

Parallel Exploitation in Estimated Basins of Attraction: A New Derivative-free Optimization Algorithm

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ABSTRACT

Direct search (DS) and evolutionary algorithms (EAs) are two of the most representative branches of derivative-free optimization methods. However, traditional DS becomes deficient in multimodal problems, while EAs suffer from long computational time due to the blind search caused by randomness in evolutionary operators. This paper proposes a new derivative-free optimization algorithm that addresses both the above issues, avoiding prematurity while maintaining fast convergence speed. The new algorithm first estimates basins of attractions in the search space by analyzing samples of the objective function. An adaptive exploitation method with the ability to predict promising search directions is then applied to search the estimated basins in parallel. The new algorithm is evaluated on both unimodal and multimodal benchmark functions. Experimental results show that the algorithm is a promising global optimizer with fast convergence speed.

Categories and Subject Descriptors

I.2.8 [Artificial Intelligence]: Problem Solving, Control Methods, and Search – *heuristic methods, scheduling.*

General Terms

Algorithms, Management, Experimentation

Keywords

Derivative-free optimization; direct search (DS); evolutionary algorithms (EAs); global optimization

1. INTRODUCTION

Global optimization of numerical problems is a fundamental issue in computational science and engineering. With the growing sophistication of science and technology, problems to be optimized become more and more complex. Situations that traditional derivative-based algorithms cannot be applied frequently occur, for calculating derivatives of the objective functions in such complex problems is difficult or even impossible. In this case, derivative-free algorithms are preferred. However, one loses plenty of information

about the problem by not having derivatives. Designing effective and efficient derivative-free algorithms for global optimization is therefore an important and challenging task.

Direct search (DS) and evolutionary algorithms (EAs) form two of the most representative branches of modern derivative-free algorithms. In general, DS is an iterative optimization procedure without any explicit or implicit derivative approximation or modal building [1]. In each iteration, DS samples the objective function at a finite number of points. The next action of DS is determined solely based on the function values of the trial points. Representative DS includes the Nelder-Mead simplex algorithm [2] and the mesh-adaptive direct search method [3], etc. Despite the fast convergence speed of DS, they experience difficulty in solving multimodal problems [4]. Although some specially-design DS may address certain type of multimodal problems, they still suffer from prematurity in the others.

Different from DS, EAs imitate the biological evolution procedure to approximate the global optimum. With certain encoding scheme, EAs encode a solution in the search space into a chromosome. A number of chromosomes compose a population, which evolves towards the global optimum through a series of evolutionary operators iteratively performed in EAs. EAs such as genetic algorithms (GAs) [5][6] estimation of distribution algorithms (EDAs) [7][8], and particle swarm optimization (PSO) [9][10], etc., are well-known for their easy implementation and flexibility to adapt different problems. However, most EAs cannot avoid blind search during the optimization process due to the randomness in evolutionary operators. Long computational time is required in order to find a solution with satisfying accuracy.

This paper proposes a new derivative-free optimization algorithm, aiming to integrate the fast convergence feature of DS and the flexibility of EAs. The new algorithm comprises a sampling step, a step to estimate basins of attractions based on the obtained samples, and a step to exploit the estimated basins in parallel. The proposed algorithm can avoid prematurity through the parallel search mechanism in possible basins of attraction. Although it is also a stochastic iterative search procedure like EAs, the proposed algorithm reduces the chance of blind search by employing an exploitation method with the ability to predict promising search directions. Experimental results on a number of benchmark functions with unimodal and multimodal characteristics show that the proposed algorithm, termed parallel exploitation in estimated basins of attraction (PE-EBA), is a promising global optimizer with fast convergence speed.

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The rest of this paper is organized as follow. Section 2 introduces the general framework and implementation details of PE-EBA. Section 3 applies the PE-EBA with a projection method to solve high-dimensional problems. Experimental results and algorithm comparisons are displayed in Section 4. Conclusion and guidelines for future work are summarized in Section V.

2. PE-EBA

Given a numerical optimization problem, it can be presented in the form of a minimization problem with an n -dimensional search domain Ω and an objective function f . The goal of the problem is to find a global optimum $\mathbf{x}^* \in \Omega$ such that

$$f(\mathbf{x}^*) = \min_{\mathbf{x} \in \Omega} f(\mathbf{x}). \quad (1)$$

In this section, the general framework of PE-EBA is first introduced in the context of the minimization problem in (1). The implementation details will be clarified afterwards.

2.1 General Framework of PE-EBA

The fundamental idea behind PE-EBA is to estimate basins of attraction in the search domain by analyzing samples of the objective function and then to locate the global optimum by exploiting the estimated basins with a powerful exploitation method.

In order to implement the above idea, the PE-EBA maintains a set $\mathbf{R} = \{R_1, R_2, \dots, R_N\}$, where R_k is a record of area k in the search domain, $k=1, 2, \dots, N$, and N is the number of areas. Each record R_k is composed of five members, i.e., $R_k = (\mathbf{l}^{(k)}, \mathbf{u}^{(k)}, \mathbf{p}^{(k)}, \rho^{(k)})$. $\mathbf{l}^{(k)}$ and $\mathbf{u}^{(k)}$ are n -dimensional vectors, whose i -th elements, denoted by $l_i^{(k)}$ and $u_i^{(k)}$, are the lower and upper bounds of area k on the i -th dimension, $i=1, 2, \dots, n$. $\mathbf{p}^{(k)} \in [\mathbf{l}^{(k)}, \mathbf{u}^{(k)}]$ is the best solution found in area k . $\rho^{(k)} \in (0, 1)$ is termed the exploitation rate, which measures the desirability of exploiting area k based on the quality of $\mathbf{p}^{(k)}$.

At the beginning of PE-EBA, the set \mathbf{R} is initialized as $\{R_1\}$ with R_1 as a record of Ω . $\mathbf{l}^{(1)}$ and $\mathbf{u}^{(1)}$ are set according to the bounds of Ω , while $\mathbf{p}^{(1)}$ and $\rho^{(1)}$ are set as undefined. The PE-EBA then manipulates \mathbf{R} through the following steps to find the global optimum \mathbf{x}^* .

1) *Sampling*. In this step, a non-empty subset of areas is selected from \mathbf{R} . A sample of solutions is generated in each selected areas for providing data to estimate the basins of attraction.

2) *Area division*. For each area that has been sampled, basins of attraction are estimated through area division. Each estimated basin is considered as a new area in the following search. The remaining sub-areas appear to be not so promising, but they should not be ignored as the sample only contains a finite number of discrete points. Therefore, the remaining sub-areas are also merged according to some criteria to form new areas. With the above operations, each sampled area is further divided into several new areas. The new areas generated by the area division step must not overlap and their union should cover the whole sampled area.

3) *Exploitation*. After area division, the exploitation rate is calculated for each area in \mathbf{R} . Areas with better solutions have higher exploitation rates because they are more likely to contain the global optimum. The PE-EBA randomly selects several areas to exploit based on the exploitation rates. Records of areas involved in the exploitation are updated accordingly.

The above three steps are performed iteratively until the termination criterion is met, e.g., the evaluation number of the objective function reaches a predefined upper bound. Then the PE-EBA terminates and returns the best solution among the records in \mathbf{R} as the result. Figure 1 depicts the above framework of PE-EBA. The implementation details of the sampling step, the area division step, and the exploitation step are introduced in the following parts.

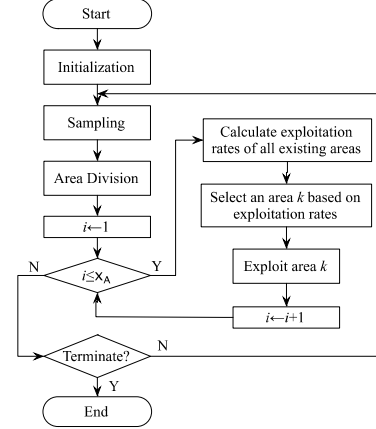


Figure 1. The general framework of the proposed PE-EBA.

2.2 The Sampling Step

Sampling is a preparation step for estimating basins of attraction. Areas with better best solutions are given priority to be sampled first.

In this paper, we adopt a common sample strategy such that solutions in the resulting sample are evenly distributed in the sampled area. Suppose the sampling granularity is m and the sampling interval is $\mathbf{w}^{(k)} = (\mathbf{u}^{(k)} - \mathbf{l}^{(k)})/m$. Then the sample of area k can be written as

$$\mathbf{S}^{(k)} = \{\mathbf{x} | x_i \in V_i^{(k)}, i=1, 2, \dots, n\}, \quad (2)$$

where $V_i^{(k)}$ is a set of m values calculated by $v_{ij}^{(k)} = l_i^{(k)} + w_i^{(k)}(2j-1)/2$, $j=1, 2, \dots, m$. Each sampled solution can define a neighborhood as a region centered at itself with radius as $\mathbf{w}^{(k)}/2$. As shown in Figure 2, the neighborhoods of different sampled solutions do not overlap and their union covers area k .

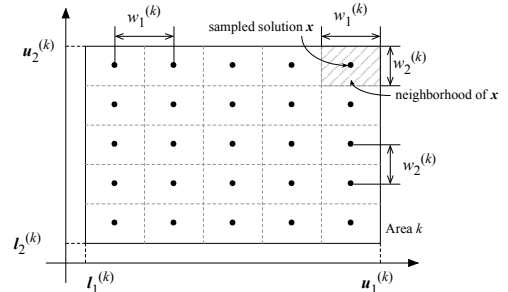


Figure 2. An example of sampling in a 2-dimensional area.

The above sample strategy offers uniform information about the sampled area. However, it suffers from the curse of dimensionality as the sample size grows exponentially with the area dimension ($|\mathbf{S}^{(k)}| = m^n$). When the problem dimension is high, the search domain must be projected onto a lower dimensional space before sampling. We will introduce a projection method in Section 3.

be mapped to an operation on a variable value. Suppose the size of a search step on the i -th dimension of area k is $\lambda_i^{(k)}$. The three directions can be mapped to the operations of changing the variable value x_i to $x_i + \lambda_i^{(k)}$, $x_i - \lambda_i^{(k)}$, and keeping x_i unchanged. Therefore, the search direction at a point in area k can be formulated as an n -dimensional vector $\mathbf{d}^{(k)}$ with each element $d_i^{(k)} \in \{\lambda_i^{(k)}, 0, -\lambda_i^{(k)}\}$, $i=1, 2, \dots, n$. If we check all the search directions to find a promising direction at one point, the sample size will be 3^n . The cost of sampling will quickly become too expensive when the number of dimensions grows. In order to reduce computational cost for predicting promising search directions, the FME procedure employs the orthogonal design method. Please refer to [11] for details of the orthogonal design method.

3. PE-EBA in High Dimensional Problems

The PE-EBA introduced in Section 2 can be directly used to solve low-dimensional numerical problems. However, as the sample size grows exponentially with the dimension of the search domain, the current sampling strategy makes it difficult to apply the PE-EBA in high-dimensional space. There are two ways to conquer this disadvantage. The first way is to derive a sampling strategy that can relieve the curse of dimensionality. The second way is to project the search domain onto a low-dimensional space. In this paper, a simple but effective projection method is introduced for projecting an n -dimensional ($n \geq 3$) search domain to a 2-dimensional plane.

Take a minimization problem with a 3-dimensional search domain as an example. The projection method converts the 3-dimensional objective function f into a combination of two 2-dimensional functions Φ_1 and Φ_2 as $\Phi_1(x_1, \Phi_2(x_2, x_3))$. The PE-EBA is first applied to find a solution (x_1^*, y^*) that minimizes the function value of Φ_1 . Then the PE-EBA searches for a solution (x_2^*, x_3^*) so that $\Phi_2(x_2^*, x_3^*)$ approximate y^* . (x_1^*, x_2^*, x_3^*) becomes the global optimum of f if Φ_1 and Φ_2 satisfy the following conditions:

- The range of Φ_1 is identical with the range of the objective value;
- The search domain of Φ_1 is $\Omega_1 \times Y$, where Ω_1 is the domain of x_1 in f and Y is the range of Φ_2 ;
- Every value in Y can be obtained by Φ_2 with $x_2 \in \Omega_2$ and $x_3 \in \Omega_3$.

Similar to the above example, the PE-EBA can also solve n -dimensional problems by converting the objective function into a combination of $(n-1)$ 2-dimensional functions. The flowchart is shown in Figure 5.

Note that the above projection method may not be applied in all cases. There are situations that the objective function cannot be converted in such a projection method. Depending on the characteristics of the objective function, different types of numerical problems may require different projection methods.

4. Experiments and Discussions

In this section, we first study the effectiveness of the PE-EBA in estimating basins of attractions in 2-dimensional benchmark functions. Then the PE-EBA and the PE-EBA with the projection method (termed p-PE-EBA) are applied to low-dimensional ($n=2$) and high-dimensional ($n=30$) benchmark functions, respectively. In order to validate the effectiveness and efficiency of the PE-EBA, the

results of PE-EBA are compared with the EDA [7] and the global PSO (GPSO) [9].

Table 1 tabulates the benchmark functions employed in experiments [12]. $f_1 \sim f_4$ are unimodal functions, while $f_5 \sim f_{10}$ are multi-modal functions with a number of local optima. The minimum function values of all the benchmark functions are zero. Random vectors are used to shift the benchmark functions for avoiding obtaining good results due to the positions of the global optima.

4.1 Effectiveness of the Area Division Step

Using the unimodal function f_1 and the multimodal function f_5 as examples, Figure 6 shows how the area division step helps to estimate the basins of attraction in the search domain.

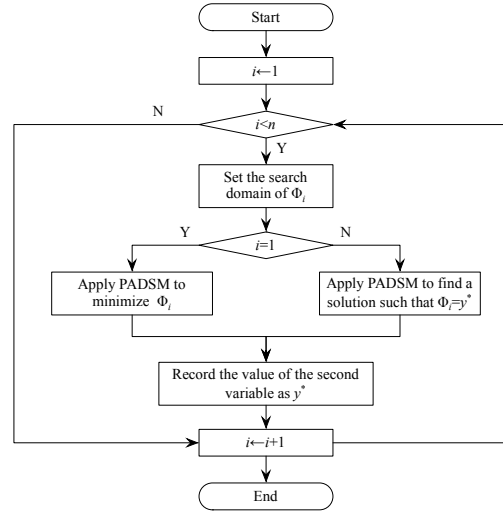


Figure 5. Flowchart of PE-EBA in high-dimensional problems

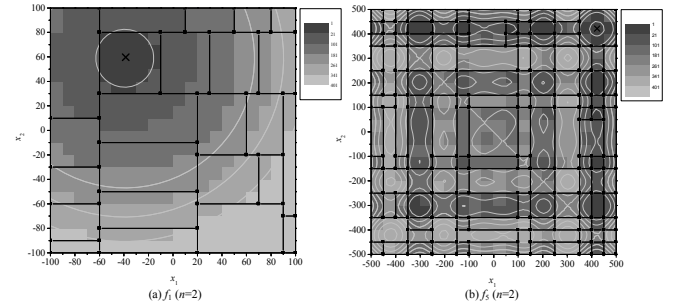


Figure 6. Examples of the area division

Each rectangle in Figure 6 denotes an area obtained after performing the area division step on the search domain of f_1 and f_5 . With $m=20$, the neighborhoods of the 400 sampled solutions are colored according to the solutions' ranks. The neighborhood of a better solution is in darker grey. With $\zeta_1=0.05$, the best 20 sampled solutions are selected for estimating basins of attraction. In Figure 6 (a), the neighborhoods of the 20 best solutions (colored by the darkest gray) form one continuous area. Thus we estimate that only one basin of attraction exists in the search domain of f_1 , which is consistent with the fact that f_1 is a unimodal functions. Moreover, the extent of the estimated basin well approximates the region circled by the contour (denoted by light grey line) with the minimum contour value.

Table 1. List of Benchmark Functions

(n =problem dimension, Ω =predefined search domain, x^* ($x_1^*, x_2^*, \dots, x_n^*$)=global optimum, o (o_1, o_2, \dots, o_n)=random shift vector)

Functions	n	Ω	x_i^*
$f_1(x) = \sum_{i=1}^n (x_i - o_i)^2$	2, 30	$[-100, 100]^n$	o_i
$f_2(x) = \sum_{i=1}^n x_i - o_i + \prod_{i=1}^n x_i - o_i $	2	$[-10, 10]^n$	o_i
$f_3(x) = \sum_{i=1}^n \left[\sum_{j=1}^n (x_j - o_j) \right]^2$	2	$[-100, 100]^n$	o_i
$f_4(x) = \sum_{i=1}^{n-1} \left[100(x_{i+1} - x_i^2) + (x_i - 1)^2 \right]$	2	$[-30, 30]^n$	1
$f_5(x) = \sum_{i=1}^n -x_i \sin(\sqrt{ x_i }) + 418.2829n$	2, 30	$[-500, 500]^n$	420.97
$f_6(x) = \sum_{i=1}^n \left[(x_i - o_i)^2 - 10 \cos 2\pi(x_i - o_i) + 10 \right]$	2, 30	$[-5.12, 5.12]^n$	o_i
$f_7(x) = -20 \exp \left(-0.2 \sqrt{1/30} \sum_{i=1}^n (x_i - o_i)^2 \right) - \exp \left[1/30 \sum_{i=1}^n \cos 2\pi(x_i - o_i) \right]$	2	$[-32, 32]^n$	o_i
$f_8(x) = 1/4000 \sum_{i=1}^n x_i^2 - \prod_{i=1}^n \cos(x_i/\sqrt{i}) + 1$	2	$[-600, 600]^n$	o_i
$f_9(x) = \pi/30 \left\{ 10 \sin^2(\pi y_i) + \sum_{j=1}^{n-1} (y_j - 1)^2 \left[1 + \sin^2(\pi y_{j+1}) \right] + (y_n - 1)^2 \right\} + \sum_{i=1}^n u(x_i - o_i, 10, 100, 4)$	2	$[-50, 50]^n$	$o_i - 1$
$f_{10}(x) = \sum_{i=1}^n u(x_i - o_i, 5, 100, 4) + \pi/10 \left\{ 10 \sin^2 3\pi(x_i - o_i) + \sum_{j=1}^{n-1} (x_j - o_j - 1)^2 \left[1 + \sin^2 3\pi(x_{j+1} - o_{j+1}) \right] + (x_n - o_n - 1)^2 \left[1 + \sin^2 2\pi(x_n - o_n) \right] \right\}$	2	$[-50, 50]^n$	$o_i + 1$

Thus, it can be told that the area division step can effectively discover the area where the global optimum (denoted by a black cross) exists in unimodal functions. In Figure 6 (b), the neighborhoods of the 20 best solutions scatter over the search domain. Thus there are multiple basins of attraction in the search domain of f_5 , which is consistent with the fact that f_5 is a multimodal function. By comparing the estimated basins (containing one or more darkest squares) with the actual contours, it can be observed that the area division step can capture the locations of the global optimum as well as some local optima. The effectiveness of the area division step in estimating basins of attraction in multimodal problems is therefore revealed.

4.2 Low-dimensional Problems

In this part, the PE-EBA are compared with the EDA and GPSO on the nine benchmark functions with $n=2$. The termination criterion of all the algorithms is set the same, i.e., the maximum number of function evaluations is $10000n$. Table 2 tabulates the parameter settings of the three algorithms. To make the results more general, each algorithm is run for 30 times independently. Average results are used for comparison.

Table 3 compares the average results of the four algorithms. The best results are marked in bold. From Table 3, it can be observed that PE-EBA can find the global optima for three of the four unimodal functions. Although GPSO performs better than the PE-EBA on f_4 , it suffers from early convergence on multimodal functions f_5 and f_8 . The PE-EBA, in contrast, can obtain the global optima for all the six multimodal functions. In conclusions, the PE-EBA outperforms the other three algorithms in terms of solution accuracy.

Table 2. Parameter Settings (PS=population size)

Algorithms	Parameters
EDA	PS=1000, no. of fittest individuals=200
GPSO	PS=10, inertia weight=0.794, $c_1=c_2=1.49445$, constrained factor=0.2
PE-EBA	$m=50$, $\xi_1=0.05$, $\xi_2=0.2$, $\xi_3=3$, $\xi_4=3$, $\mu=0.9$, $\alpha_1=0.2$, $\alpha_2=0.9$, $\alpha_3=0.2$, $\alpha_4=3$

Table 3. Comparison on 2-dimensional Benchmark Functions

	Unimodal Functions			Multimodal Functions		
	Func	Average	Std. Dev.	Func	Average	Std. Dev.
EDA	f_1	7.25×10^{-19}	7.05×10^{-19}	f_6	0.000511	0.00192
GPSO		0	0		0	0
PE-EBA		0	0		0	0
EDA	f_2	1.81×10^{-10}	9.08×10^{-11}	f_7	8.71×10^{-10}	5.13×10^{-10}
GPSO		0	0		4.44×10^{-16}	0
PE-EBA		0	0		4.44×10^{-16}	0
EDA	f_3	2.74×10^{-16}	7.03×10^{-16}	f_8	0.00214	0.00193
GPSO		0	0		0.00205	0.00349
PE-EBA		0	0		0	0
EDA	f_4	0.00018	0.000156	f_9	8.44×10^{-20}	9.56×10^{-20}
GPSO		3.28×10^{-29}	9.88×10^{-29}		1.57×10^{-32}	8.35×10^{-48}
PE-EBA		2.55×10^{-5}	0		1.35×10^{-31}	6.68×10^{-47}

Figure 7 depicts the convergence curves of EDA, GPSO, and PE-EBA with f_1, f_3, f_5, f_6, f_9 , and f_{10} as examples. The convergence curves of PE-EBA are the steepest among the three algorithms, indicating that the PE-EBA only needs a small computational cost for evolving to a high accuracy level. This is because once the basin containing the global optimum is found, the exploitation step in the PE-EBA can quickly locate the global optimum by adaptively adjusting the search direction and the search step size. Compared to

the other algorithms, the PE-EBA uses the smallest number of function evaluations to find solutions with the same precision. The PE-EBA converges faster than the other algorithms.

Based on the above results, it can be concluded that the PE-EBA can outperform the other algorithms in both terms of solution accuracy and convergence speed. It is an effective and efficient for solving both unimodal and multimodal problems.

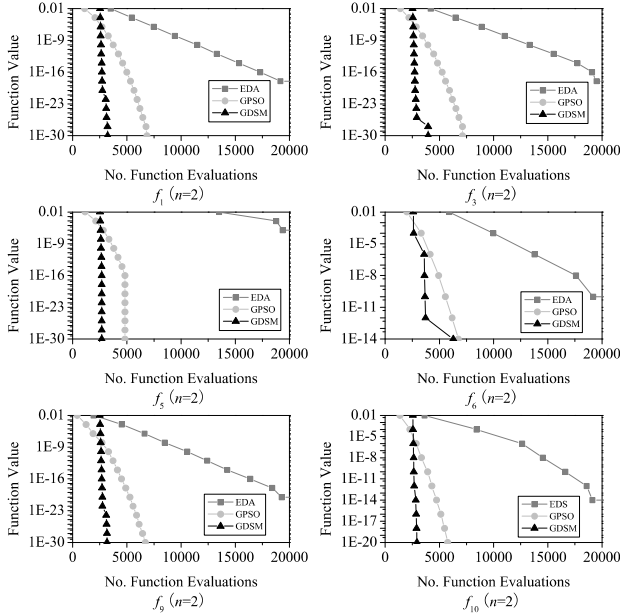


Figure 7. Comparison of convergence speed

4.3 High-dimensional Problems

The projection method introduced in Section 4 cannot solve all the benchmark functions in Table 2. The p-PE-EBA is tested on functions f_1 , f_5 , and f_6 with $n=30$. The parameter settings remain unchanged.

Table 4 tabulates the average results of the three algorithms over 30 independent runs. The best results are shown in bold. From the table, it can be observed that the p-PE-EBA outperforms the other algorithms on all the test functions. The advantage of p-PE-EBA becomes more obvious on multimodal functions. Both GPSO and EDA suffer prematurity, while p-PE-EBA avoids such a problem and locates the global optimum precisely. The experimental results on 30-dimensional benchmark functions show that the PE-EBA is also promising for high-dimensional problems.

Table 4. Comparison on 30-dimensional Problems

	Func	Average	Std. Dev.	Func	Average	Std. Dev.
EDA	f_1	3.57×10^{-25}	3.81×10^{-26}	f_6	152	9.3
GPSO		4.46×10^{-18}	2.44×10^{-17}		46.6	16.9
p-PE-EBA		7.72×10^{-25}	2.72×10^{-25}		0	0
EDA	f_5	8340.00	280			
GPSO		3940.00	443			
p-PE-EBA		0.000382	0			

5. Conclusion

This paper proposes a new derivative-free optimization algorithm for global optimization. The basic idea is to estimate basins of attraction that are likely to contain the global optimum by analyzing

the samples of the objective function. An exploitation method with the ability to predict promising search direction is also introduced for probing the basins efficiently. Experiments on benchmark functions show that the proposed algorithm is able to discover the basins of attraction in both cases of unimodal and multimodal problems. Once the basins are identified, the proposed algorithm can locate the global optimum quickly and accurately.

The study of the PE-EBA is still in the early stage. For future work, a more general strategy is needed for further extending the proposed algorithm to high-dimensional space. The influence of the control parameters on the proposed method needs to be studied. We also look forwards to test the performance of the proposed method on practical problems.

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