Use RBF as a sampling method in Multistart global optimization method

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Abstract

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Keywords: Global optimization, stochastic methods, termination rules.

1 Introduction

A novel method to draw samples for global optimization methods is presented here. The process of locating the global minimum of a continuous and differentiable function $f : S \to R, S \subset R^n$ is described as, determine

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

with S:

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

The above problem is commonly used to describe problems in economics [1, 2, 3], physics [4, 5, 6], chemistry [7, 8, 9], medicine [10, 11] etc. The global optimization methods have two major categories: deterministic and stochastic methods. The most common methods of the first category are the so called Interval methods [12, 13, 14], 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. The majority of the methods belong to the second category where the reader can found Controlled Random Search methods [15, 16, 17], Simulated Annealing methods [18, 19], Differential Evolution methods [20, 21], Genetic algorithms [22, 23, 24], Particle Swarm optimization methods [25, 26], Ant Colony methods [27, 28] etc. Also, may hybrid stochastic methods have been appeared recently in the relevant literature such as methods that combine

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Particle Swarm Optimization and Simulated Annealing [29, 30], methods that combine Genetic Algorithms and Differential Evolution [31, 32], combinations of Genetic Algorithms and Particle Swarm Optimization [33] etc. Also, due to the wide spread of parallel architectures in recent years as well as the widespread use of GPUs, many methods have emerged that exploit such architectures [34, 35, 36].

This paper proposes an innovative sampling technique for the Multistart stochastic global sampling method. The Multistart technique is one of the simplest stochastic global optimization techniques and is the basis for many modern global optimization methods. In the Multistart method, a series of random samples are taken from the objective function and then a local optimization method is started from each sample. Regarding its simplicity, the method have been used with success in a wide area of practical applications such as the TSP problem [37], the vehicle routing problem [38], the facility location problem [39], the maximum clique problem [40], the maximum fire risk insured capital problem [41], aerodynamic shape problems [42] etc. In addition, the Multistart method has been thoroughly studied by many researchers in recent years, and many works have been proposed on this method, such as methods for finding all local minima of a function [43, 44, 45], hybrid techniques [46, 47], GRASP methods[48], new termination rules [49, 50, 51], parallel techniques[52, 53]. Usually in the Multistart method, samples are used from the objective function using some distribution such as the uniform distribution. In the present work, it is proposed that these samples are obtained from a radial basis network [54] (RBF), which has already been trained on a limited number of real samples from the objective function. RBF networks have been widely used in many real world problems such as face recognition [55], function approximation [56], image classification [57], water quality prediction [58] etc.

The rest of this article is organized as follows: in section 2 the proposed sampling technique is outlined in detail, in section 3 the test functions used as well the experimental results are listed and finally in section 4 some conclusions are presented.

2 Method description

2.1 The Multistart method

A commonly used representation of the Multistart method is shown in Algorithm 1. In practice, the method takes N samples at each iteration and starts a local minimization method from each sample, without doing any other checking. However, despite its simplicity, it has two key components which, with proper adaptation, can make the method extremely efficient. The first component is the termination method used and the second is the sampling method within the central iteration. The local search procedure used here is an adaptation of the BFGS method [59]. The used termination rule was also used in a variety of global optimization methods [60, 61]. This termination method is outlined in

Algorithm 1 Representation of the Multistart algorithm.

1. **Initialization** step.
   (a) **Set** N the number of samples, that will taken in every iteration.
   (b) **Set** $\textbf{ITER}_{\textbf{MAX}}$, the maximum number of allowed iterations.
   (c) **Set** Iter=0, the iteration number.
   (d) **Set** (x^*, y^*) as the global minimum. Initialy $y^* = \infty$
2. **Evaluation** step.
   (a) **Set** Iter=Iter+1
   (b) **For** $i = 1 \ldots N$ **Do**
      i. **Take** a new sample $x_i \in S$
      ii. $y_i = \mathrm{LS}(x_i)$. Where LS(x) is a predefined local search method.
      iii. **If** $y_i \leq y^*$ then $x^* = x_i, y^* = y_i$
   (c) **EndFor**
3. **Termination** check. The termination criteria are checked and if they are true, then the method terminates.

subsection 2.2 The second point, which this paper focuses on, is the sampling method. Usually sampling is done with random samples from some distribution such as the uniform one. In this paper sampling will be used from an approximation of the objective function $f(x)$ constructed using a neural network. This approach is discussed in subsection 2.3.

2.2 The used termination rule

2.3 Rbf networks

An RBF neural network typically is expressed as a function:

$$y(\overrightarrow{x}) = \sum_{i=1}^{k} w_i \phi\left(\|x - c_i\|\right) \tag{2}$$

where the vector $\overrightarrow{x}$ stands for the input vector of the network and the vector $\overrightarrow{w}$ is called weight vector with k elements. Typically, the function $\phi(x)$ is the so - called Gaussian function defined as:

$$\phi(x) = \exp\left(-\frac{(x-c)^2}{\sigma^2}\right) \tag{3}$$

where the value $\phi(x)$ depends mainly on the distance between x and x. The vector $\overrightarrow{c}$ is called centroid and the vector $\overrightarrow{\sigma} = (\sigma_1, \sigma_2, \ldots, \sigma_k)$ is considered as the variance vector. A typical plot of this function is shown in Figure 1.

The network of equation 2 can be used to appoximate functions $f(x),\ x \in S \subset R^n$ by minimizing the error:

$$E\left(y\left(\overrightarrow{x}\right)\right) = \sum_{i=1}^{M} \left(y\left(x_i\right) - f\left(x_i\right)\right)^2 \tag{4}$$

where the variable M denotes the number of training samples provided for the function $f(x)$. The RBF network is shown graphically in Figure 2. During a traininig procedure, the parameters of the RBF network are adapted in order to minimize the error of equation 4 .The RBF network us trained using a two - phase methodology:

1. During the first phase the k centers of and the associated variances are calculated through K-Means algorithm [62].
2. During the second phase, the weight vector $\overrightarrow{w} = (w_1, w_2, \ldots, w_k)$ is calcuated by solving a linear system of equations with the following procedure:
   (a) **Set** $W = w_{kj}$, the matrix for the k weights
   (b) **Set** $\Phi = \phi_j\left(x_i\right)$
   (c) **Set** $T = \left\{t_i = f\left(x_i\right), i = 1, .., M\right\}$.
   (d) The system to be solved is defined as:

   $$\Phi^T\left(T - \Phi W^T\right) = 0 \tag{5}$$

   The solution is:

   $$W^T = \left(\Phi^T \Phi\right)^{-1} \Phi^T T = \Phi^{\dagger} T \tag{6}$$

   The matrix $\Phi^{\dagger} = \left(\Phi^T \Phi\right)^{-1} \Phi^T$ is the so - called pseudo-inverse of Φ, with the property

   $$\Phi^{\dagger} \Phi = I \tag{7}$$

In the proposed technique, the previously defined network constructs an approximation of the objective function $f(x)$ and subsequently the method Multistart takes samples from the approximation of the objective function. **.........**

3 Experiments

3.1 Test function

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

Figure 1: Typical plot of the Gaussian function.

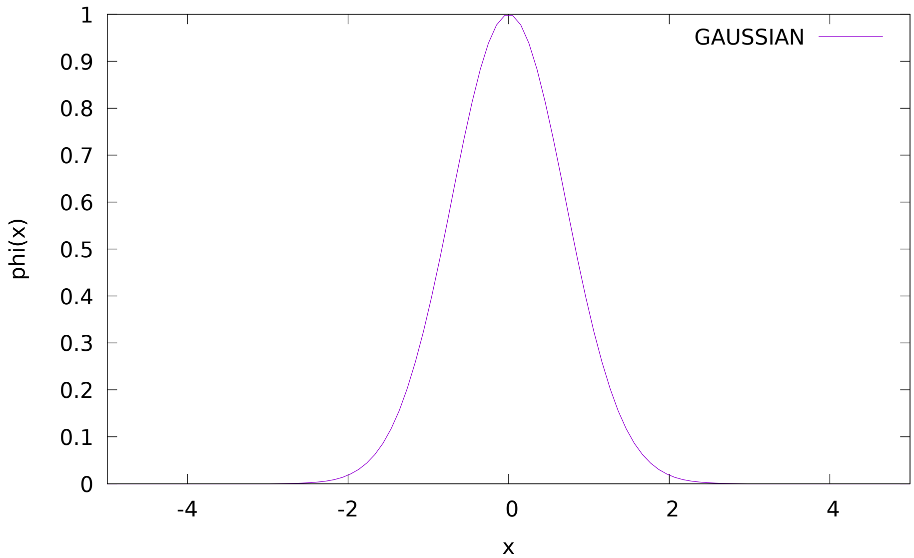
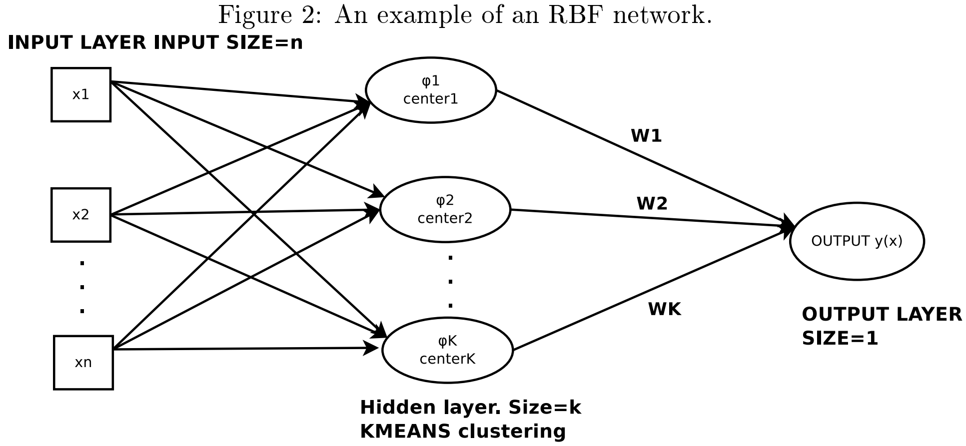


Figure 2: An example of an RBF network.



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

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 $n = 4$. The corresponding function is denotes as CM4

- **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 $f(x^*) = -1.0316$

- **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 $n = 2, 4, 8, 16, 32, 64, 100$ and the corresponding functions are denoted by the labels EXP2, EXP4, EXP8, EXP16, EXP32, EXP64 and EXP100.

- **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.

- **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.

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

$$V_{LJ}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{8}$$

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

- **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

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

  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 $n = 7$.

- **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

3.2 Experimental results

4 Conclusions

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Table 1: Experimental results for the Multistart method.

FUNCTION	SAMPLES=20	SAMPLES=50
BF1	3004	5975
BF2	2828	5826
BRANIN	2409	5415
CAMEL	2661	5599
CM4	3551(0.87)	6431(0.80)
EXP2	2688	5677
EXP4	2769	5772
EXP8	2805	5807
EXP16	2836	5837
EXP32	2842	5843
EXP64	2912	5914
EXP100	2967	5959
GRIEWANK2	3938(0.40)	6572(0.30)
GRIEWANK10	4536(0.97)	7520
POTENTIAL3	3121	6120
POTENTIAL5	4363	7320
HANSEN	5344(0.93)	9536(0.90)
HARTMAN3	2618	5608
HARTMAN6	3014	6037
RASTRIGIN	3850(0.83)	6401(0.77)
ROSENBROCK4	6456	8584
ROSENBROCK8	7646	10095
SHEKEL5	3144	6215
SHEKEL7	3354	6508
SHEKEL10	3388	6860
SINU4	3935	6670(0.97)
SINU8	5547	8056
SINU16	19313	35751(0.97)
TEST2N4	3035(0.87)	6002(0.97)
TEST2N5	3127(0.73)	6042(0.67)
TEST2N6	3393(0.40)	6169(0.47)
TEST2N7	4075(0.37)	6443(0.33)
TEST30N3	3723	6322
TEST30N4	3736	6465
TOTAL	**138927(0.923)**	**251391(0.916)**

Table 2: Experimental results for the proposed method with SAMPLES=20

FUNCTION	ISAMPLES=100	ISAMPLES=200	ISAMPLES=500
BF1	1086	1159	1500
BF2	922	1026	1304
BRANIN	503	590	899
CAMEL	670	756	1060
CM4	1583(0.83)	1716(0.83)	1861(0.90)
EXP2	570	672	966
EXP4	766	803	1049
EXP8	868	947	1237
EXP16	912	1009	1303
EXP32	958	1059	1354
EXP64	968	1070	1359
EXP100	1042	1147	1445
GRIEWANK2	2409(0.53)	1641(0.40)	2069(0.57)
GRIEWANK10	2607(0.97)	2609	2902(0.93)
POTENTIAL3	1211	1297	1613
POTENTIAL5	2414	2521	2835
HANSEN	6079(0.87)	4785(0.83)	6504(0.77)
HARTMAN3	729	830	1143
HARTMAN6	1111(0.90)	1290(0.93)	1525(0.97)
RASTRIGIN	1727(0.57)	1043(0.87)	1386
ROSENBROCK4	4111	2672	4357
ROSENBROCK8	5417	6253	5609
SHEKEL5	1751(0.73)	2152(0.90)	1245(0.90)
SHEKEL7	1667(0.87)	1627(0.83)	1676(0.93)
SHEKEL10	2329(0.80)	2946(0.73)	3678(0.77)
SINU4	938	991	1227
SINU8	1194	1360	1479
SINU16	14305(0.87)	32647(0.97)	21363(0.97)
TEST2N4	904(0.57)	936(0.73)	1227
TEST2N5	1881(0.80)	1218	1351
TEST2N6	1092(0.67)	1224(0.87)	1435(0.97)
TEST2N7	1452(0.70)	1397(0.80)	1477(0.90)
TEST30N3	1244	2054	2584
TEST30N4	2027	2644	2638
TOTAL	**69447(0.902)**	**88091(0.932)**	**86660(0.958)**

Table 3: Experimental results for the proposed method with SAMPLES=50

FUNCTION	ISAMPLES=100	ISAMPLES=200	ISAMPLES=500
BF1	1093	1175	1527
BF2	943	1022	1319
BRANIN	502(0.97)	594	900
CAMEL	642	729	1046
CM4	1491(0.87)	1884(0.90)	1799(0.97)
EXP2	522	621	923
EXP4	766	827	1050
EXP8	865	946	1231
EXP16	912	1007	1298
EXP32	961	1057	1349
EXP64	983	1064	1358
EXP100	1053	1129	1442
GRIEWANK2	1788(0.50)	1762(0.43)	2345(0.50)
GRIEWANK10	2505	2677	2868
POTENTIAL3	1244	1313	1609
POTENTIAL5	2420	2502	2795
HANSEN	6711(0.70)	4278(0.70)	7264(0.67)
HARTMAN3	728	830	1144
HARTMAN6	1027(0.93)	1202(0.93)	1492
RASTRIGIN	977(0.53)	1269(0.77)	1397(0.97)
ROSENBROCK4	2348	2453	3278
ROSENBROCK8	3928	4461	4865
SHEKEL5	5630(0.67)	7498(0.87)	1510(0.93)
SHEKEL7	2135(0.67)	1973(0.67)	1815(0.97)
SHEKEL10	1864(0.73)	1245(0.60)	3165(0.83)
SINU4	984	1020	1355
SINU8	10502	1517	1456
SINU16	95225(0.83)	21658(0.90)	21330(0.87)
TEST2N4	820(0.63)	1079(0.90)	1274
TEST2N5	1140(0.67)	1107(0.80)	1333
TEST2N6	1203(0.73)	1371(0.97)	1440(0.97)
TEST2N7	1602(0.50)	1200(0.77)	1618(0.97)
TEST30N3	1494	1903	2279
TEST30N4	1164	2287	2284
TOTAL	**158172(0.880)**	**78660(0.918)**	**85158(0.960)**

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