An improved multistart based method for global optimization problems

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Abstract

There is a great need to discover the global optimum of multimodal functions that arises from many scientifical and practical problems. A base method used to solve this problem is the Multistart method. The proposed method extends the traditional method by adding two major features: the first one is a rejection mechanism to prevent the method from spending time in unnecessary function evaluations and the second is a stopping rule aimed to terminate the method when the global minimum has been located with some certainty. The proposed method has been evaluated on a series of global optimization functions from the relevant literature and it is compared against some other optimization methods and the experimental results are presented.

Keywords: Global optimization, stochastic methods, termination rules.

1 Introduction

A novel 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:

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

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

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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 Annealing methods [14, 15, 16], Differential Evolution methods [17, 18], Particle Swarm Optimization methods [19, 20, 21], Ant Colony Optimization [22, 23], Genetic algorithms [24, 25, 26] etc. Also many hybrid methods have been proposed such as combing the Simplex method and Inductive search [27], methods that using PSO in conjuction with other methods [28, 29], etc. Recently many works have been appeared that take advantage of the GPU processing units to implement parallel global optimization methods [30, 31, 32].

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 starts a local optimization method from different random samples 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 [33], the vehicle routing problem [34], the facility location problem [35], the maximum clique problem [36], the maximum fire risk insured capital problem [37], aerodynamic shape problems [38] etc. During the past year, the method multistart has been enhanced in the relevant literature with methods that target to discover all the local minima of a function [40, 41, 42], hybrid multistart techniques [43, 44], GRASP methods[45], new stopping rules [46, 47, 48], parallel techniques[49, 50], methods that utlize the modern GPU architectures to execute [51, 52], methods that introduces sampling in the multistart method using Neural Networks [53] 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

At every iteration of the proposed method a number of samples is taken in the bounding box 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, defined in subsection 2.2 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.

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), used to reject points from being start points of the local search procedure.

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 $(x - z)^T (\nabla f(x) - \nabla f(z)) > 0$ **then return** true
4. **else return** false

end gradientCheck

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

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

  where the local search procedure $L(x)$ initiates from x_i and x_{iL} is the outcome of $L(x_i)$. 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 local minimum z is defined as:

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

- 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:

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

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

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

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

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

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

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

The distance r_C is used with conjunction with equation 7 to reject a point. The method rejects points from being start points if they are close enough to some other located local minima and in the same time equation 7 holds. A measure to identify if a point is close enough to some other located local minima is the distance r_C calculated after every local minimization.

In order to measure the efficiency of the above rejection procedure two tests were performed on two benchmark functions: Rastrigin and Exp16. In these test the proportion of local search starts over total number of samples were measured. The plot of this measurement for 20 iterations is plotted in Figures 1 and 2 respectively.

Figure 1: Plot for the proportion of local search starts over total number of samples for the Rastrigin function for the first 20 iterations.

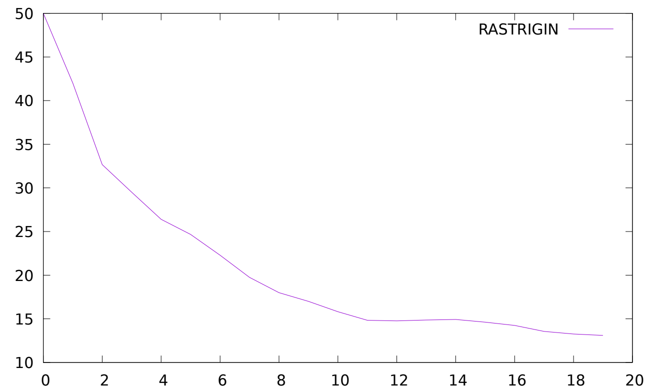


Figure 2: Plot for the proportion of local search starts over total number of samples for the EXP16 function for the first 20 iterations.

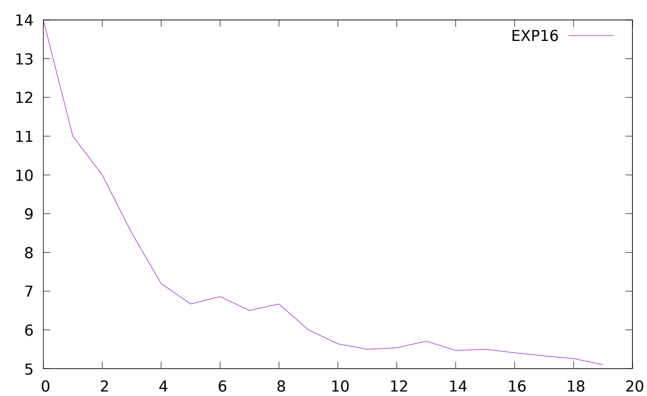
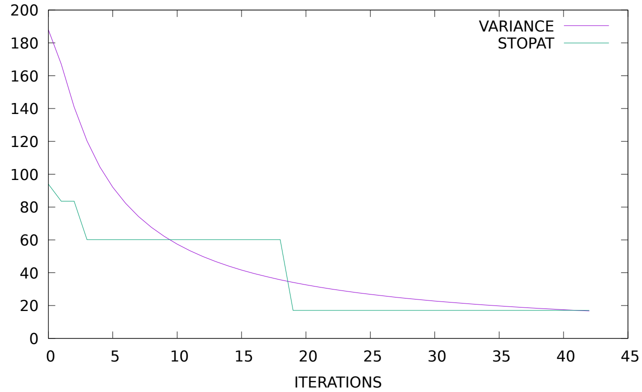


Figure 3: Plot of variance along with the stopping quantity for the problem of Potential with 20 atoms.



2.2 Stopping rule

A common way to terminate a global optimization procedure is to use the maximum number of allowed iterations, i.e. stop when iter $\geq K$. Although, it is a simple criterion but is not an efficient one since, if K is tool small, then the algorithm will terminate without locating the global optimum. Also, when K is too high, the optimization algorithm will spend computation time in unnecessary function calls. The termination rule used here is derived from [54]: denote with $\sigma^{(k)}$ the variance of $f(x^*)$, where k is the current iteration and x^* is the so far located global minimum. If the algorithm did not manage to locate new minimum for a number of generations, then probably the algorithm has located the global minimum and it should terminate. The termination rule stops the algorithm when

$$k \geq k_{\mathrm{min}} \text{ AND } \sigma^{(k)} \leq \frac{\sigma^{\left(k_{\mathrm{last}}\right)}}{2} \tag{8}$$

where k_{last} stands for iteration where a new minimum was found. The value k_{min} is a predefined minimum number of iterations, in order to prevent the algorithm from premature termination. In figure 3 the values $\sigma^{(k)}$ denoted as VARIANCE and the value $\frac{\sigma^{\left(k_{\mathrm{last}}\right)}}{2}$ denoted as STOPAT are plotted. The objective function used is the EXP8 function. 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.

2.3 Constrained optimization problems

The proposed method can also be used to constrained optimization problems, which general formulation is:

$$\begin{aligned} \min_x \quad & f(x) \quad \text{subject to} \\ & g_i(x) \leq 0 \quad i = 1, \ldots, m \\ & h_j(x) = 0 \quad j = 1, \ldots, p \end{aligned} \tag{9}$$

where $x_i \in [a_i, b_i]$, $i = 1, \ldots, n$, which finds application in many practical fields such as physics [62], astronomy [63], chemistry [64], biology [65] etc. Many methods have been proposed to tackle this problem such as Lagrange multiplier methods [66], Trust region methods [67], interval methods [68], methods based on differential evolution [69] etc. The constrained optimization problem can transformed to a single function for the proposed method. The transformation is performed in a way that when a solution is infeasible then the function value is penalized according to the constraint violations. The steps for the transformation are the following:

1. **Set** $v_1(x) = f(x)$
2. **Set** $v_2(x) = \sum_{i=1}^{p} h_i^2(x)$
3. **Calculate** for the inequality constraints $g_i(x),\ i = 1, ..., m$ the quantity

   $$v_3(x) = \sum_{i=1}^{m} G_i^2\left(g_i(x)\right) \tag{10}$$

   where the function $G(x)$ is defined as follows:

   $$G(x) = \begin{cases} 0, & x \leq 0 \\ x, & x > 0 \end{cases} \tag{11}$$

4. The transformed objective function for the proposed method is given by:

   $$v(x) = v_1(x) + \lambda v_2(x) + \lambda v_3(x) \tag{12}$$

   where $\lambda > 0$.

3 Experiments

The proposed method was tested on a series of unconstrained and constrained optimization functions that are listed in the Appendix. The local search procedure in all experiments and methods was a BFGS variant of Powell[55]. Two series of test were performed. In the first series the proposed method was tested against some other restarting techniques from the relevant literature and the results are listed in Table 1. These methods are:

1. Multistart method. This is simple method, who samples a series of points each time (the same number as the proposed method) and performs a local search procedure from every sample. In order to be the results comparable against the proposed method the same stopping rule was used also in the Multistart method. The code was implemented in ANSI C++.

2. Multistart method with the repulsion sampling technique [57] (title MREP). During the repulsion sampling, any produced sample is repelled to a new location by the old starting points, in order to avoid already visited regions of attraction.

3. The Topographical Multilevel Single Linkage (TMLSL) method proposed in [40]. This is another enhancement of the Multistart method, that is based on the discovery of the so - called graph minima in order to reduce the number of function calls. The implemented TMLSL algorithm uses the suggested $N = 10n$ value for the number of samples used in every iteration of the method.

In the second series of experiments the method was tested against some state of the art methods from the relevant literature:

1. Controlled Random Search denoted as CRS in the results. The implementation used here is based on the algorithm of Price[11] made in Ansi C++. The method uses the suggested $N = 25n$ from price value for the initial number of samples in the set. Also, the implementation utilizes the application of the Local search procedure after the termination of the algorithm to enhance the located global optimum.

2. Simulated Annealing, denoted as SA in the results. The used software here is the work of Corana[56].

3. Particle swarm optimization[19], denoted as PSO in the results. The implemented software here is coded in ANSI C++ and utilizes the same stopping rule as in the proposed method.

The experimental results for the second series of the experiments are reported in Table 2. The number in the cells denotes average function calls for 30 runs using with seed for the random generator each time. The fraction in parentheses stands for the fraction of runs where the global optimum was found. If this number is missing then the global minimum was discovered in every independent run (100% success). The parameters used in the experiments are listed in Table 3. The bold letters were used to demonstrate the method that achieved the best average result.

The proposed method seems to require less number of function calls than the other methods and the PSO technique shown to work well for small problems like BF1 or BRANIN but failed to work on bigger problems such Potential20, a problem with dimension 60 and thousands of local minima. Also, in some small problems the TMLSL required less function calls than the other methods, but in the majority of cases TMLSL did not manage to discover the global minimum of the mentioned test functions in every run. On the other hand, the Simulated Annealing managed to solve with success all the optimization problems, although it requires more function calls than the proposed method and the same holds for the simple Multistart method. Also, the Repulsion method seems to overcome the simple Multistart but in the majority of cases require significant more function calls than the proposed method.

In Table 4 the results from the comparison of Multistart and the proposed method for the constrained optimization test problems are listed. Again, the proposed method has managed to handle the test problems using less number of function evaluations than the Multistart method. The value of $\lambda = 100$ was used for the conducted experiments. Again, the proposed method overcomes the Multistart method to solve constrained optimization problems.

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 4. 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 5. 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.

To compare the proposed method with all the rest methods for different function calls, the Wilcoxon signed-rank test was used. The results obtained with this statistical test are shown in Figure 6. The results indicate that the proposed method is superior than the most of unconstrained optimization function (multistart, CSA and SA). There was not, however, a significant difference between PSO and the proposed method.

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.

Table 1: Comparison results between the proposed method and other restart methods.

PROBLEM	MULTISTART	MREP	TMLSL	PROPOSED
BF1	22533	5767	601(0.8)	**2833**
BF2	18809	4873	575(0.83)	**2629**
BRANIN	9735	4221	**498**	1753
CM4	27037	15216	1125(0.4)	**2293**
CAMEL	13688	4828	**503**	**1732**
DIFFPOWER10	1194776	67129	48847	**19572**
EASOM	5372	3834	471	**199**
EXP8	12022	7226	**1675**	2830
EXP32	18294	7600	6462	**3265**
GKLS250	17333(0.77)	3854	3980	**2415**
GKLS350	10104	5081	776(0.97)	**243**
GRIEWANK2	13003	5031	520(0.20)	**1786**
GRIEWANK10	53372	28289	2182(0.40)	**7184**
HANSEN	15294	5268(0.97)	702(0.97)	**1510**
HARTMAN3	14815	5807	**1366**	11463
HARTMAN6	19459	7598	**2762**	3740
POTENTIAL5	111631	29281	**7196**	49601
POTENTIAL10	208405	**73080**	125410(0.93)	91094
POTENTIAL20	280575	**135164**	143930	170524(0.97)
RASTRIGIN	16968	4706	637(0.40)	**675**
SHEKEL5	19224	6456	**1020**	3465
SHEKEL7	20985	7116	1035(0.90)	**2976**
SHEKEL10	20284	6968	1060(0.90)	**3566**
SINU8	21860	13183	5489(0.93)	**549**
SINU32	39905	92562	111042(0.93)	**1296**
TEST2n4	15938	9860	1257(0.93)	**2890**
TEST2n5	18085	11190	2173(0.73)	**3262**
TEST2n6	19879	13185	2113(0.23)	**3451**
TEST2n7	21432	14579	8989(0.50)	**4002**
TEST30n3	24450	13644	**916**	10818
TEST30n4	26514	12004	**1592**	13320

Table 2: Average number of function calls for the proposed functions. Comparison between the proposed method and some state of the art global optimization methods.

PROBLEM	CRS	SA	PSO	PROPOSED
BF1	2218	3845	**2494**	2833
BF2	2207	3340	2641	**2629**
BRANIN	1744	4816	**1636**	1753
CM4	4746	9652	2988	**2293**
CAMEL	1882	4820	**1639**	1732
DIFFPOWER10	78634	25918	15500(0.87)	**19572**
EASOM	588	4807	866	**199**
EXP8	13239	19233	3084	**2830**
EXP32	93520	76842	5055	**3265**
GKLS250	1633	4120	**1459**	2415
GKLS350	3329	7229	2259(0.97)	**243**
GRIEWANK2	2111	3830	2595(0.83)	**1786**
GRIEWANK10	32037	24118	8378(0.25)	**7184**
HANSEN	3348	3323	4284	**1510**
HARTMAN3	2898	7227	**2448**	11463
HARTMAN6	9276	14440	4645	**3740**
POTENTIAL5	95027	36084	**20100**	49601
POTENTIAL10	193066	172166	19610(0.13)	91094
POTENTIAL20	189591(0.53)	244314	18466(0.03)	170524(0.97)
RASTRIGIN	1906	3343	2258	**675**
SHEKEL5	6345	9635	4791	**3465**
SHEKEL7	6528	9334	5722	**2976**
SHEKEL10	6477	9998	5354	**3566**
SINU8	16950	19241	5398	**549**
SINU32	100887	13858	6887	**1296**
TEST2n4	6754	9631	5219	**2890**
TEST2n5	12717	12036	7672	**3262**
TEST2n6	12822	14438	8039	**3451**
TEST2n7	18620	16840	8220	**4002**
TEST30n3	2768	9616	**2456**	10818
TEST30n4	**3894**	10617	4528	13320

Table 3: Parameter values for the experiments. The parameters are hold for Multistart, the Repulsion method and the proposed method.

PARAMETER	VALUE
K	200
N	25
$k_{\min}$	20

Figure 4: Average number of function calls for the function Exponential, as the dimension of the function increases.

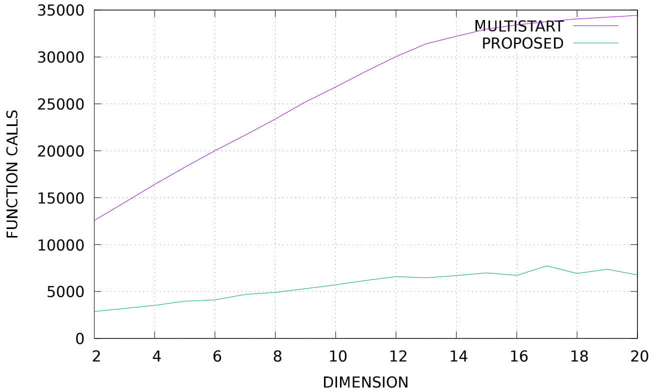


Figure 5: Average number of function calls as the number of samples increases for the function EXP10.

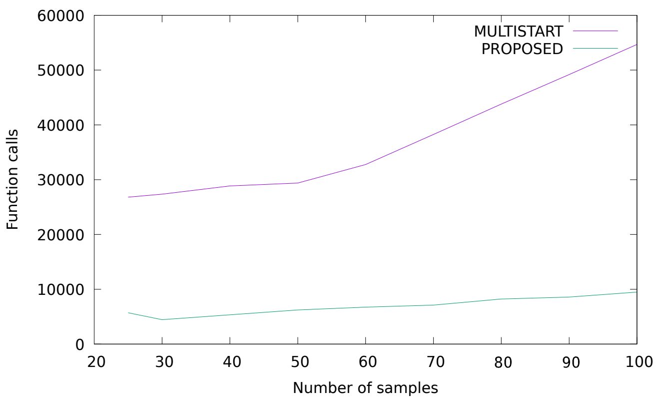
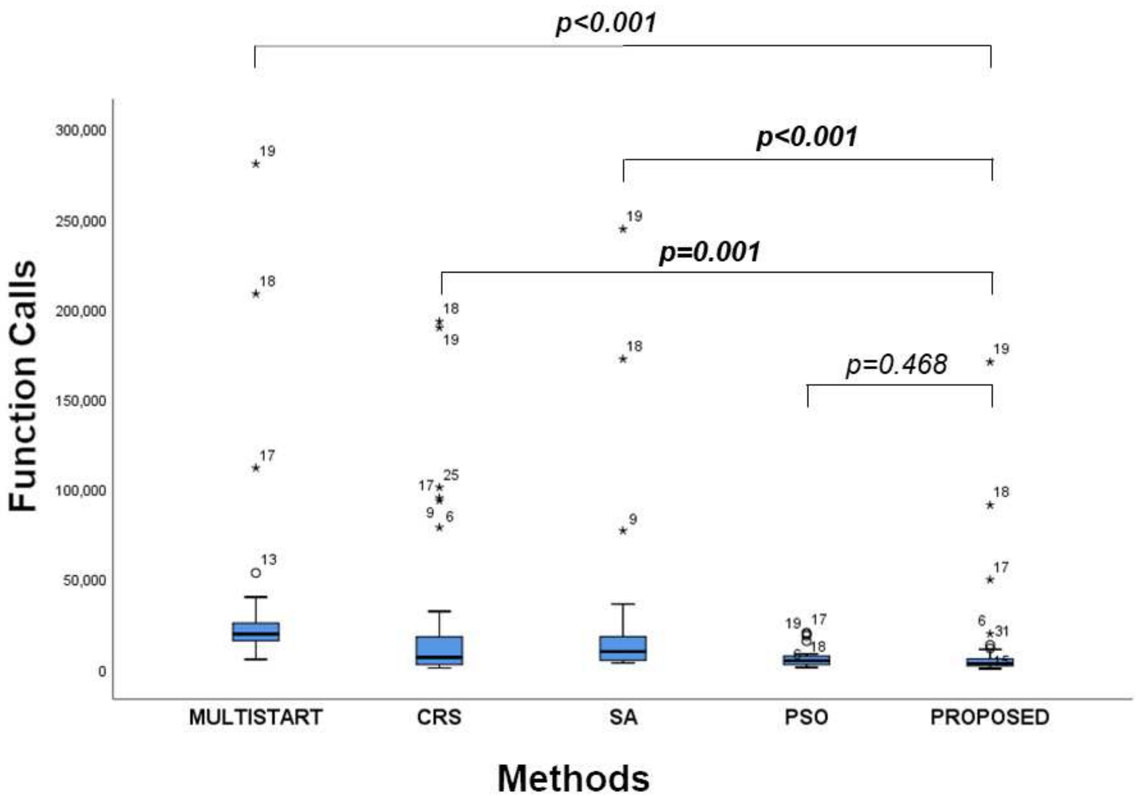


Table 4: Average function calls from comparisons of the proposed method and Multistart for the constrained optimization problems.

PROBLEM	MULTISTART	PROPOSED
Levy	17491	1301
Salkin	48816	1010
Hess	27775	9524
Chootinan1	293459	15035
G15	318162	63542

Figure 6: Box plot representation and Wilcoxon rank-sum test results of the comparison between the multistart, CRS, SA, and PSO method and the proposed method. A p-value of less than 0.05 (2-tailed) was used for statistical significance and has been marked with bold.



Appendix - Test functions

In order to measure the effectiveness of the proposed approach we utilize several benchmark functions from the relevant literature [58, 59].

Unconstrained optimization functions

- **Bf1** function. The function Bohachevsky 1 is given by the equation

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

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

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

  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.

- **CM** function. The Cosine Mixture function is given by the equation

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

  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 $f(x^*) = -1.0316$

- **DiffPower** function. The Sum of Different Powers function is defined

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

  and the global minimum is is $f(x^*) = 0$. 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

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

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** function. 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. $f(x) = \mathrm{Gkls}(x, n, w)$, is a function with w local minima, described in [60] 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. $f(x) = \sum_{i=1}^{5} i\cos[(i-1)x_1 + i]\sum_{j=1}^{5} j\cos[(j+1)x_2 + j]$, $x \in [-10, 10]^2$. 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.

- **Hartman 6** function.

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

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[61] is used as a test case here. The function to be minimized is given by:

$$V_{LJ}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{13}$$

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.

- **Shekel 7** function.

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

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** function.

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

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 10** function.

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

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

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

  The global minimum is located at $x^* = (2.09435, 2.09435, ..., 2.09435)$ with $f(x^*) = -3.5$. 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

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

  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

Constrained optimization test fuctions

The following functions were used from the relevant literature.

- **Levy** function. This problem is described in [70] and it is given by:

$$\min_x f(x) = -x_1 - x_2$$

  with $x \in [0, 1]^2$, subject to

$$g_1(x) = \left\lfloor (x_1 - 1)^2 + (x_2 - 1) \right\rfloor \left(\frac{1}{2a^2} - \frac{1}{2b^2}\right) + (x_1 - 1)(x_2 - 1)\left(\frac{1}{a^2} - \frac{1}{b^2}\right) - 1 \geq 0$$

  with $a = 2,\ b = 0.25$. The value of global minimum is $f_{\text{min}} = -1.8729$.

- **Salkin** function. This problem is described in [71] and it is given by:

$$\max_x f(x) = 3x_1 + x_2 + 2x_3 + x_4 - x_5$$

  with $1 \leq x_1 \leq 4,\ 80 \leq x_2 \leq 88,\ 30 \leq x_3 \leq 35,\ 145 \leq x_4 \leq 150,\ 0 \leq x_5 \leq 2$ subject to

$$\begin{aligned}
g_1(x) &= 25x_1 - 40x_2 + 16x_3 + 21x_4 + x5 \leq 300 \\
g_2(x) &= x_1 + 20x_2 - 50x_3 + x_4 - x_5 \leq 200 \\
g_3(x) &= 60x_1 + x_2 - x_3 + 2x_4 + x_5 \leq 600 \\
g_4(x) &= -7x_1 + 4x_2 + 15x_3 - x_4 + 65x_5 \leq 700
\end{aligned}$$

  This global maximum is $f_{\text{max}} = 320$.

- **Hess** function. This problem is described in [72] and it is given by:

$$\max_x f(x) = 25\,(x_1-2)^2+(x_2-2)^2+(x_3-1)^2+(x_4-4)^2+(x_5-1)^2+(x_6-4)^2$$

with $0 \le x_1 \le 5,\ 0 \le x_2 \le 1,\ 1 \le x_3 \le 5,\ 0 \le x_4 \le 6,\ 0 \le x_5 \le 5,\ 0 \le x_6 \le 10$ subject to:

$$\begin{aligned} g_1(x) &= x_1 + x_2 - 2 \ge 0 \\ g_2(x) &= -x_1 + x_2 + 6 \ge 0 \\ g_3(x) &= x_1 - x_2 + 2 \ge 0 \\ g_4(x) &= -x_1 + 3x_2 + 2 \ge 0 \\ g_5(x) &= (x_3-3)^2 + x_4 - 4 \ge 0 \\ g_6(x) &= (x_5-3)^2 + x_6 - 4 \ge 0 \end{aligned}$$

The value of global maximum is $f_{\max} = 310$.

- **Chootinan1** function. This problem is described in [73] and it is given by:

$$\min_x f(x) = 5\sum_{i=1}^{4} x_i - 5\sum_{i=1}^{4} x_i^2 - \sum_{i=1}^{13} x_i$$

with $0 \le x_i \le 1$ for $i = 1,..,9,13$, $0 \le x_i \le 100$ for $i = 10,11,12$ with the following constraints:

$$\begin{aligned} g_1(x) &= 10 - (2x_1 + 2x_2 + x_{10} + x_{11}) \ge 0 \\ g_2(x) &= 10 - (2x_1 + 2x_3 + x_{10} + x_{12}) \ge 0 \\ g_3(x) &= 10 - (2x_2 + 2x_3 + x_{11} + x_{12}) \ge 0 \\ g_4(x) &= 8x_1 - x_{10} \ge 0 \\ g_5(x) &= 8x_2 - x_{11} \ge 0 \\ g_6(x) &= 8x_3 - x_{12} \ge 0 \\ g_7(x) &= 2x_4 + x_5 - x_{10} \ge 0 \\ g_8(x) &= 2x_6 + x_7 - x_{11} \ge 0 \\ g_9(x) &= 2x_8 + x_9 - x_{12} \ge 0 \end{aligned}$$

The value of global minimum is $f_{\min} = -15.0$.

- **G15** function. This problem is described in [74] and it is given by:

$$\min_x f(x) = 1000 - x_1^2 - 2x_2^2 - x_3^2 - x_1x_2 - x_1x_3$$

with $x \in [0,10]^3$ subject to the following constraints:

$$\begin{aligned} h_1(x) &= x_1^2 + x_2^2 + x_3^2 - 25 = 0 \\ h_2(x) &= 8x_1 + 14x_2 + 7x_3 - 56 = 0 \end{aligned}$$

The value of the global minimum is $f_{\min} = 961.7150$

Compliance with Ethical Standards

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

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