D$, where D is the dimensionality of the search space.

We articulate TER with three heuristics, including LS1 (LS) in (LaTorre, Muelas, and Pena 2012), Cooperative Coevolution with random grouping (CC) in (Omidvar et al. 2010) and Global Search (GS) in (Molina, LaTorre, and Herrera 2018), with the same configurations from the original papers. There are mainly three reasons for which we choose these heuristics: 1) These heuristics are used in literature and have

Table 2: Scalability Tests on LSO08

Problem	1000		2500		5000		10000	
	mean	std	mean	std	mean	std	mean	std
f_1	0.00e0	0.00e0	0.00e0	0.00e0	0.00e0	0.00e0	0.00e0	0.00e0
f_2	2.60e1	2.53e0	8.58e1	2.12e0	1.25e2	1.97e0	1.44e2	7.53e-1
f_3	3.26e0	3.67e0	5.81e2	5.99e2	1.68e3	1.18e3	1.61e3	1.84e3
f_4	0.00e0	0.00e0	0.00e0	0.00e0	0.00e0	0.00e0	0.00e0	0.00e0
f_5	3.67e-15	1.80e-16	1.83e-14	1.55e-15	4.06e-14	1.58e-15	9.57e-14	1.17e-14
f_6	1.04e-12	5.37e-14	5.50e-13	2.01e-14	1.15e-12	3.64e-14	2.70e-12	1.62e-13

f_7 is excluded since we do not know its global minimum.

shown powerful empirical performance, *s.t.* we can refer the knowledge of finetuning these heuristics to their satisfactory configurations; 3) These heuristics have wide intersections with the existing meta-heuristics, which makes the comparison more reasonable. The details of the heuristics are presented in the Appendix.

After a coarse hyperparameter search, we chose $\langle \tau, w \rangle = \langle 1/5, 5 \rangle$. This pair gives the probability of exploration approximately in the interval (0.01, 0.45). We offer more details for in the Appendix.

Validation

Comprehensive Abilities We validate the effectiveness of TER by comparing it with several baselines that articulate the same heuristics. We run TER and the baselines on the 15 test cases in LSO13 for 20 times and the obtained results are listed in Table 1. The operation of "RAN" means purely random choices for actions. The "BEK" means the best known average performance achieved by using from LS, CC and GS. The best known decision sequences come from many random runs using the three heuristics¹. The performance obtained using the "BEK" baseline indicates the full potential of the articulated framework and serves as the approximate lower bound of the error obtained by TER. We also present the decision sequence similarity

¹The BEK sequences will be released together with the source code.

Table 3: Similarity Scores for LSO08 problems

		f_2					f_4					f_6				
1k	1k	52.14%	48.34%	23.07%	1k	1k	66.63%	24.13%	12.75%	1k	1k	70.13%	66.75%	62.11%	1k	1k
2.5k	85.40%	2.5k	46.26%	31.68%	2.5k	55.12%	2.5k	42.67%	19.57%	2.5k	71.33%	2.5k	72.25%	69.33%	2.5k	2.5k
5k	78.46%	81.33%	5k	43.49%	5k	43.09%	5k	33.26%	5k	51.24%	5k	60.01%	5k	68.24%	5k	5k
10k	71.98%	75.47%	77.35%	10k	10k	24.25%	32.75%	54.33%	10k	10k	33.26%	39.66%	44.25%	10k	10k	10k
		f_1					f_3					f_5				

Each entry is the mean similarity score of decision sequences for a problem explained by the row dimensionality indicator and the column dimensionality indicator. For example, the bottom left 71.98% is the mean value of similarity scores of the 20 sequences under $D = 1k$ to the 20 sequences under $D = 10k$. The greener the cell is shaded, the more similar the corresponding decision sequences are.

Table 4: Comparative Results on LSO13 Problems

LSO13	TER		MTS		MOS		CSO		CC-CMA-ES		DECC-DG2		DECC-D	
	mean	std	mean	std	mean	std	mean	std	mean	std	mean	std	mean	std
f_1	0.00e0	0.00e0	0.00e0	0.00e0	0.00e0	0.00e0	0.00e0	0.00e0	3.01e-2	1.22e-1	9.54e5	1.57e6	4.23e-12	9.08e-13
f_2	8.69e0	2.78e0	7.98e2	5.41e1	1.93e1	4.16e0	7.25e2	2.72e1	1.97e3	2.73e2	1.38e4	1.78e3	1.16e3	2.92e1
f_3	9.83e-13	5.27e-14	9.18e-13	6.31e-14	0.00e0	0.00e0	1.19e-12	2.11e-14	1.20e-13	3.08e-15	1.07e1	8.71e-1	8.52e-10	5.18e-11
f_4	6.98e8	2.51e8	2.47e10	1.32e10	1.34e10	7.69e9	1.13e10	1.29e9	1.13e10	9.91e9	5.15e8	2.39e8	3.81e10	1.61e10
f_5	2.68e6	4.38e5	1.02e7	1.17e6	1.11e7	1.76e6	7.66e5	1.17e5	8.72e6	2.52e6	2.51e6	4.49e5	9.71e6	1.77e6
f_6	4.44e4	3.42e4	8.84e5	1.66e5	9.85e5	3.22e3	4.36e-8	1.58e-9	7.55e5	3.65e5	1.25e5	2.01e4	1.57e4	2.88e4
f_7	1.58e5	3.68e4	7.08e7	7.60e7	2.31e7	4.12e7	7.94e6	2.88e6	5.37e6	1.15e7	1.54e7	1.01e7	3.29e9	1.14e9
f_8	1.24e11	9.29e10	1.71e15	5.60e14	1.64e15	1.66e15	3.07e14	7.64e13	5.87e14	2.02e14	9.35e13	4.28e13	1.92e15	9.47e14
f_9	2.36e8	2.61e7	7.32e8	9.60e7	8.97e8	1.39e8	4.59e7	8.57e6	5.19e8	1.70e8	3.06e8	7.37e7	7.18e8	1.14e8
f_{10}	7.64e5	5.90e5	2.16e6	2.45e6	6.05e7	2.91e7	5.35e-5	2.19e-4	7.11e7	2.94e7	1.43e2	1.87e1	1.03e3	1.65e3
f_{11}	3.33e7	1.08e7	6.26e9	1.64e10	4.01e10	1.23e11	3.87e8	1.13e8	4.52e8	1.18e9	8.82e9	2.60e10	4.13e10	9.40e10
f_{12}	6.27e2	2.11e2	1.03e3	8.70e2	8.63e1	7.71e1	1.43e3	8.80e1	1.24e3	8.61e1	1.51e8	3.64e8	1.36e3	1.32e2
f_{13}	1.14e7	2.20e6	1.30e9	1.51e9	1.13e9	7.71e8	5.65e8	1.87e8	7.42e9	4.97e9	9.62e8	3.80e8	4.33e10	9.30e9
f_{14}	4.35e7	6.85e6	4.11e10	7.79e10	6.89e9	1.41e10	6.62e10	1.30e10	8.06e9	2.05e10	3.39e10	2.15e9	7.86e11	2.91e11
f_{15}	3.66e6	2.32e5	4.07e7	1.23e7	1.31e8	6.02e7	1.59e7	1.06e6	3.51e6	1.02e6	1.55e7	1.36e6	5.39e7	4.53e6
t-test	< / ≈ / >		11/3/1		10/3/2		10/1/4		11/3/1		11/2/2		12/1/2	
F-rank	2.033		4.833		4.500		2.933		4.033		4.067		5.600	

The greener the indicator, the better the performance. The best performance is in bold and shaded grey. Friedman test: $\chi^2 = 27.73$, $p = 1.0541 \times 10^{-4}$; If TER performs better in terms of t -test results, the corresponding “l/u/g” string is in bold type and shaded grey.

scores of TER with respect to the sequences used in the BEK baseline. The sequence similarity scores are computed as mean values of the local alignment scores via the Smith-Waterman method (Smith and Waterman 1981). The higher the similarity scores, the more similar the decision sequences are to the best known sequence. Some additional curves are provided in the Appendix.

To show the general performance rankings of algorithms, Friedman tests are conducted with significance level $\alpha = 0.05$. If Friedman tests tell $p < \alpha$, we can conclude that the given performance rankings are statistically meaningful. To show one-on-one performance differences of algorithms, paired t -tests are also conducted with significance level of $\alpha = 0.05$. We give collective t -test results in the format of a “< / ≈ / >” string. < represents the number of test cases in which we are highly-confident that the first algorithm gives smaller results than the second one. > represents the opposite of <. ≈ represents the number of test results with no confident difference. We obtain the following observations:

1. According to the statistics, TER achieves significantly better performance than the 4 baselines (RAN, LS, CC and GS); This in a way shows the effectiveness of the online decisions.
2. In terms of decision similarity, TER is significantly more similar to BEK, than the other baselines. This indicates that TER may be more able to excavate effective sequences of actions.

Scalability

We test if TER has stable behavior to achieve satisfactory performance within wide range of problem dimensionality by validating it on the 6 scalable benchmark functions in LSO08 with $D \in \{1000, 2500, 5000, 10000\}$. maxFEs scales linearly with problem dimensionality, which means that the length of the decision sequence on different dimensions are roughly the same and thus are comparable. In Table 2, the means and stds obtained over 20 independent runs on each case are given. In Table 3, the similarity score matrices of the decision sequences are presented.

From the similarity matrices, it can be observed that generally the larger difference in problem dimensionality, the less similar the sequences are. However, these dissimilarities still leads to similar results: on 4 of 6 problems, the global optima are found. This indicates that, though the patterns of sequences are not similar when the problem dimensionality changes, the qualities of the decisions remain strong.

Comparisons with Existing Algorithms

Comprehensive Abilities On the LSO13 benchmark problems, we compare the performance of TER with some competitive algorithms, including MOS (LaTorre, Muelas, and Pena 2012), MTS (Tseng and Chen 2008), CSO (Cheng and Jin 2015), CC-CMA-ES (Liu and Tang 2013), DECC-DG2 (Omidvar et al. 2017) and DECC-D (Omidvar, Li, and Yao 2010). Under the CEC’2018

Table 5: Comparative Results on LSO08 Problems

LSO08	D	TER		MTS		CSO		CC-CMA-ES		DECC-DG2		DECC-D	
		mean	std	mean	std	mean	std	mean	std	mean	std	mean	std
f_1	1000	0.00e0	0.00e0	0.00e0	0.00e0	0.00e0	0.00e0	0.00e0	0.00e0	1.08e2	4.40e2	0.00e0	0.00e0
	2500	0.00e0	0.00e0	0.00e0	0.00e0	1.48e-20	7.71e-22	0.00e0	0.00e0	1.11e5	1.25e5	0.00e0	0.00e0
	5000	0.00e0	0.00e0	0.00e0	0.00e0	5.32e-18	4.63e-19	0.00e0	0.00e0	6.46e5	6.31e4	0.00e0	0.00e0
	10000	0.00e0	0.00e0	0.00e0	0.00e0	1.64e-17	2.02e-18	0.00e0	0.00e0	6.47e7	6.94e5	0.00e0	0.00e0
f_2	1000	2.60e1	2.53e0	1.12e2	8.86e0	8.04e1	2.43e0	1.62e2	7.74e0	7.40e1	1.66e0	5.65e1	4.63e0
	2500	8.58e1	2.12e0	1.47e2	1.30e0	4.61e1	1.28e0	1.82e2	1.14e1	1.39e2	2.96e0	6.72e1	4.56e0
	5000	1.25e2	1.97e0	1.59e2	1.12e0	8.26e1	1.30e0	1.90e2	5.81e0	1.44e2	3.78e0	8.21e1	4.23e0
	10000	1.44e2	7.53e-1	1.69e2	1.32e0	1.23e2	1.48e0	1.95e2	5.27e-1	1.96e2	8.58e-1	8.69e1	4.21e0
f_3	1000	3.26e0	3.67e0	1.69e2	1.27e2	1.26e3	1.42e2	1.02e3	2.87e1	5.49e6	1.71e7	1.23e3	1.10e2
	2500	5.81e2	5.99e2	7.68e2	2.50e2	2.54e3	2.48e1	2.82e3	8.96e1	7.37e9	4.93e9	3.16e3	4.91e2
	5000	1.68e3	1.18e3	1.35e3	3.55e2	5.45e3	1.36e2	5.75e3	1.89e2	2.22e11	6.49e10	6.19e3	4.41e2
	10000	1.61e3	1.84e3	2.04e3	6.95e2	1.57e4	8.75e2	1.16e4	2.97e2	8.39e13	1.21e12	1.22e4	4.06e2
f_4	1000	0.00e0	0.00e0	0.00e0	0.00e0	7.05e2	3.00e1	1.93e3	1.29e2	4.63e3	4.91e2	5.21e2	2.27e1
	2500	0.00e0	0.00e0	7.96e-1	4.45e-1	1.22e3	4.07e1	5.31e3	2.48e2	1.68e4	1.63e3	1.23e3	6.12e1
	5000	0.00e0	0.00e0	3.98e0	1.22e0	2.84e3	3.29e1	1.10e4	1.39e2	4.09e4	3.73e3	2.38e3	6.84e1
	10000	0.00e0	0.00e0	8.29e0	3.91e0	9.19e3	1.63e2	2.22e4	5.49e2	2.62e5	3.92e2	4.68e3	5.64e1
f_5	1000	3.67e-15	1.80e-16	3.71e-15	1.37e-16	2.22e-16	0.00e0	2.71e-3	5.92e-3	4.46e-1	5.78e-1	1.72e-15	9.17e-17
	2500	1.83e-14	1.55e-15	1.92e-14	4.78e-16	4.44e-16	0.00e0	1.97e-3	4.41e-3	1.35e3	2.05e2	3.45e-3	7.70e-3
	5000	4.06e-14	1.58e-15	6.53e-14	3.24e-16	6.66e-16	0.00e0	2.11e-14	6.97e-15	1.65e4	1.23e3	1.17e-14	1.45e-16
	10000	9.57e-14	1.17e-14	7.07e-5	1.58e-4	1.13e-15	4.97e-17	4.02e-14	2.48e-14	5.85e5	5.46e3	2.35e-14	1.57e-16
f_6	1000	1.04e-12	5.37e-14	9.22e-13	4.28e-14	1.20e-12	1.61e-14	1.17e-13	3.25e-15	1.09e1	7.98e-1	1.05e-13	2.65e-15
	2500	5.50e-13	2.01e-14	2.31e-12	4.63e-13	2.92e-12	4.44e-14	3.61e0	8.07e0	1.46e1	2.93e-1	2.62e-13	6.16e-15
	5000	1.15e-12	3.64e-14	3.53e-12	8.94e-13	4.51e-11	7.07e-13	1.82e1	8.90e-2	1.75e1	9.26e-1	5.13e-13	5.55e-15
	10000	2.70e-12	1.62e-13	5.65e-12	2.53e-13	1.66e-10	2.62e-11	1.85e1	7.29e-1	2.16e1	6.60e-3	1.03e-12	1.29e-14
t -test	1000	~	~	2/3/1	~	4/1/1	~	3/2/1	~	5/1/0	~	3/1/2	~
	2500	~	~	5/1/0	~	4/0/2	~	5/1/0	~	6/0/0	~	3/1/2	~
	5000	~	~	4/2/0	~	4/0/2	~	4/1/1	~	6/0/0	~	2/1/3	~
	10000	~	~	3/3/0	~	4/0/2	~	4/1/1	~	6/0/0	~	2/1/3	~
F -rank	1000	2.25	~	3.08	~	3.67	~	4.00	~	5.50	~	2.50	~
	2500	1.92	~	2.92	~	2.83	~	4.42	~	5.67	~	3.25	~
	5000	2.42	~	3.08	~	3.17	~	4.42	~	5.50	~	2.42	~
	10000	2.25	~	3.08	~	3.50	~	3.92	~	6.00	~	2.25	~

MOS is excluded because we have trouble reproducing the algorithm and cannot find the related results; All Friedman tests satisfy $p \ll 5\%$. The best ranking is in **bold** type and shaded grey; If TER performs better in terms of t -test results, the corresponding "l/u/g" string is in **bold** type and shaded grey.

competition standards, we run each algorithm independently for 20 times on each benchmark function. We present the results in Table 4.

The statistics show that TER achieves the best results within the compared algorithms. Furthermore, on 6 test cases, TER achieved errors at least one order of magnitude lower than all the others. Since we do not add any additional prior-dependent components such as restart mechanisms to further enhance the performance, such performance can be highlighted.

Scalability

For this part, we adopt the same problem settings as in the scalability validation. We compare the performance of TER against the other algorithms, whose results are listed in Table 5. The statistics show TER achieves the best performance, exhibiting less performance deterioration than other algorithms with the increment of problem dimensionality. Some additional curves are provided in the Appendix.

Conclusion

Purposely for addressing the existing problems of meta-heuristic frameworks, this paper formulates a methodology of transforming zero-order optimization problems into decision processes, in which during dif-

ferent stages for decision, different articulated heuristics are initiated as actions.

With such methodology, a solution using local reward estimation is proposed, with the hypothesis that the problem can be approximately addressed from the perspective of multi-armed bandits with non-stationary reward distributions. The temporal estimation is implemented using a simple window. With the local estimations, the problem is then addressed using Boltzmann exploration. This proposed solution enables robust interfaces for practical use and simplicity to ensure easy generalization, accompanied with bounds for the behavior and the guidelines for hyperparameter tuning. Empirically, the proposed TER, when articulated with three heuristics, has shown significant performance when compared to baselines on many benchmark problems, without embedding prior-dependent components. When compared to other competitive existing methods, it shows nearly state-of-the-art performance.

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