An improved multistart based method for global optimization problems

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Abstract

The problem of locating the global minimum of a function finds application in many scientific and real world problems. One of the most used and simplest method to tackle this problem is the so called Multistart method. This article proposes novel method based on the Multistart, that utilizes a mechanism to prevent unnecessary local optimization calls as well as an asymptotic stopping rule. The proposed method is tested against Multistart on a wide set of well - known benchmark optimization problems from the relevant literature and the results are reported.

Keywords: Global optimization, stochastic methods, termination rules.

1 Introduction

A new method for the task of locating the global minimum of a continuous and differentiable function $f : S \to R, S \subset R^n$ is introduced here. The task of locating the global optimum can be formulated as, determine

$$x^* = \arg\min_{x \in S} f(x) \tag{1}$$

with S:

$$S = [a_1, b_1] \otimes [a_2, b_2] \otimes \ldots [a_n, b_n]$$

Methods that discover the global minimum can be used in many areas such as: economics [1, 2], physics [3, 4], chemistry [5, 6], medicine [7, 8] etc. Global optimization methods usually are divided into two main categories: deterministic and stochastic methods. The most common methods of the first category are the so called Interval methods [9, 10], where the set S is divided iteratively in subregions and some subregions that not contain the global solution are discarded using some pre defined criteria. On the other hand, in the second category there are Controlled Random Search methods [11, 12, 13], Simulated

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Annealing methods [14, 15], Differential Evolution methods [16, 17], Particle Swarm Optimization methods [18, 19], Ant Colony Optimization [20, 21], Genetic algorithms [22, 23, 24] etc.

This article introduces a novel method which is based on the multistart method to discover the global minimum of continuous functions. The method incorporates an efficient stopping rule as well as an asymptotic criterion to prevent the algorithm from unnecessary local optimization calls. The multistart method is one of the simplest global optimization technique which start a local search optimizer such as BFGS from different random points and yields the lowest discovered minimum as the global one. Due to its simplicity the method has been used in many problems such as the TSP problem [25], the vehicle routing problem [26], the facility location problem [27], the maximum clique problem [28] etc. The method multistart has been extended in the relevant literature with methods aim to discover all the local minima of a function [30, 31, 32], hybrid multistart techniques [33, 34], GRASP methods[35], new stopping rules [36, 37, 38], parallel techniques[39, 40] etc.

The rest of this article is organized as follows: in section 2 the proposed method is described in detail, in section 3 the experimental results are demonstrated and finally in section 4 some conclusions and guidelines for future work are provided.

2 Method description

The proposed method works for a predefined number of iterations. At every iteration a number of samples is taken in the feasible region of the objective problem. Some of them are considered as starting points for a local search procedure and the rest are discarded. The method continues until the maximum number of iterations is reached or an asymptotic termination rule is satisfied. The main steps of the proposed algorithm are outlined in Algorithm 1. In the following subsection the main parts of the proposed algorithm which are the discarding procedure and the proposed stopping rule are described in detail.

2.1 Discarding procedure

The discarding procedure has two major elements:

- The first is the typical distance that is calculated after every local search and it is given by

$$r_C = \frac{1}{M}\sum_{i=1}^{M}\left\|x_i - x_{iL}\right\| \tag{2}$$

where x_i are starting points for the local search procedure $L(x)$ and x_{iL} is the outcome of $L\left(x_i\right)$. If a point x is close enough to an already discovered local minima then it is highly possible that the point belongs to the so called region of attraction of the minima. The region of attraction of a

Algorithm 1 The main steps of the proposed algorithm.

```
1. Initialization Step
    (a) Set $K$, the maximum number of allowed iterations.
    (b) Set $N$, the number points that will be samples at each iteration.
    (c) Set $r_C = 0$, the distance for the gradient check algorithm.
    (d) Set $X^* = \emptyset$, the set of local minima discovered by the local search
        procedure.
2. Main Step
    (a) For $i = 1..N$ do
        i. Sample randomly a point $x \in$S.
        ii. Check if $x$ is a valid starting point for the local search procedure
            using the method gradientCheck(x) given in algorithm 2.
        iii. If gradientCheck(x)=false then
            A. Start a local search procedure $y = L(x)$
            B. Update the distance $r_C$ using the equation 2.
            C. If $x \notin X^*$ then $X^* = X^* \cup x$
        iv. End if
    (b) End For
3. Termination Check Step. Check the termination rule as described in
   subsection 2.2.
    (a) If the termination rule holds then terminate
    (b) else goto 2
    (c) End if
```

Algorithm 2 The procedure gradientCheck(x).

```
boolean gradientCheck(x)
    1. Set $d = \min_{y \in X^*} \|y - x\|$
    2. Set $z = \arg\min_{y \in X^*} \|y - x\|$
    3. If $d < r_C$ AND $(x - z)^T \left(\nabla f(x) - \nabla f(z)\right) > 0$ then return true
    4. else return false
end gradientCheck
```

local minimum z is defined as:

$$A\left(z\right)=\left\{ x:x\in S,\ L(x)=z\right\} \tag{3}$$

- The second element is a gradient check performed between a candidate starting point and an already discovered local minimum. The value of the objective function $f(x)$ near to an already discovered local minimum can be calculated using:

  $$f(x)\simeq f(z)+\frac{1}{2}\left(x-z\right)^{T}B\left(x-z\right) \tag{4}$$

  where B is the Hessian matrix at the minimum z. By taking gradients in both sides of Equation 4 we obtain:

  $$\nabla f(x)\simeq B\left(x-z\right) \tag{5}$$

  Of course equation 5 holds for any other point y near to z

  $$\nabla f(y)\simeq B\left(y-z\right) \tag{6}$$

  By subtracting the equation 6 from 5 and by multiplying with $\left(x-y\right)^{T}$ we have the following equation:

  $$\left(x-y\right)^{T}\left(\nabla f(x)-\nabla f(y)\right)\simeq\left(x-y\right)^{T}B\left(x-y\right)^{T}>0 \tag{7}$$

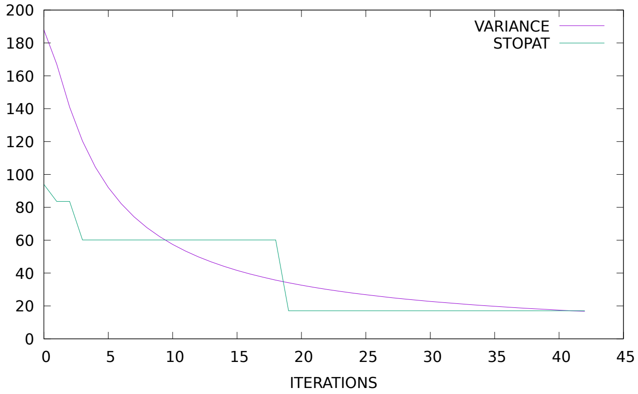
From the above two points a criterion to reject a point x from being a starting point for the local search procedure could be the equation 7. Although, the point x should be close enough to some local minimum and for this purpose the equation 2 is used as a distance measure.

2.2 Stopping rule

A common way to terminate a global optimization procedure is to use the maximum number of allowed iterations, i.e. terminate when iter $\ge K$. Although, this may be a simple criterion but is not an efficient one since, small values of the parameter K mean that the algorithm probably should terminate prematurely. On the other hand higher values for this parameter require more function calls function calls and higher computation times. The termination rule used here is derived from [41]: At every iteration k the variance of $f\left(x^{*}\right)$ is measured, where $x^{*}$is the located global minimum so far. Denote this variance with $\sigma^{(k)}$. If there is no any new minimum found for a number of generations, then it is highly possible that the algorithm has found the global minimum and hence it should terminate. The algorithm terminates when

$$k\ge k_{\mbox{min}}\mbox{ AND }\sigma^{(k)}\le\frac{\sigma^{\left(k_{\mbox{last}}\right)}}{2} \tag{8}$$

Figure 1: Plot of variance along with the stopping quantity for the problem of Potential with 20 atoms.



where k_{last} is the last iteration where a new minimum was found and k_{min} is a predefined minimum number of iterations, in order to prevent the algorithm from premature termination. In figure the values $\sigma^{(k)}$ denoted as VARIANCE and the value $\frac{\sigma^{\left(k_{\text{last}}\right)}}{2}$ denoted as STOPAT are plotted. The objective function used is the EXP8 function given by:

$$f(x) = -\exp\left(-0.5\sum_{i=1}^{8} x_i^2\right), \quad -1 \le x_i \le 1 \tag{9}$$

The value of k_{min} is set to 20 iterations and the maximum number of iterations is 200. The algorithm terminates successfully in 40 generation without spending unnecessary function calls for about 160 generations.

3 Experiments

In order to measure the effectiveness of the proposed approach we utilize several benchmark functions from the relevant literature [42, 43].

3.1 Benchmark functions

Bf1 Function

The function Bohachevsky 1 is given by the equation

$$f(x) = x_1^2 + 2x_2^2 - \frac{3}{10}\cos\left(3\pi x_1\right) - \frac{4}{10}\cos\left(4\pi x_2\right) + \frac{7}{10}$$

with $x \in [-100, 100]^2$. The value of global minimum is 0.0.

Bf2 Function

The function Bohachevsky 2 is given by the equation

$$f(x)=x_1^2+2x_2^2-\frac{3}{10}\cos\left(3\pi x_1\right)\cos\left(4\pi x_2\right)+\frac{3}{10}$$

with $x\in[-50,50]^2$. The value of the global minimum is 0.0.

Branin function

The function is defined by
$f(x)=\left(x_2-\frac{5.1}{4\pi^2}x_1^2+\frac{5}{\pi}x_1-6\right)^2+10\left(1-\frac{1}{8\pi}\right)\cos(x_1)+10$ with $-5\le x_1\le 10,\ 0\le x_2\le 15$. The value of global minimum is 0.397887.with $x\in[-10,10]^2$. The value of global minimum is -0.352386.

Cosine Mixture function (CM)

The function is given by the equation

$$f(x)=\sum_{i=1}^{n}x_i^2-\frac{1}{10}\sum_{i=1}^{n}\cos\left(5\pi x_i\right)$$

with $x\in[-1,1]^n$. The value of the global minimum is -0.4 and in our experiments we have used $n=4$.

Camel function

The function is given by

$$f(x)=4x_1^2-2.1x_1^4+\frac{1}{3}x_1^6+x_1x_2-4x_2^2+4x_2^4,\quad x\in[-5,5]^2$$

The global minimum has the value of $f\left(x^*\right)=-1.0316$

DiffPower function

The Sum of Different Powers function is defined

$$f(x)=\sum_{i=1}^{n}\left|x_i\right|^{i+1}$$

and the global minimum is is $f\left(x^*\right)=0$. The value $n=10$ was used in the conducted experiments and the associated function is denoted as Diffpower10.

Easom function

The function is given by the equation

$$f(x)=-\cos\left(x_1\right)\cos\left(x_2\right)\exp\left(\left(x_2-\pi\right)^2-\left(x_1-\pi\right)^2\right)$$

with $x\in[-100,100]^2$. The value of the global minimum is -1.0

Exponential function.

The function is given by

$$f(x) = -\exp\left(-0.5\sum_{i=1}^{n} x_i^2\right), \quad -1 \le x_i \le 1$$

The global minimum is located at $x^* = (0, 0, ..., 0)$ with value -1. In our experiments we used this function with $n = 8, 32$ and the corresponding functions are denoted by the labels EXP8,EXP32.

Griewank2 function.

The function is given by

$$f(x) = 1 + \frac{1}{200}\sum_{i=1}^{2} x_i^2 - \prod_{i=1}^{2}\frac{\cos(x_i)}{\sqrt{(i)}}, \quad x \in [-100, 100]^2$$

The global minimum is located at the $x^* = (0, 0, ..., 0)$ with value 0.

Griewank10

The function is given by the equation

$$f(x) = \sum_{i=1}^{n}\frac{x_i^2}{4000} - \prod_{i=1}^{n}\cos\left(\frac{x_i}{\sqrt{i}}\right) + 1$$

In our experiments we have used $n = 10$ and the global minimum is 0.0 The function has several local minima in the specified range.

Gkls function.

$f(x) = \text{Gkls}(x, n, w)$, is a function with w local minima, described in [44] with $x \in [-1, 1]^n$ and n a positive integer between 2 and 100. The value of the global minimum is -1 and in our experiments we have used $n = 2, 3$ and $w = 50$. The corresponding functions are denoted by the labels GKLS250 and GKLS350.

Hansen function

$f(x) = \sum_{i=1}^{5} i\cos\left[(i-1)x_1 + i\right]\sum_{j=1}^{5} j\cos\left[(j+1)x_2 + j\right]$, $x \in [-10, 10]^2$. The global minimum of the function is -176.541793.

Hartman 3 function

The function is given by

$$f(x) = -\sum_{i=1}^{4} c_i \exp\left(-\sum_{j=1}^{3} a_{ij}\left(x_j - p_{ij}\right)^2\right)$$

with $x \in [0,1]^3$ and $a = \begin{pmatrix} 3 & 10 & 30 \\ 0.1 & 10 & 35 \\ 3 & 10 & 30 \\ 0.1 & 10 & 35 \end{pmatrix}$, $c = \begin{pmatrix} 1 \\ 1.2 \\ 3 \\ 3.2 \end{pmatrix}$ and

$$p = \begin{pmatrix} 0.3689 & 0.117 & 0.2673 \\ 0.4699 & 0.4387 & 0.747 \\ 0.1091 & 0.8732 & 0.5547 \\ 0.03815 & 0.5743 & 0.8828 \end{pmatrix}$$

The value of global minimum is -3.862782.

Hartman6

$$f(x) = -\sum_{i=1}^{4} c_i \exp\left(-\sum_{j=1}^{6} a_{ij}\left(x_j - p_{ij}\right)^2\right)$$

with $x \in [0,1]^6$ and $a = \begin{pmatrix} 10 & 3 & 17 & 3.5 & 1.7 & 8 \\ 0.05 & 10 & 17 & 0.1 & 8 & 14 \\ 3 & 3.5 & 1.7 & 10 & 17 & 8 \\ 17 & 8 & 0.05 & 10 & 0.1 & 14 \end{pmatrix}$, $c = \begin{pmatrix} 1 \\ 1.2 \\ 3 \\ 3.2 \end{pmatrix}$

and

$$p = \begin{pmatrix} 0.1312 & 0.1696 & 0.5569 & 0.0124 & 0.8283 & 0.5886 \\ 0.2329 & 0.4135 & 0.8307 & 0.3736 & 0.1004 & 0.9991 \\ 0.2348 & 0.1451 & 0.3522 & 0.2883 & 0.3047 & 0.6650 \\ 0.4047 & 0.8828 & 0.8732 & 0.5743 & 0.1091 & 0.0381 \end{pmatrix}$$

The value of global minimum is -3.322368.

Potential function.

The molecular conformation corresponding to the global minimum of the energy of N atoms interacting via the Lennard-Jones potential[45] is used as a test case here. The function to be minimized is given by:

$$V_{LJ}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{10}$$

In the current experiments three different cases were studied: $N = 5,\ 10,\ 20$

Rastrigin function.

The function is given by

$$f(x) = x_1^2 + x_2^2 - \cos(18x_1) - \cos(18x_2), \quad x \in [-1,1]^2$$

The global minimum is located at $x^* = (0,0)$ with value -2.0.

Shekel7

$$f(x) = -\sum_{i=1}^{7} \frac{1}{(x-a_i)(x-a_i)^T + c_i}$$

with $x \in [0,10]^4$ and $a = \begin{pmatrix} 4 & 4 & 4 & 4 \\ 1 & 1 & 1 & 1 \\ 8 & 8 & 8 & 8 \\ 6 & 6 & 6 & 6 \\ 3 & 7 & 3 & 7 \\ 2 & 9 & 2 & 9 \\ 5 & 3 & 5 & 3 \end{pmatrix}$, $c = \begin{pmatrix} 0.1 \\ 0.2 \\ 0.2 \\ 0.4 \\ 0.4 \\ 0.6 \\ 0.3 \end{pmatrix}$. The value of global minimum is -10.342378.

Shekel 5

$$f(x) = -\sum_{i=1}^{5} \frac{1}{(x-a_i)(x-a_i)^T + c_i}$$

with $x \in [0,10]^4$ and $a = \begin{pmatrix} 4 & 4 & 4 & 4 \\ 1 & 1 & 1 & 1 \\ 8 & 8 & 8 & 8 \\ 6 & 6 & 6 & 6 \\ 3 & 7 & 3 & 7 \end{pmatrix}$, $c = \begin{pmatrix} 0.1 \\ 0.2 \\ 0.2 \\ 0.4 \\ 0.4 \end{pmatrix}$. The value of global minimum is -10.107749.

Shekel 7

$$f(x) = -\sum_{i=1}^{7} \frac{1}{(x-a_i)(x-a_i)^T + c_i}$$

with $x \in [0,10]^4$ and $a = \begin{pmatrix} 4 & 4 & 4 & 4 \\ 1 & 1 & 1 & 1 \\ 8 & 8 & 8 & 8 \\ 6 & 6 & 6 & 6 \\ 3 & 7 & 3 & 7 \\ 2 & 9 & 2 & 9 \\ 5 & 3 & 5 & 3 \end{pmatrix}$, $c = \begin{pmatrix} 0.1 \\ 0.2 \\ 0.2 \\ 0.4 \\ 0.4 \\ 0.6 \\ 0.3 \end{pmatrix}$. The value of global minimum is -10.342378.

Shekel 10

$$f(x) = -\sum_{i=1}^{10} \frac{1}{(x-a_i)(x-a_i)^T + c_i}$$

with $x \in [0,10]^4$ and $a = \begin{pmatrix} 4 & 4 & 4 & 4 \\ 1 & 1 & 1 & 1 \\ 8 & 8 & 8 & 8 \\ 6 & 6 & 6 & 6 \\ 3 & 7 & 3 & 7 \\ 2 & 9 & 2 & 9 \\ 5 & 5 & 3 & 3 \\ 8 & 1 & 8 & 1 \\ 6 & 2 & 6 & 2 \\ 7 & 3.6 & 7 & 3.6 \end{pmatrix}$, $c = \begin{pmatrix} 0.1 \\ 0.2 \\ 0.2 \\ 0.4 \\ 0.4 \\ 0.6 \\ 0.3 \\ 0.7 \\ 0.5 \\ 0.6 \end{pmatrix}$. The value of global minimum is -10.536410.

Sinusoidal function.

The function is given by

$$f(x) = -\left(2.5 \prod_{i=1}^{n} \sin\left(x_i - z\right) + \prod_{i=1}^{n} \sin\left(5\left(x_i - z\right)\right)\right), \quad 0 \le x_i \le \pi.$$

The global minimum is located at $x^* = (2.09435, 2.09435, ..., 2.09435)$ with $f\left(x^*\right) = -3.5$. In our experiments we used $n = 8, 32$ and $z = \frac{\pi}{6}$ and the corresponding functions are denoted by the labels SINU8 and SINU32 respectively.

Test2N function.

This function is given by the equation

$$f(x) = \frac{1}{2} \sum_{i=1}^{n} x_i^4 - 16x_i^2 + 5x_i, \quad x_i \in [-5, 5].$$

The function has 2^n in the specified range and in our experiments we used $n = 4, 5, 6, 7$. The corresponding values of global minimum is -156.664663 for $n = 4$, -195.830829 for $n = 5$, -234.996994 for $n = 6$ and -274.163160 for $n = 7$.

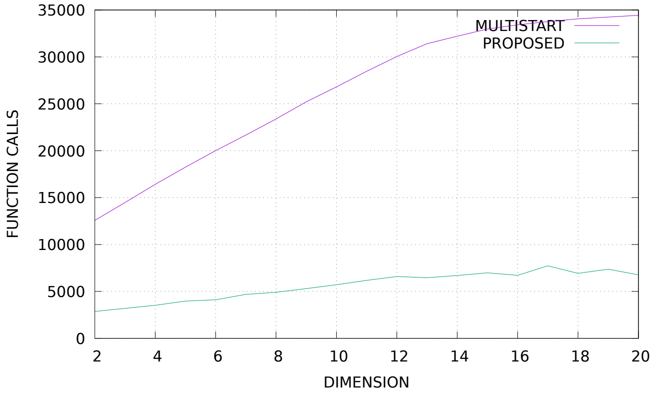
Test30N function.

This function is given by

$$f(x) = \frac{1}{10} \sin^2\left(3\pi x_1\right) \sum_{i=2}^{n-1} \left(\left(x_i - 1\right)^2 \left(1 + \sin^2\left(3\pi x_{i+1}\right)\right)\right) + \left(x_n - 1\right)^2 \left(1 + \sin^2\left(2\pi x_n\right)\right)$$

with $x \in [-10, 10]$. The function has 30^n local minima in the specified range and we used $n = 3, 4$ in our experiments. The value of global minimum for this function is 0.0

Figure 2: Average number of function calls for the function Exponential.



3.2 Experimental results

The proposed method is compared against the multistart method with the same number of samples at every generation and the same stopping rule and the results are reported in Table 1. The column PROBLEM denotes the objective function, the column MULTISTART denotes the average function calls for the multistart method and the PROPOSED column denotes the average function calls for the proposed method. The number in the cells denotes average function calls for 30 independent runs using different seed for the random generator each time. The numbers in parentheses denote the fraction of runs where the global minimum was located. If this number is missing then the global minimum was discovered in every independent run (100% success). The last row in all tables (denoted by TOTAL) is the total number of function calls for listed test problems. The parameters used in the experiments are listed in Table 2. As it is evident from the conducted experiments there is a significant improvement in terms of function evaluations at about 80%.

Also, in order to measure the efficiency of the proposed method for as the dimension of the objective functions increases an additional experiments was conducted: The function Exponential was used with different values of the dimension n from 2 to 20. The proposed method is tested against Multistart and the results are plotted in Figure 2. The average function calls required by the proposed method are in the range [4000,6000] when the Multistart requires 5 or 6 times more function calls.

Additionally another experiment was conducted using the Exponential function with $n = 10$ with different values for the number of samples N and the results are plotted in Figure 3. Again the Multistart requires much more function calls than the proposed method and also the Multistart function calls tends to increase very rapidly as compared to the calls of the proposed method.

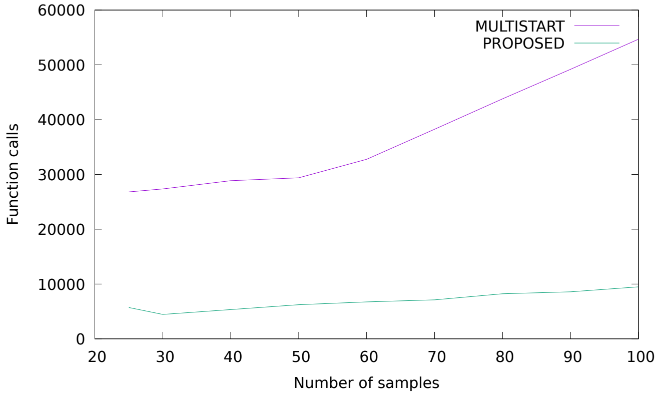
Table 1: Average number of function calls for the proposed functions.

PROBLEM	MULTISTART	PROPOSED
BF1	22533	2833
BF2	18809	2629
BRANIN	9735	1753
CM4	27037	2293
CAMEL	13688	1732
DIFFPOWER10	1194776	19572
EASOM	5372	199
EXP8	12022	2830
EXP32	18294	3265
GKLS250	17333(0.77)	2415(0.93)
GKLS350	10104	243
GRIEWANK2	13003	1786
GRIEWANK10	53372	7184
HANSEN	15294	1510
HARTMAN3	14815	11463
HARTMAN6	19459	3740
POTENTIAL5	111631	49601
POTENTIAL10	208405	91094
POTENTIAL20	280575	170524(0.97)
RASTRIGIN	16968	675
SHEKEL5	19224	3465
SHEKEL7	20985	2976
SHEKEL10	20284	3566
SINU8	21860	549
SINU32	39905	1296
TEST2n4	15938	2890
TEST2n5	18085	3262
TEST2n6	19879	3451
TEST2n7	21432	4002
TEST30n3	24450	10818
TEST30n4	26514	13320
TOTAL	**2231781**	**426666**

Table 2: Parameter values for the experiments.

PARAMETER	VALUE
K	200
N	25
k_{min}	20

Figure 3: Average number of function calls as the number of samples increases for the function EXP10.



4 Conclusions

A novel multistart based method is described and tested here for global optimization problems. The method utilizes an efficient discarding procedure to prevent the method from unnecessary function calls and an asymptotic stopping rule to stop the algorithm where there is a good probability that the global optimum has been discovered. The method was tested on a series of well known optimization problems from the relevant literature and proved to be efficient and fast.

Compliance with Ethical Standards

All authors declare that they have no has no conict of interest.

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