MinCenter: a novel clustering technique for global optimization

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Abstract

A common problem arises in many scientific fields is that of locating the global minimum of a multimodal function. A novel clustering technique that tackles this problem is introduced here. The proposed method creates clusters from uniform samples of the objective function with the usage of the Kmeans clustering technique. For every cluster a center is created. Finally, a simple rejection procedure is applied to the created clusters in order to remove clusters that are close to others. The proposed method is tested on a series of well - known optimization problems from the relevant literature and the results are reported and compared against the simple Multistart global optimization method.

Keywords: Global optimization, clustering, hubrid methods, numerical methods.

1 Introduction

A novel method that estimates the global minimum of a continuous and differentiable function $f : S \to R, S \subset R^n$ is proposed in the current article. The global optimum location problem is usually defined as:

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

where S is

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

A review of the recent advantages in the area of the Global Optimization can be found in [1]. Methods that discover the global minimum can be used in many areas such as: economics [2, 3], physics [4, 5], chemistry [6, 7], medicine [8, 9] etc. Global optimization methods usually are divided into two main categories:

*Corresponding author. Email: itsoulos@uoi.gr deterministic and random search methods. Common methods of the first category are the so called Interval methods [10, 11], where the set S is divided iteratively in subregions using some criteria. On the other hand, random search methods are used in the majority of cases, because they can be implement easy and they do not depend on a some a priori information about the objective function. A small set of random search methods may include Controlled Random Search methods [12, 13, 14], Simulated Annealing methods [15, 16], Differential Evolution methods [17, 18], Particle Swarm Optimization methods [19, 20], Ant Colony Optimization [21, 22], Genetic algorithms [23, 24, 25] etc.

A subclass of random search methods are the clustering techniques as proposed by Rinnooy Kan [26], Ali [27], Tsoulos [28], etc. These methods are try to estimate the clusters of function in order to minimize the effort required to compute the global minimum or all the local minima of the function. The term cluster refers to a set of points that are believed, under some asymptotic considerations, to belong to the same region of attraction of the function. The region of attraction for a local minimum x^* is defined as:

$$A\left(x^*\right) = \left\{x:\ x \in S \subset R^n,\ L(x) = x^*\right\} \tag{2}$$

where $L(x)$ is a local search procedure that starts from a given point x and terminates when a local minimum is discovered. Common local search procedures are BFGS[29, 30], Steepest Descent[31], L-Bfgs [32] for large scaled functions etc. The proposed method creates clusters iteratively using the well - known technique of the K-Means clustering introduced by MacQueen[33]. For every cluster a representative is constructed using the K-means method and afterwards a rejection procedure is utilized in order to reduce the number of representatives. Finally, for every remain point a local search procedure is started to locate the global minimum of the function.

The rest of this article is organized as follows: in section 2 the proposed method is described in detail, in section 3 some experimental test functions from the relevant literature are described and a series of test are performed on those functions and finally in section 4 some conclusions are discussed as well as some guidelines to improve the proposed method.

2 Method description

The proposed method is initially based on the commonly used global optimization method named Multistart. The proposed method creates clusters from the objective function. 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. As it was demonstrated by various researchers [34, 35], if the number of local minimum is finite then Multistart method is capable to locate the global minimum. Due to its simplicity, the Multistart method is the base method for a series of stochastic methods in the relevant literature such as hybrid methods[36, 37],

Figure 1: The main steps of the Multistart method.

```
1. Initialization step.
    (a) Set $M$ as the total number of samples.
    (b) Set $(x^*, y^*)$ as the global minimum. Initialize $y^*$ to a very large value.
2. Sampling step.
    (a) For $i = 1 \ldots M$ Do
        i. Sample a point $x_i \in S$
        ii. $y_i = \mathrm{LS}(x_i)$. Where LS(x) is a local search procedure.
        iii. If $y_i \leq y^*$ then $x^* = x_i, y^* = y_i$
    (b) EndFor
```

GRASP methods[38] etc. The main steps of a typical Multistart procedure are shown in Figure 1.

The proposed method replaces the sampling step of the Multistart method with the usage of centroids constructed by Kmeans clustering. The main steps of the Kmeans method are given in Figure 2. The estimated centroids are iteratively enhanced with Kmeans and new samples that added each time for a predefined number of times. Having created the centroids a rejection procedure is applied to reduce the number of centroids. The rejection procedure removes from the set of centers, points that have many neighbors in a predefined radius. The rejection procedure is necessary to remove from the set samples, that possible will yeld the same local optimum after the application of the local search procedure. The proposed method is described in Figure 3.

3 Experiments

3.1 Test functions

In order to measure the effectiveness of the proposed approach we utilize several benchmark functions from the relevant literature [39, 40].

3.2 Benchmark functions

Bf1 Function

The function Bohachevsky 1 is given by the equation

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

Figure 2: The algorithm Kmeans.

```
1. Repeat
   (a) $S_j = \{\}, \ j = 1..K$
   (b) For every sample $x_i$ Do
       i. Set $j^* = \min_{i=1}^{K} \{D(x_i, c_j)\}$, where $j^*$ is the nearest center for
          sample $x_i$.
       ii. Set $S_{j^*} = S_{j^*} \cup \{x_i\}$.
   (c) EndFor
   (d) For every center $c_j$ Do
       i. Set $M_j$=number of elements in $S_j$
       ii. Update $c_j$
           $$c_j = \frac{1}{M_j} \sum_{i=1}^{M_j} x_i$$
   (e) EndFor
2. Terminate when $c_j$ no longer change.
```

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 $-5 \leq x_1 \leq 10, \ 0 \leq x_2 \leq 15$. 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

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

Figure 3: The proposed method.

```
1. Initialization step.
   (a) Set $M$ as the number of samples.
   (b) Set $(x^*, y^*)$ as the global minimum. Initialize $y^*$ to a very large value.
   (c) Set $K$ the number of teams, where $K < M$.
   (d) Set $K_{\text{MAX}}$ the number of construction iterations for the KMeans algorithm.
   (e) Set $C = \{\}$, as the set of constructed centers.
2. Construction step.
   (a) For $i = 1..K_{\text{MAX}}$ Do
       i. Sample $M$ points from the objective function $S = \{x_1, x_2, \ldots, x_M\}$
       ii. Update the centers $C$ with the set $S$, using Kmeans.
   (b) EndFor
3. Create the set $R$ from $C$ using the rejection algorithm of Figure 4.
4. Evaluation step.
   (a) For $i = 1 \ldots |R|$ Do
       i. Set $x_i = R_i$
       ii. $y_i = \text{LS}\left(x_i\right)$. Where LS(x) is a local search procedure.
       iii. If $y_i \le y^*$ then $x^* = x_i, y^* = y_i$
   (b) EndFor
```

Figure 4: The rejection algorithm.

```
1. Set $C$ the set of centers.
2. Set $R = \emptyset$ the outcome of the rejection algorithm.
3. Set $D_{\text{min}} = \min_{i \neq j} \|c_i - c_j\|$
4. Set $F > 1$, a double value.
5. Set $N_{\text{min}} > 1$, an integer value.
6. For every center $c_i$ Do
   (a) Set $N = 0$
   (b) For every center $c_j,\ i \neq j$ Do
       i. If $\|c_i - c_j\| \leq F D_{\text{min}}$ then $N = N + 1$
   (c) EndFor
   (d) If $N < N_{\text{min}}$ then $R = R \cup c_i$
7. EndFor
8. Return $R$
```

with $x \in [-1, 1]^n$. The value of the global minimum is -0.4 and in our experiments we have used $n = 4,\ 8$.

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

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 [41] 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 $w = 50,\ 100$. The corresponding functions are denoted by the labels GKLS250, GKLS350 and GKLS3100.

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

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

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

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

$$V_{LJ}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{3}$$

In the current experiments three different cases were studied: $N = 3,\ 5,\ 10$.

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 $n = 4, 8, 16$ and $z = \frac{\pi}{6}$ and the corresponding functions are denoted by the labels SINU4, SINU8 and SINU16 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 $n = 7$.

Table 1: The values for the parameters used in the conducted experiments.

PARAMETER	VALUE
K	100
K_{max}	100
F	1.5
N_{min}	3

3.3 Experimental Results

The proposed method was tested against the traditional multistart global optimization method on the series of benchmark problems. The parameters used in the conducted experiments are listed in Table 1. The method was coded using the OpenMP library[43] in order to take advantage of multi - core modern computing systems and the experiments were conducted on a cluster of systems running the Linux operating system. The results from the experiments are listed in Tables 2 and 3. 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 local search procedure used (denotes as LS(x)) was a BFGS variant due to Powell[30].

In Table 2 the results for the Multistart global optimization procedure are shown. The column $M = 100$ denotes the application of the algorithm given in Figure 1 with $M = 100$ samples. The column $M = 200$ stands for the Multistart algorithm using 200 samples. The last column stands for the results of the Multistart method with 100 samples and the application of the proposed rejection procedure of algorithm in Figure 4 in the samples before the application of the local search procedure. It is evident that the application of the rejection procedure does not reduce significantly the number of function calls for the multistart case.

In Table 3 the experimental results for the proposed method are listed. The column $M = 100$ stands for the usage of 100 samples in the proposed method (parameter M) and the column $M = 200$ for 200 samples. The proposed method has significantly lower number of function calls than the Multistart method and as the number of samples increases (parameter M) the method requires lower amount of function calls to estimate the global minimum. This means that the method tends to create more accurate clusters (clusters that emulate the true regions of attraction) of the objective function as the number of samples increases.

Table 2: Multistart results.

Function	$M = 100$	$M = 100$	$M = 100$,Rejection
B2	4518	8849	4472
Easom	943	1949	933
Bf1	4508	9300	4469
Bf2	3750	7621	3666
Branin	1948	3855	1938
Camel	2669	4983	2502
CM4	5714	11783	5644
CM8	7341(0.33)	14813(0.60)	7289(0.33)
DIFFPOWER10	123729	248924	121012
ELP4	1203	2474	1158
ELP8	1721	3395	1652
ELP16	2789	5485	2252
EXP4	3646	7063	3609
EXP8	3723	7447	3651
EXP16	3835	7486	3310
GKLS250	1486	2928	1426
GKLS350	1030(0.97)	2007	913(0.87)
GKLS3100	1020(0.77)	2005	1018(0.77)
GRIEWANK2	3131(0.70)	6197(0.97)	3048(0.70)
GRIEWANK10	10449	20763	10226
HANSEN	2482	4997	2422
HARTMAN3	2911	5753	2868
HARTMAN6	3825	7875	3787
POTENTIAL3	5237	10784	5178
POTENTIAL5	11594	22331	10127
POTENTIAL10	20361	40592	5089(0.70)
RASTRIGIN	2345	4731	2242(0.93)
SHEKEL5	3852	7841	3730
SHEKEL7	3951	7149	3885
SHEKEL10	3982	6987	3890
SINU4	3317	6624	3246
SINU8	4883	10015	4791
SINU16	8731	17005	8692
TEST2n4	3258	6608	3216
TEST2n5	3565	7128	3534
TEST2n6	3804(0.90)	7790	3850(0.90)
TEST2n7	4203(0.83)	8501(0.97)	4155(0.77)
TOTAL	**281454(0.93)**	**562038(0.98)**	**259160(0.92)**

Table 3: The proposed method with $K = 100$ centers.

Function	$M = 100$	$M = 200$
B2	4073	3886
Easom	830	782
Bf1	4046	3864
Bf2	3346	3153
Branin	1699	1623
Camel	2338	2237
CM4	4434	4043
CM8	3084(0.63)	1819(0.50)
DIFFPOWER10	26726	17980
ELP4	971	908
ELP8	601	338
ELP16	139	100
EXP4	2764	2522
EXP8	1564	943
EXP16	245	179
GKLS250	1337	1275
GKLS350	911(0.93)	777(0.83)
GKLS3100	939(0.97)	796(0.97)
GRIEWANK2	2812(0.77)	2684(0.70)
GRIEWANK10	1812	1152(0.80)
HANSEN	2210	2077
HARTMAN3	2400	1993
HARTMAN6	2707	2369
POTENTIAL3	1246	714
POTENTIAL5	752	664
POTENTIAL10	1621(0.23)	1045(0.10)
RASTRIGIN	2016	1917
SHEKEL5	3520	3116
SHEKEL7	3515	3113
SHEKEL10	3586	3237
SINU4	2548	2268
SINU8	2121	1624
SINU16	546	358
TEST2n4	2436	2198
TEST2n5	2186(0.97)	1840(0.97)
TEST2n6	2648(0.80)	2300(0.83)
TEST2n7	2469(0.77)	2173(0.73)
TOTAL	**103198(0.95)**	**84067(0.93)**

4 Conclusions

A new clustering method was introduced in this article to tackle to global optimization problem. For every cluster gradually a representative is created using the well - known Kmeans method. Afterwards, the clusters are reduced in number using a simple rejection procedure. The proposed method was tested on a series of benchmark problems from the relevant literature and it is compared against the Multistart method and the results are reported. Judging from the reported results, the proposed method seems to be very promising and a series of enhancements could be applied on the method such as:

1. Dynamic selection of K in Kmeans algorithm.
2. Better estimation of the critical distance between clusters in the rejection procedure.
3. Usage of more efficient stopping rules to prevent the method from unnecessary local searches, that could lead to the same global optimum many times.

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Compliance with Ethical Standards

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

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