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Stability Index Method for Global Minimization

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Abstract. The Stability Index Method (SIM) combines stochastic and deterministic algorithms to find global minima of multidimensional functions. The functions may be non-smooth and may have multiple local minima. The method examines the change of the diameters of the minimizing sets for its stopping criterion. At first, the algorithm uses the uniform random distribution in the admissible set. Then normal random distributions of decreasing variation are used to focus on probable global minimizers. To test the method, it is applied to seven standard test functions of several variables. The computational results show that the SIM is efficient, reliable and robust.

Key words: global minimization, random sample, stability index

1. Introduction

Given a function $f\colon A \to \mathbb{R}$, our goal is to minimize it over an admissible set A assumed to be a bounded set in a metric space X. Typically, the structure of the objective function f is quite complicated. In particular, it can have many local minima and a non unique global minimum. To better understand the structure of the minima, let us introduce the minimizing sets S_ϵ of f. Let $m = \inf\{f(x) : x \in A\}$. Given an $\epsilon > 0$ define

$$S_\epsilon = \{x \in A\colon\ f(x) < m + \epsilon\} \tag{1.1}$$

or

$$S_\epsilon = \{x \in A\colon\ f(x) < f(x_p) + \epsilon\}, \tag{1.2}$$

if the problem admits a global minimizer $x_p \in A$.

DEFINITION. Given an $\epsilon > 0$, let D_ϵ be the diameter of the minimizing set S_ϵ, which we call the **Stability Index** D_ϵ of the minimization problem (1.1).

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We are interested in the behavior of D_ϵ as $\epsilon \to 0$. So, one can properly say that the problem (1.1) possesses a set of Stability Indices $\{D_\epsilon : \epsilon > 0\}$, and the above definition should be understood in this sense.

One would expect to obtain a stable identification for minimization problems with small (relative to the admissible set) stability indices. Minimization problems with large stability indices either have distinct global minimizers, or the function f is nearly flat in a neighborhood of the global minimizer x_p. In this situation, and with no additional information known, one has an uncertainty of the minimizer's choice. The stability index provides a quantitative measure of this uncertainty or instability of the minimization.

In a practical minimization problem one constructs a sequence of minimizers $\{x_1, x_2, \dots\} \subset A$, and makes a decision when to terminate the iterations according to a stopping criterion. We assert that the knowledge of the Stability Index provides a valuable tool for the formulation of such a stopping criterion.

In this paper we choose to present a particular implementation of the Stability Index Method (SIM). Its numerical performance on a variety of standard test functions found in the literature is described in the Numerical Results section. The algorithm shows how to iteratively estimate the Stability Indices D_ϵ, and how to use them in a stopping criterion. Clearly, one can combine this idea with other minimization methods to obtain different implementations.

Originally, we applied the Stability Index minimization method to inverse scattering problems arising in quantum mechanical scattering (Gutman et al., 2002). Such potential scattering problems are important in quantum mechanics, where they appear in the context of scattering of particles bombarding an atom nucleus. One is interested in reconstructing the scattering potential from the results of a scattering experiment. Assuming a particular structure of the potential, the scattering results can be computed and compared to the given scattering data. Thus the inverse scattering problem is reduced to the minimization of the discrepancy (best fit to data) (see Gutman et al., 2002; Ramm and Gutman, 2005 for details).

2. Stability Index Method

The goal of the SIM algorithm is to find a minimizing set S_ϵ that fits within a small portion of the computational domain $A \subset \mathbb{R}^N$. Practically, we assume that $A = [-M, M]^N \subset \mathbb{R}^N$, for an $M > 0$. If it is desirable to introduce different scales for the variables, then the algorithm should be modified accordingly.

Let $0 < \delta < 1$. The minimization is stable if, given a global minimizer x_p, we are able to find a minimizing set $S_\epsilon \subset C[x_p, \delta]$, where $C[x_p, \delta]$ is the cube centered at $x_p \in A$ with the side equal to $2\delta M$.

The next step is to define a sequence of normal distributions T_n with the variances $\mu_n \to 0$, as $n \to \infty$. Thus we fix an $0 < \alpha < 1$, and let $\mu_n = \alpha^n$, $n = 1, 2, \ldots$

Initially, for $n = 0$, let the T_0 be the uniform random distribution in A. A special algorithm SMS, described below, determines a finite Stable Minimizing Set (SMS) $S_0 \subset A$. Let $x_0 \in S_0$ be the minimizer in S_0, that is

$$f(x_0) = \min\{f(x) : x \in S_0\}. \tag{2.1}$$

If $S_0 \subset C[x_0, \delta]$, then the minimization is stable and the global minimizer $x_p = x_0$.

If, on the other hand, the above inclusion is not achieved, then one continues with another application of the **SMS**, this time using the normal distribution T_1 with the mean at x_0, and the variance μ_1, etc. The iterations continue until either $S_n \subset C[x_n, \delta]$ or $3\mu_n < 2\delta M$. The last condition is needed to prevent all the trial points to be chosen too close to x_n, thus preventing a reasonable estimate for the diameter of S_n.

Stability Index Method (SIM)

Fix $0 < \alpha, \delta < 1$. Suppose that $A = [-M, M]^N$.

(1) Initialization. Let $n = 0$. Use the **SMS** algorithm with the uniform random distribution T_0 in A to determine the minimizing set $S_0 \subset A$ and the minimizer $x_0 \in S_0$. Go to the Stopping Criterion (step 3) to check if additional iterations are needed.

(2) (nth iteration). Let $\mu_n = \alpha^n$. Use the **SMS** algorithm with the normal random distribution T_n with the mean at x_{n-1} and the variance μ_n to determine the minimizing set $S_n \subset A$ and the minimizer $x_n \in S_n$.

(3) Stopping criterion. Let $C[x_n, \delta]$ be the cube centered at $x_n \in A$ with the side equal to $2\delta M$.

If $S_n \subset C[x_n, \delta]$, then stop. The minimization is stable. The estimated global minimizer x_p is x_n.

If $S_n \not\subset C[x_n, \delta]$ and $3\mu_n < 2\delta M$, then stop. The minimization is unstable. The diameter (Stability Index) D_n of S_n is a measure of the instability of the minimization.

Otherwise, increase n by 1, and return to Step 2 to do another iteration.

Note that the obtained point x_p is an estimated global minimizer. See Section 5 for a convergence analysis of the method. A somewhat different implementation of the SIM is described in Gutman et al. (2002) and Ramm and Gutman (2005). The version of the SIM presented in this paper is more efficient due to a smaller number of local minimizations, fewer number of parameters, and other improvements.

3. Stable Minimizing Set (SMS) algorithm

The main part of the SIM is the **SMS** algorithm, which determines stable minimizing sets S_n, corresponding to the random distributions T_n. These distributions are either uniform in A or normal with a given variation μ_n.

The SMS algorithm is, in itself, an iterative algorithm. It can be classified as an Iterative Reduced Random Search method. Choose an integer $K>0$ from the consideration that K random points in S_ϵ are sufficient to estimate its diameter D_ϵ. If $n \geqslant 1$, then the calling algorithm SIM provides the minimizing set S_{n-1}, its minimizer x_{n-1}, and the variance μ_n.

Let a batch $H^1 \subset A$ of $L>K$ trial points be generated in the admissible set A according to the random distribution T_n. If $n=0$, then T_0 is just the uniform random distribution in A. If $n \geqslant 1$, then T_n is the normal distribution with the variance μ_n, and the mean at x_{n-1}. Let Q_U^1 be the subset of K points from H^1 where the objective function f attains its K smallest values. That is

$$\max\{f(u_i): u_i \in Q_U^1\} \leqslant \min\{f(u_i): u_i \notin Q_U^1\}. \tag{3.1}$$

Use each point $u_i \in Q_U^1$ as the initial guess for a Local Minimization Method (LMM) of your choice, e.g. the conjugate gradient method, etc. The specific LMM used by us is described in the next section. While the use of a local minimization is not, strictly speaking, necessary for the SIM, it provides a significant improvement in the performance of the algorithm, and is highly recommended. Thus for each starting point $u_i \in Q_U^1$ the LMM produces a minimizer $v_i \in A$. Let Q_V^1 be the set of all such minimizers. Let Q^1 be the subset of $Q_U^1 \cup Q_V^1$ containing K points with the smallest values of f, and q^1 be the minimizer in Q^1. Define the radius of Q^1 by

$$R^{(1)} = \max\{\|z_i - q^1\| : z_i \in Q^1,\ i=1,2,\ldots,K\}. \tag{3.2}$$

The idea of the SIM is to iteratively construct subsets Q^j until their diameters are stabilized. Practically, one can achieve the same goal by estimating and examining the radius $R^{(j)}$ of the sets Q^j. This also requires less computational effort.

To construct the next set Q^2 generate another batch $H^2 \subset A$ of L trial points according to the uniform random distribution, if $n=0$, or, for $n \geqslant 1$, according to the normal distribution T_n with the variance μ_n, and the mean at q^1. Let Q_U^2 be the subset of K points from $H^2 \cup Q^1$ having the smallest K values of f. Apply the LMM to produce the set of minimizers Q_V^2.

Of course, if some point $u_i \in Q_U^2$ has already been used as an initial guess for the LMM in the previous iteration, it is excluded from the LMM application. Let Q^2 be the subset of $Q_U^2 \cup Q_V^2$ containing K points with the smallest values of f. Let q^2 be the minimizer in Q^2, and $R^{(2)} = \max\{\|z_i - q^2\| : z_i \in Q^2, i = 1, 2, \dots, K\}$ be its radius, etc.

This way one produces a sequence of the minimizing sets Q^j, $j = 1, 2, \dots$. Let $0 < \gamma < 1$, and P be a positive integer. The iterations are terminated if the maximum number of iterations $N_{\max}$ is exceeded or the following Stopping Criterion is satisfied:

$$\left| R^{(j)} - \frac{1}{P} \sum_{i=j-P+1}^{j} R^{(i)} \right| < 2\gamma M . \tag{3.3}$$

In either case, when the last iteration j is determined from (3.3) or $j = N_{\max}$, we let $S_n = Q^j$ and $x_n = q^j$.

Stable Minimizing Set (SMS) algorithm

Fix $0 < \gamma < 1$, and integer $K, L > K, P, N_{\max}$. Constant M, normal random distribution T_n, its variance μ_n (for $n \geqslant 1$), the minimizing set S_{n-1}, and the minimizer x_{n-1} are supplied by the calling algorithm SIM.

(1) Initialization. Let $j = 1$.
- For $n = 0$. Generate a batch H^1 of L trial points in $A \subset \mathbb{R}^N$ using the uniform random distribution. Let Q_U^1 be the subset of K points from H^1 where the objective function f attains its K smallest values. Go to step 4.
- For $n \geqslant 1$. Generate a batch H^1 of L trial points in $A \subset \mathbb{R}^N$ using the normal distribution T_n with the variance μ_n and the mean at x_{n-1}. Let Q_U^1 be the subset of K points from $H^1 \cup S_{n-1}$ where the objective function f attains its K smallest values. Go to step 4.

(2) Iterative step ($j \geqslant 2$).
- For $n = 0$. Generate a batch H^j of L trial points in $A \subset \mathbb{R}^N$ using the uniform random distribution.
- For $n \geqslant 1$. Generate a batch H^j of L trial points in $A \subset \mathbb{R}^N$ using the normal distribution T_n with the variance μ_n and the mean at q^{j-1}.

(3) Let Q_U^j be the subset of K points from $H^j \cup Q^{j-1}$, where the objective function f attains its K smallest values.

(4) Local minimization. Use each unflagged point $u_i \in Q_U^j$ as the initial guess for a Local Minimization Method (LMM). Let $v_i \in A$ be the resulting minimizer. Let Q_V^j be the set of all such minimizers resulting from the application of LMM to Q_U^j. Flag all points in Q_U^j and Q_V^j.

(5) Let Q^j be the subset of $Q_U^j \cup Q_V^j$ containing K points with the smallest values of f and q^j be the minimizer in Q^j. Define the radius of Q^j by

$$R^{(j)} = \max\{\|z_i - q^j\| : z_i \in Q^1,\ i = 1, 2, \ldots, K\}.$$

(6) Stopping criterion.
- If $j < P$, increase j by 1 and return to step 2 for another iteration.
- If $j \geqslant P$, compute the average radius during the last P iterations:

$$R_a = \frac{1}{P} \sum_{i=j-P+1}^{j} R^{(i)}.$$

- Termination. If $|R^{(j)} - R_a| \leqslant 2\gamma M$, or $j \geqslant N_{\max}$, let $S_n = Q^j$, $x_n = q^j$ and exit the procedure.
- Otherwise, increase j by 1 and return to step 2 for another iteration.

The implementation of the SMS involves a combination of stochastic (global) and deterministic (local) minimization methods. Such hybrid procedures are becoming increasingly popular (Ramm and Gutman, 2005; Yiu et al., 2004). Generally, local searches offer more precision and speed than their global counterparts, so that adding a local step to a global minimization algorithm should yield improvement in both areas. Likewise, by itself, a LMM will very often produce points of considerable distance from the actual global minimizer, that is it would be trapped in one of many local minima of the objective function f. Adding a global step helps the algorithm escape from local minima, and explore the entire admissible set A. The use of various normal distributions of decreasing variance is similar to ideas of the simulated annealing method (Kirkpatrick, 1984).

4. Local Minimization Method (LMM)

The particular LMM used in the numerical experiments was a modification of Powell's minimization method in $\mathbb{R}^N$ (Brent, 1973). It was chosen with applications in mind, for which the objective function f does not have a convenient expression for its gradient. Either a Golden Search or Brent's method can be used for one-dimensional minimizations (Miller, 2000; Press et al., 1992).

Modified Powell's Method

(1) Choose the set of directions u_i, $i=1,2,\dots,N$ to be the standard basis in $\mathbb{R}^N$

$$u_i=(0,0,\dots,1,\dots,0)\,,$$

where 1 is in the ith place.
(2) Save the starting point p_0.
(3) For $i=1,\dots,N$ move from p_{i-1} along the direction u_i and find the point of minimum p_i.
(4) Set $v=p_N-p_0$.
(5) Move from p_0 along the direction v and find the minimum. Call it p_0 again. It replaces p_0 from step 2.
(6) Repeat the above steps until a stopping criterion is satisfied. The resulting point is $p_{\min}$.

Note that $f(p_{\min})\leqslant f(p_0)$ for any objective function f used in the LMM.

5. Convergence Analysis

In this section we prove some results on the properties of the SIM algorithm, and the minimizing sets S_ϵ.

THEOREM 5.1 Let $f\colon A\to\mathbb{R}$ be the objective function, and $\{x_n,\ n=0,1,\dots\}$ be the sequence of minimizers produced by the SIM algorithm. Then

$$f(x_{n+1})\leqslant f(x_n) \tag{5.1}$$

for $n=0,1,\dots$

Proof According to the SIM algorithm, the sequence of minimizers x_n, $n=0,1,\dots$ is produced by a repeated application of the SMS procedure. Since the analysis of the SMS when $n=0$ is basically the same as for $n\geqslant 1$, we only consider the later case. Among the input data supplied by the SIM to SMS are the normal random distribution T_n, its variance μ_n, the minimizing set S_{n-1}, and the minimizer x_{n-1}.

To simplify the notation we will write

$$\min f(Q)=\min\{f(x)\ :\ x\in Q\}.$$

By construction, if $j=1$ we have $\min f(Q_U^1)\leqslant \min f(H^1\cup S_{n-1})\leqslant f(x_{n-1})=\min f(S_{n-1})$. Furthermore, $\min f(Q_V^1)\leqslant \min f(Q_U^1)$ since the LMM does not increase the value of the objective function f. Finally in this step, the set Q^1 is chosen to contain the minimizer of $Q^1_U \cup Q^1_V$. Thus $f(q^1) = \min f(Q^1) \leqslant f(x_{n-1})$.

Arguing similarly, for $j > 1$ we have $\min f(Q^j_U) \leqslant \min f(H^j \cup Q^{j-1}) \leqslant f(q^{j-1}) = \min f(Q^{j-1})$. Next $\min f(Q^j_V) \leqslant \min f(Q^j_U)$ and $f(q^j) = \min f(Q^j)$. Thus $f(q^j) \leqslant f(q^{j-1})$.

When the SMS procedure is terminated it assigns $x_n = q^j$. Therefore $f(x_n) \leqslant f(x_{n-1})$ and the proof is completed. □

Recall that the minimizing sets S_ϵ were defined in (1.2). From the definition $S_\mu \subset S_\nu$ for $\nu \geqslant \mu$. Next theorem shows that for a continuous function with a unique minimizer x_p one can always find a minimizing set with an arbitrarily small diameter. Thus, in principle, the SIM can estimate the global minimizer with arbitrary precision as long as it is able to approximate the minimizing sets S_ϵ.

THEOREM 5.2 Suppose that $f: A \to \mathbb{R}$ is a continuous function on a compact set A in a normed space, and $x_p \in A$ is its unique global minimizer. Then for any $\delta > 0$ there exists $\epsilon > 0$ such that *diam* $S_\epsilon < \delta$.

Proof. Let

$$G_n = S_{1/n} = \left\{ x \in A\colon\ f(x_p) \leqslant f(x) < f(x_p) + \frac{1}{n} \right\}, \quad n = 1, 2, 3 \ldots \tag{5.2}$$

Then

$$x_p = \bigcap_{n=1}^{\infty} G_n, \tag{5.3}$$

since $x_p \in G_n$ for any n, and the global minimizer x_p is assumed to be unique.

Suppose that the conclusion of the theorem is not valid. Then there exists $\delta > 0$ such that for any positive integer n one can find $z_n \in G_n$ such that $\|z_n - x_p\| \geqslant \delta$. Since the set A is compact one can find a convergent subsequence in $\{z_n\} \subset A$. Let its limit point be $z_p \in A$. Then $f(z_p) = f(x_p)$ from the continuity of f, and $\|z_p - x_p\| \geqslant \delta$, but this is impossible since the minimizer x_p is unique. □

Clearly, when the parameters in any minimization method are fixed, one can design a function for which the method fails. On the other hand, suppose that it is known that the objective function f is Lipschitz continuous with $|f(x) - f(y)| \leqslant \gamma |x - y|$, $\gamma > 0$. Let $H \subset A \subset \mathbb{R}^N$ be a rectangular lattice in which the closest points are separated by the distance $h < \epsilon/\gamma$ for an $\epsilon > 0$. Then $H \cap S_\epsilon \neq \emptyset$. This implies an estimate on the lattice size $|H|$ that assures the value of the global minimum $f(x_p)$ is being determined within the ϵ accuracy. Practically, this gives very large sample sizes and it is not suitable for computations.

6. Numerical Results

The SIM described in the previous sections was tested on seven functions designed to test and compare various minimization algorithms. The experiments were conducted on a 2.8 GHz PC with 256 MB RAM.

In all the numerical experiments we used the same parameter values: $\alpha = 0.8, \delta = 0.001, \gamma = 0.001, K = 30, L = 5000, P = 6$, and $N_{\max} = 30$. For each test function the admissible set A is a cube $[-M, M]^N$ provided in the function's description together with its global minimizer.

Test Function 1

$$f(x, y) = \left(\sum_{i=1}^{5} i\cos[(i+1)x + i]\right)\left(\sum_{i=1}^{5} i\cos[(i+1)y + i]\right) + 0.5((x + 1.4213)^2 + (y + 0.80032)^2).$$

The minimum is sought on $[-5, 5] \times [-5, 5]$. This function has a global minimum at $(-1.42513, -0.80032)$ with a function value of -186.73091 (Yiu et al., 2004).

Test Function 2

$$f(x, y) = e^{\sin(50x)} + \sin(60e^y) + \sin(70\sin x) + \sin(\sin(80y)) - \sin(10(x + y)) + (x^2 + y^2)/4.$$

The minimum is sought on $[-1, 1]^2$. According to Bornemann et al. (2004), the minimum occurs at approximately $(-0.0244031, 0.2106124)$ with a function value of -3.30686865.

Test Function 3

$$f(x) = \frac{\pi}{N}\left(10\sin^2(\pi y_1) + \sum_{i=1}^{N-1}(y_i - 1)^2(1 + 10\sin^2(\pi y_i + 1)) + (y_N - 1)^2\right),$$

where $x = (x_1, x_2, \ldots, x_N) \in \mathbb{R}^N$, $y_i = 1 + 0.25(x_i - 1)$, $i = 1, 2, \ldots, N$. The minimum is sought on $[-10, 10]^N$. This function has a global minimum at $x = (1, 1, \ldots, 1)$ with a function value of 0 (Yiu et al., 2004).

Test Function 4

$$f(x) = -20\exp\left(-0.2\sqrt{\frac{1}{N}\sum_{i=1}^{N}|x_i|}\right) - \exp\left(\frac{1}{N}\sum_{i=1}^{N}\cos(2\pi x_i)\right) + 20 + e,$$

where $x=(x_1,x_2,\dots,x_N)\in\mathbb{R}^N$, $i=1,2,\dots,N$. The minimum is sought on $[-32.768,32.768]^N$. This function has a global minimum at $x=(0,0,\dots,0)$ with a function value of 0 (Bagirov et al., preprint).
Test Function 5

$$f(x)=\frac{1}{400}\sum_{i=1}^{N}|x_i|-\prod_{i=1}^{N}\cos\left(\frac{x_i}{\sqrt{i}}\right)+1,$$

where $x=(x_1,x_2,\dots,x_N)\in\mathbb{R}^N$. The minimum is sought on $[-500,500]^N$. This function has a global minimum at $x=(0,0,\dots,0)$ with a function value of 0 (Bagirov et al., preprint).
Test Function 6

$$f(x)=\frac{\pi}{N}\left(10|\sin(\pi y_1)|+\sum_{i=1}^{N-1}|y_i-1|(1+10|\sin(\pi y_i+1)|)+|y_N-1|\right),$$

where $x=(x_1,x_2,\dots,x_N)\in\mathbb{R}^N$, $y_i=1+0.25(x_i-1)$, $i=1,2,\dots,N$. The minimum is sought on $[-10,10]^N$. This function has a global minimum at $x=(1,1,\dots,1)$ with a function value of 0 (Yiu et al., 2004).
Test Function 7

$$\begin{aligned}f(x,y,z)=\,&e^{\sin(50x)}+\sin(60e^{y})\sin(60z)+\sin(70\sin x)\cos(10z)\\&+\sin(\sin(80y))-\sin(10(x+y))+(x^2+y^2+z^2)/4.\end{aligned}$$

The minimum is sought on $[-0.5,0.5]^3$ According to Bornemann et al. (2004), the minimum occurs at approximately $(-0.15804, 0.29102, -0.28930)$ with a function value of -3.32834.

The results of the minimization using the SIM for all seven test functions are shown in Table 1. The algorithm was run 20 times on each function. It found the correct global minimum most of the time. The "success rate" column in Table 1 shows the percentage of trials in which the global minimum was found exactly. The "Function evaluation" column shows the average number of times the objective function was evaluated. Finally, Table 1 shows the average run time, in seconds, for a single trial run.

The table shows that in every trial run for function no. 4 the minimum value was found within 0.004 of the actual minimum of 0.00000. In all trial runs for function no. 7 the minimum values were less than -3.3205, and the actual minimum of -3.3283 was found in 85% of the runs. The performance of the method deteriorates for higher dimensional problems.

Table 1. Results of the computational experiments

Function	Dimension N	Actual minimum	Found minimum	Success rate (%)	Function evaluation	Average run time (seconds)
1	2	−186.731	−186.731	100	341454	2
2	2	−3.30687	−3.30687	100	384937	2
3	5	0.00000	0.00000	100	1029801	7
3	10	0.00000	0.00000	100	2423475	16
3	20	0.00000	0.00000	100	4194304	50
4	2	0.00000	<0.00362	100	508266	2
4	3	0.00000	<0.00345	100	1005597	4
5	2	0.00000	0.00000	100	1169491	4
6	5	0.00000	0.00000	100	1517361	8
6	10	0.00000	0.00000	95	2765348	19
6	20	0.00000	0.10003	0	4088200	45
7	3	−3.32834	−3.32834	85	655776	4

7. Conclusions

The SIM is a robust and efficient algorithm for global minimization. Its efficiency comes from a combined use of global and local minimization. The global (stochastic) part employs uniform and normal random distributions. It can be combined with local (deterministic) methods appropriate for the objective function. The diameters of the minimizing sets (Stability Index) are used for a self-contained stopping criterion. The computational experiments show that the method was successful for various standard test functions over multidimensional domains. No adjustment of parameters was needed in different tests. The method is well suited for low dimensional minimization problems. Its performance deteriorates for higher dimensional problems. The SIM is a valuable addition to already existing global minimization methods.

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