A finite-step convergent derivative-free method of unconstrained optimization

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Abstract

In our previous work [Y. Q. Huang and K. Jiang, Advances in Applied Mathematics and Mechanics, 2017, 9: 307-323], a useful derivative-free algorithm, the hill-climbing method with a stick (HiCS), has been proposed to treat unconstrained optimization. Numerical results have been demonstrated its wonderful performance. However, there are two issues required to be solved: convergent analysis and a extension to high dimensional problems. In this paper, we will give a rigorous theory to ensure finite-step convergence with mild conditions. Meanwhile, an economic sampling strategy using regular simplex of evaluating function values is proposed to treat high dimensional optimization. Finally, we use several standard numerical examples to demonstrate its efficiency.

Keywords: Hill-climbing method with a stick (HiCS), Finite-step convergence, Suspected minimum point, Simplex sampling, High-dimensional unconstrained optimization

1. Introduction

Derivative-free optimization is an area of long history and current rapid growth, fueled by a growing number of applications that range from science problems to medical problems to engineering design and facility location problems. In general, derivative-free optimization does not use derivative information to find optimal solution.

The derivative-free optimization algorithms can mainly be classified as direct and model-based. Direct algorithms usually determine search directions by evaluating the function f directly, whereas model-based algorithms construct and utilize a surrogate model of f to guide the search process. A detailed review about this kind of approaches was presented by Rios and Sahinidis [6]. Recently developed methods based trust-region using interpolation model belong to model-based methods [7, 8, 9, 10]. In practical implementation, heuristic algorithms, such as simulated annealing, genetic algorithm [11], have been also developed to solve derivative-free optimization. Here we focus our attention on the direct search algorithms.

In our previous work [1], we proposed a derivative-free optimization method, i.e., hill-climbing method with a stick (HiCS), to treat unconstrained optimization. The main idea of the algorithm,

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at each iteration, is comparing function values on a surface surrounding the current point, rather than a neighbourhood of current node. It has many good properties, such as easily to implement, a unique parameter required to be modulated, and having capacity for find local and global maxima. However, it still lacks rigorous theoretical explanation. In this paper, we will give the convergence analysis and related properties of this algorithm. Meanwhile, a new strategy will be proposed to sample the search surface to deal with high dimension optimization problems.

In the following, we will briefly introduce the HiCS algorithm and prove its finite-step convergence in Sec. 2. The algorithm implementation is presented in Sec. 3. In particular, the new sampling strategy using regular simplex is also given in this section. The numerical experiments including high dimensional optimization problems are showcased in Sec. 4. Finally the conclusion and discussions are given in Sec. 5.

2. Algorithm description and convergence analysis

Before going further, a short introduction of the HiCS method is necessary. We consider an unconstrained optimization problem

$$\min_{x\in\Omega\subset\mathbb{R}^d} f(x), \tag{1}$$

where the objective function $f(x):\mathbb{R}^n\to\mathbb{R}$ is continuous. Let ρ be a search radius, $O(x_k,\rho)=\{x : |x-x_k|=\rho\}$ be the search surface in the k-th iteration with radius ρ. $U(x_k,\rho)$ is the neighbourhood of x_k with radius of ρ. To illustrate the algorithm to be more precision, an useful concept of suspected extreme point is introduced.

Definition 1. *For a given objective function $f(x)$ and a positive constant $\rho>0$, $\tilde{x}$ is a suspected extreme point if $f(\tilde{x})<f(x)$ or $f(\tilde{x})>f(x)$, for $\forall x\in O(\tilde{x},\rho)$. If $f(\tilde{x})<f(x)$ for all $x\in O(\tilde{x},\rho)$, $\tilde{x}$ is the suspected minimum point (SMP).*

Certainly, $\tilde{x}$ is a SMP if $\tilde{x}$ is a minimizer in the neighborhood of $U(\tilde{x},\rho)$. The opposite is not always true. The definition can be extended to describe suspected maximum point. With these notations, the HiCS algorithm can be presented more precisely as

Algorithm 1 Stick Hill-Climbing (HiCS) Algorithm

1: **Initialization:** Choose x_0 and ρ.
2: **For** $k=0,1,2,\dots$
3: Try to find $\bar{x}\in O(x_k,\rho)$, s.t. $f(\bar{x})<f(x_k)$.
If such a point is found, then set $x_{k+1}=\bar{x}$.
Otherwise, a SMP is found, and declare the iteration successful.

From our experience, the HiCS approach usually terminates in finite steps. It is an amazing property. In what follows, we will give the condition to ensure the finite-step convergence.

Theorem 1 (Finite-step convergence)**.** *Assume that objective function $f(x)$ is continuous and the search domain Ω is a compact set. If there are not two SMPs x_* and x^* satisfying $\|x_*-x^*\|=\rho$ and $f(x^*)=f(x_*)=\alpha$. Then Algorithm 1 converges in finite steps.*

Proof. Assume that the HiCS method produces an infinite pair sequence $\{x_n, f(x_n)\}_{x=0}^{\infty}$. From assumption, it is obvious $f(x)$ is bounded. The decreasing sequence $\{f(x_n)\}_{n=0}^{\infty}$ converges, and the bounded $\{x_n\}_{n=0}^{\infty}$ has a convergent subsequence $\{x_{n_k}\}_{k=0}^{\infty}$. Assume that $f(x_n) \to \alpha$ and $x_{n_k} \to x^*$.

In accordance with the subsequence $\{x_{n_k}\}_{k=0}^{\infty}$, we can always have an another bounded subsequence $\{x_{n_k-1}\}_{k=0}^{\infty} \subset \{x_n\}$ satisfying $\|x_{n_k-1} - x_{n_k}\| = \rho$. Due to the boundedness of iteration sequence, $\{x_{n_k-1}\}_{k=0}^{\infty}$ has a convergent subsequence $\{x_{n_m}\}_{m=0}^{\infty}$. Let $x_{n_m} \to x_*$ when $m \to \infty$. From $\{x_{n_m}\}_{m=0}^{\infty}$, it alway has a subsequence $\{x_{n_m+1}\}_{m=0}^{\infty} \subset \{x_{n_k}\}_{k=0}^{\infty}$ satisfying $\|x_{n_m+1} - x_{n_m}\| = \rho$ for any m. Obviously, $x_{n_m+1} \to x^*$. Due to $\|x^* - x_*\| = \rho$, but $f(x^*) = f(x_*) = \alpha$, it results in contradiction. $\square$

3. Algorithm implementation

As mentioned above, the HiCS algorithm can converge within finite steps with mild assumptions and has a unique parameter of search radius ρ required to adjust. However in practice, the search surface $O(x_k, \rho)$ in each iteration shall be discretized to $O_h(x_k, \rho)$ in numerical implementation. The discretization strategy can not only has a major impact on the efficiency of capturing the SMP, but also concerns solving high-dimensional optimization problems. Without a priori knowledge of objective function, the principles of sampling strategy should include:

- Symmetry;
- Uniform distribution;
- As few discretization points as possible.

Our previous work has demonstrated that uniformly distributed sampling points were useful to find the SMP when without a priori knowledge of objective functions [1]. However, sampling points of the bisection sampling strategy based on spherical coordinates in the previous work are as large as $2m^{n-1}$ in each iteration, m is the number of refinement, n is the dimensions of optimization problems. This significantly limits the application to high-dimensional problems. To overcome this limitation, it is required to develop a new strategy to sample $O(x_k, \rho)$ with a few sampling points. A reasonable requirement is that the number of sampling points should be linear or quasi-linear growth with the increase of problem dimensions. A simple uniformly discretization method is sampling $O(x_k, \rho)$ along Cartesian coordinate axes and their opposite directions. For an n dimension objective function, the discretization points are $2n$ for each sampling. A more economic discretization method is the regular simplex approach. An n-dimension regular simplex of $\mathbb{R}^n$ is the congruent polytope of $n + 1$ vertices. In this work, we will use the regular simplex method to sample the search surface $O(x_k, \rho)$. The Cartesian coordinates of an n-dimension regular simplex with a set of points $\{a_1, \dots, a_n, a_{n+1}\}$ and all pairwise distances 1, can be obtained from the following two properties:

1. For a regular simplex, the distances of its vertices $\{a_1, \dots, a_n, a_{n+1}\}$ to its center are equal.
2. The angle subtended by any two vertices of n-dimension simplex through its center is $\arccos(-1/n)$.

In particular, the above two properties can be implemented through the Algorithm 2.

If the HiCS method has not find a better state on a regular simplex, we can add more points to refine $O(x_k, \rho)$. The newly added points should not repeat the old ones and also are uniformly

Algorithm 2 Generate n-D regular simplex coordinates

Give an $n \times (n+1)$-order zero matrix $x(1:n, 1:n+1)$
for $i = 1:1:n$ **do**
  $x(i,i) = \sqrt{1 - \sum_{k=1}^{i-1} [x(k,i)]^2}$
  for $j = i+1:1:n+1$ **do**
    $x(i,j) = \dfrac{1}{x(i,i)}\Big(-\dfrac{1}{n} - x(1:i-1,i)^T \cdot x(1:i-1,j)\Big)$
  end for
end for
Output the column vectors, and let $a_j = x(:,j)$, $j = 1,2,\ldots,n+1$.

distributed when the priori knowledge of objective function is unknown. To satisfy these requirements, we rotate the simplex through Euler angle $\theta = (\theta_1, \theta_2, \ldots, \theta_n)$. Correspondingly, the rotation matrix $\boldsymbol{R}$ is defined as

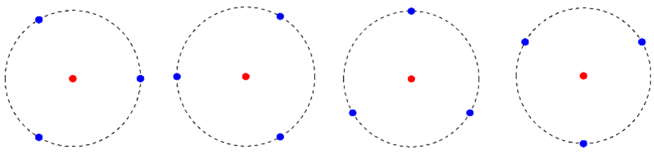
$$\boldsymbol{R} = \prod_{i=2}^{n-1} \begin{array}{c} \begin{array}{ccccccccc} & & & & i & & & & \end{array} \\ \begin{pmatrix} 1 & & & & \vdots & & & & \\ & \ddots & & & \vdots & & & & \\ & & 1 & & \vdots & & & & \\ & & & \cos\theta_i & 0 & -\sin\theta_i & & & \\ & & & 0 & 1 & 0 & & & \\ & & & \sin\theta_i & 0 & \cos\theta_i & & & \\ & & & & & & 1 & & \\ & & & & & & & \ddots & \\ & & & & & & & & 1 \end{pmatrix} \end{array} \tag{2}$$
$$\begin{pmatrix} \cos\theta_1 & -\sin\theta_1 & 0 & & \\ \sin\theta_1 & \cos\theta_1 & 0 & & \\ 0 & 0 & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{pmatrix} \begin{pmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & 0 & 0 \\ & & 0 & \cos\theta_n & -\sin\theta_n \\ & & 0 & \sin\theta_n & \cos\theta_n \end{pmatrix}.$$

Then vertices of new simplex can be obtained by

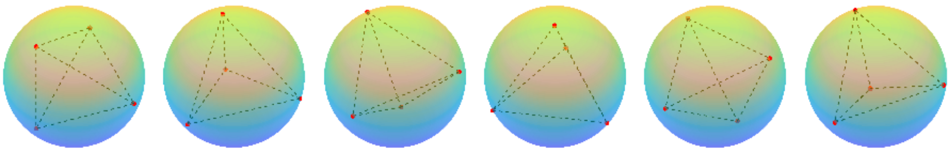
$$a_j = \boldsymbol{R} a_j + x_k \tag{3}$$

A standard schematic plots of 2-, and 3-D case are given in Fig. 1. It should be noted that there are also other strategies to rotate the regular simplex. For example, the additional simplexes can be obtained in a random way, or dependent on the known information of objective function.

In practice, we choose a dynamic refinement strategy to sample the search surface and find SMP. Based on the dynamic refinement strategy, we propose the computable HiCS method, see Algorithm 3, if we fix the maximum number of rotation $m_{\max}$. The computational amount is not larger than $m_{\max}(n+1)$ in each iteration which is linearly dependent on the dimension of objective function. Whence, it could be easy to treat high-dimensional optimization problems.



(a) 2D regular simplexes



(b) 3D regular simplexes

Figure 1: The first 2-, and 3-D regular simplexes of sampling the search set $O(x, \rho)$.

Algorithm 3 HiCS

Input x_0, ρ, and $m_{\max}$
for $k = 0, 1, 2, \cdots$ **do**
  Set $m = 0$
  if $m \le m_{\max}$ **then**
    Discretize $O(x_k, \rho)$ to obtain $O_h^m(x_k, \rho)$
    if $\exists x_j \in O_h^m(x_k, \rho)$, s.t. $f(x_j) < f(x_k)$ **then**
      Set $x_{k+1} = x_j$, and $m = m_{\max} + 1$
    else
      Set $m = m + 1$
    end if
  else
    Declare find a SMP, end program
  end if
end for

If the HiCS algorithm converges, the convergent result provides a good initial value and small search region for other optimization methods, including derivative-free approaches, or derivative-based algorithms if the objective function is differentiable. And it is evident that the search space is shrunk to a ball with the radius ρ. We will demonstrate this by several numerical experiments in Sec. 4.

Meanwhile, we can further exploit the potential of HiCS algorithm to improve the approximation precision by tuning the search radius ρ. Algorithm 4 presents a strategy to resize the search radius ρ. Significant difference of the version from Algorithm 3 is adjusting the search radius ρ when Algorithm 3 fails to find $f(\bar{x}) < f(x_k)$, $\bar{x} \in O(x_k, \rho)$ with fixed ρ. A natural stop criterion of Algorithm 4 is to terminate the run when ρ is smaller than a prescribed numerical accuracy. Certainly, the search surface can be expanded by setting control factor $\eta > 1$ if required. In fact, Algorithm 4 can provide a restart mechanism by adjusting search radius ρ.

Algorithm 4 HiCS: adjust ρ

Input $x_0, \rho, m_{\max}, \varepsilon$ and $\eta < 1$
if $\rho > \varepsilon$ **then**
  for $k = 0, 1, 2, \cdots$ **do**
    Set $m = 0$
    if $m \leq m_{\max}$ **then**
      Discrete $O(x_k, \rho)$ to obtain $O_h^m(x_k, \rho)$
      if $\exists x_j \in O_h^m(x_k, \rho)$, s.t. $f(x_j) < f(x_k)$ **then**
        Set $x_{k+1} = x_j$, and $m = m_{\max} + 1$
      else
        Set $m = m + 1$
      end if
    else
      Set $\rho = \eta\rho$
    end if
  end for
end if

4. Numerical results

In this section, we choose three kinds of test functions, including a single extreme point function, high dimensional multi-extreme points functions, and a continuous but indifferentiable function, to demonstrate the performance of the HiCS algorithm. In Algorithm 3, the sampling points of search set in each iteration are $m(n+1)$, n is the dimension of objective function. If not specified, the maximum number of refinement $m = 32$.

4.1. A single extreme point problem

The first example is a unimodal function, in particular, the Gaussian function

$$f(x) = -10 \exp\left(-\sum_{j=1}^{n} x_j^2\right), \tag{4}$$

whose global minimum is obviously $f_* = 0$ at $(0, 0, \ldots, 0)$. The objective function is differentiable in $\mathbb{R}^n$, however, it quickly diffuses out towards zero out of the upside-down "bell". Here we will illustrate the numerical behavior of HiCS method for 2 dimension Gaussian function.

We firstly investigate the convergent properties of Algorithm 1 for the Gaussian function. The function satisfies the assumptions of Theorem 1, therefore, Algorithm 1 will be convergent in finite steps theoretically. To verify this fact, we use random initial values and carry out Algorithm 1 within 30 runs. In the set of numerical experiments, the search radius ρ is fixed as 1.0, start points are randomly generated in the space $[-10, 10]^2$. For each experiment, the HiCS method indeed converges and captures a neighbourhood of the peak 0 in finite iterations. Fig. 2 gives the required iterations for convergence in 30 numerical experiments. In these 30 runs, the average iterations of convergence is about 12, while the maximum is 22, and the minimum is 1. The number of iterations is inversely proportional to the distance of the initial point and the minimizer. When the initial values are far away from the optimal point, the algorithm needs more iterations. In contrast, when the initial points are close to the minimizer, the method requires

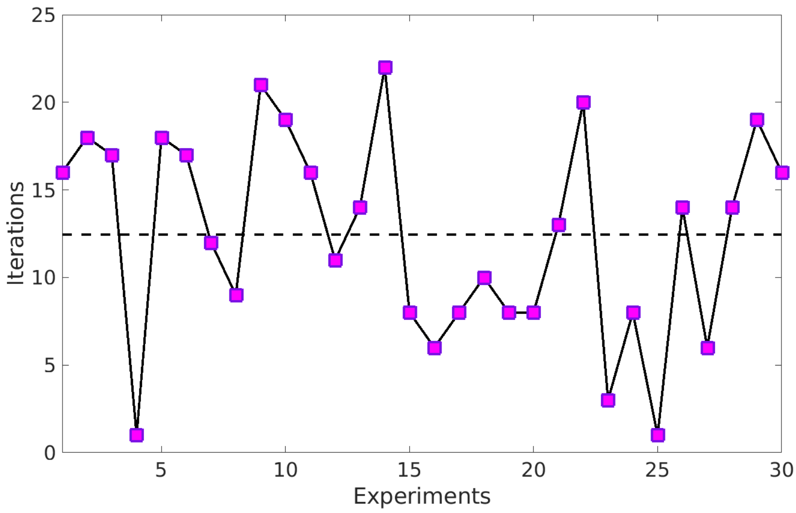


Figure 2: The iterations of convergence of the HiCS algorithm to the Gaussian function (4) in 30 runs. Start points are randomly generated in the space $(-10, 10)^2$, and $\rho = 1.0$. The flat dashed line shows the average.

less iterations. We also note that when the start point is far away from the peak, the derivative-based methods, such as steepest descent method, conjugate gradient method and Newton method, would fail since the gradient value is almost zero. However, the HiCS algorithm can always approximate the peak point. The initial values may yield a few more iterations but NOT affect the finite-step convergence as the Theorem 1 shows.

Then we take an example to further observe the numerical behavior of the HiCS algorithm. Tab. 1 shows the iterative procedure of the HiCS approach in detail when the start point is $x_0 = (6.7, -8.0)$ with fixed search radius $\rho = 1.0$. In the Tab. 1, the first and second columns show the number of iterations and rotation simplexes when applying HiCS method. The third column gives the ℓ^2-distance between iterator and the global minimizer 0, where $\|x\|_{\ell^2} = \left(\sum_{i=1}^n x_i^2\right)^{1/2}$. The fourth column is the function value on iterator. The results show that the iterates can be updated efficiently to capture a neighbourhood of the minimizer 0 within 14 steps. The convergent result reduces the search space and provides a good start position $(0.3, -0.1)$ to further approximate the minimizer to high precision with other optimization algorithms. Due to the good analytical nature of objective function, the derivative-based methods or adaptive HiCS method (see Algorithm 4) are both good choices of finding the minimizer with the above convergent results.

Table 1: The iterative procedure of HiCS algorithm with $\rho = 1.0$ when the initial value is $x_0 = (6.7, -8, 0)$.

Iteration	m	ℓ^2-distant	Function value
1	1	10.435037135	-5.1247639412e-47
2	1	9.4516450176	-1.5955605034e-38
3	1	8.4721418236	-6.7230095025e-31
4	1	7.4980517882	-3.8337625366e-24
5	1	6.5317971614	-2.9586781839e-18
6	1	5.5774517207	-3.0901622718e-13
7	1	4.6423659094	-4.3679320991e-09
8	1	3.7410098605	-8.3556743824e-06
9	1	2.9049523775	-2.1632074620e-03
10	1	2.2096021938	-7.5792437378e-02
11	1	1.8237147240	-3.5938885990e-01
12	1	1.2175146221	-2.2710521764e+00
13	1	0.96225536865	-3.9616067919e+00
14	32	0.28695270523	-9.2095707106e+00

4.2. High-dimensional multi-minimizers problems

The second tested function is the Ackley function [19], a benchmark function, widely used for testing optimization algorithms. The expression of the Ackley function can be written as

$$f(x) = -20 \cdot \exp\left(-\frac{1}{5} \cdot \sqrt{\frac{1}{n}\sum_{i=1}^{2} x_i^2}\right) - \exp\left(\frac{1}{n}\sum_{i=1}^{n} \cos(2\pi x_i)\right) + a + \exp(1), \tag{5}$$

where n is the dimension. Ackley function has many local minima and a unique global minimum of 0 with $f(0) = 0$, which poses a risk for optimization algorithms to be trapped into one of local minima, such as the traditional hill-climbing method [22]. In this subsection, we will apply the HiCS algorithm to 2, 100, and even 2500 dimension Ackley function.

Firstly we consider the 2 dimension Ackley function whose morphology can be found everywhere, such as [1]. In our previous work, we have found that the HiCS method is able to obtain a neighbourhood of the global minimum with an appropriate search radius ρ using the bisection sampling approach. In the current work, we still to examine the convergent behavior of Algorithm 1 to approximate the global minimum using the simplex sampling strategy. The first 30 numerical experiments are performed with random initial values generated in the space of $[-10, 10]^2$ when $\rho = 1.0$. The final convergent domain in each test contains the global minimizer $(0, 0)$. Fig. 3 shows the required iterations of convergence. In the 30 numerical tests, the average iterations of convergence is about 11, while the maximum number of iterations is 20 and the minimum is 4. The initial positions also only affect the speed of convergence, but not the ability of catching the neighbourhood of the global minimum.

The above tests have demonstrated that the HiCS algorithm can capture the neighbourhood of the global minimum of the Ackley function. Subsequently we plan to manifest the ability of the HiCS algorithm to obtain local minimizers. As discussed above, the unique regulatable parameter in the HiCS scheme is the search radius ρ. Therefore we will test the numerical

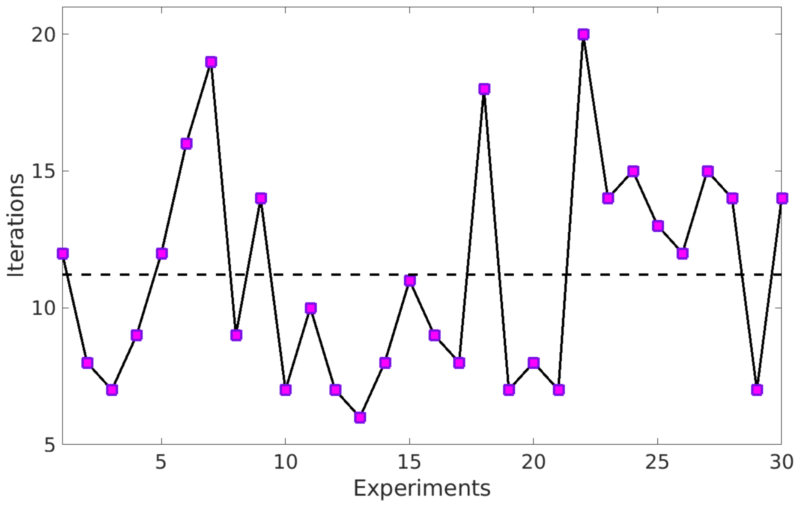


Figure 3: The required iterations of convergence by HiCS algorithm 1 for 2 dimension Ackley function (5) in 30 numerical experiments. Start points are randomly generated in the space $[-10, 10]^2$ with fixed $\rho = 1.0$. The flat dashed line shows the average.

behaviors with different size of ρ. In the set of tests, the initial value is always $x_0 = (4.1, 3.4)$. Tab. 2 gives the convergent results with different ρ. Fig. 4 marks corresponding local minima.

Table 2: The convergent results and required iterations of the HiCS algorithm with different ρ when the initial value is $x_0 = (4.1, 3.4)$. The locations of different local minima are marked in Fig. 4.

ρ	0.1	0.3	0.5	0.55	0.58	0.6	1.0
Iterations	7	3	2	6	7	15	7
Min.	Loc_1	Loc_1	Loc_1	Loc_2	Loc_3	Global	Global

From these numerical experiments, one can find that the search radius ρ plays a filter role in catching different local minimum by setting different values. When ρ is greater than 0.6, the HiCS approach can approximate the global minimum, otherwise, the method can converge to different local minima. If starting from other initial position, the HiCS method can find other minima.

Next we consider the 100 dimension Ackley function. The initial value is randomly generated in $[-10, 10]^{100}$ and the search radius is set as $\rho = 2$. The iteration detail has been listed in Tab. 3. The first and second columns show the number of iterations and rotation simplexes when applying HiCS method. The third column gives the ℓ^2-distance between the current iterator and the global minimizer 0. The fourth column is the function value on the current iterator. Obviously, HiCS algorithm converges within 365 steps and the global minimizer is contained in the convergent neighbourhood.

The convergent result by HiCS method efficiently shrinks the search region. Then we can further approximate the unique minimizer by repeatedly using HiCS with different ρ, i.e., Al-

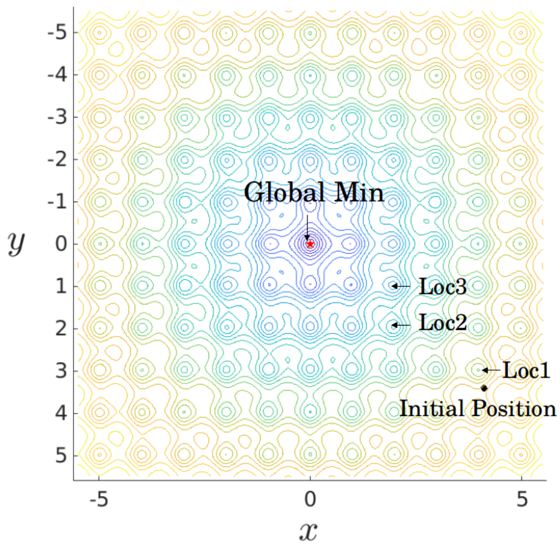


Figure 4: The locations of some local minima and the global minimum of 2 dimension Ackley function.

Table 3: The iterative procedure of HiCS algorithm with fixed $\rho = 2$ and random initial value when optimizing 100 dimension Ackley function.

Iteration	m	ℓ^2-distance	Function value
1 ↓ 353	1	43.769842839 ↓ 5.6705662388	13.402763950 ↓ 3.6500283195
354	3	5.7676753732	3.6496090883
355	5	5.8410256060	3.6457912911
356	5	5.7571725375	3.6370586909
357	1	5.7273233589	3.6315399254
358	1	5.6810640400	3.6302051882
359	6	5.6745774447	3.6065456752
360	12	5.7618050286	3.6056866282
361	5	5.8449616655	3.5967423037
362	1	5.7652804943	3.5937731951
363	1	5.7175444967	3.5927685452
364	2	5.9090844843	3.5905379762
365	32 ($m_{\max}$)	5.9376731371	3.5825199326

gorithm 4. The convergent criterion of AHiCS is $\rho < 10^{-5}$. The detail of iteration procedure is given in Tab. 4. In this table, the first and second columns give the values of search radius ρ and corresponding iterations. The third and fourth columns are the same as the third and fourth ones in Tab. 3. Obviously, for each fixed ρ, the algorithm is convergent in finite steps. The pair sequence produced by AHiCS method approximates to both the unique global minimizer and corresponding function value.

Table 4: The iterative procedure of AHiCS algorithm for optimizing 100 dimension Ackley function based on the convergent result as given in Tab. 3. The control factor $\eta = 0.5$.

ρ	Iterations	ℓ^2-distance	Function value
2.0	431	5.9376731371	3.5825199326
1.0	152	2.5717428366	2.2979795353
0.5	171	1.2147220195	1.1029637432
0.25	145	0.60161985055	0.42190311564
0.125	152	0.30400991430	0.17007648336
0.0625	105	0.14644406013	0.069957199791
0.03125	175	0.076076391231	0.033509781782
$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$
1.525879e-05	135	3.5663302607e-05	1.4265998399e-05

Finally, we apply HiCS and AHiCS algorithms to 2500 dimension Ackley function. The random initial value is randomly generated in $[-10, 10]^{2500}$, and initial search radius is $\rho = 3.5$. Due to such high dimension problem, the maximum number of rotation of simplexes is $m_{\max} = 16$ to save computational amount. The convergent criterion of AHiCS approach is that ρ is smaller than 10^{-5}. The iterative information can be found in Tab. 5. The table is the same as Tab. 4 except that 2500 dimension Ackley function is optimized. For the high dimension optimization problem, the iteration behavior is similar to previous numerical experiments. When $\rho = 3.5$, the scheme, which is actual the HiCS method, converges within 5415 steps. Keeping carrying out the HiCS algorithm by shrinking ρ, we can further approximate the global minimizer 0. After 61755 iterations, the AHiCS algorithm achieves the convergent point as shown in the last row in Tab. 5. It costs roughly 3.7 hours of real time using one Inter 3.60 GHz i7-4790 processor.

Table 5: The iterative procedure of optimizing 2500 dimension Ackley function using AHiCS algorithm with initial $\rho = 3.5$ and random initial value. The control factor $\eta = 0.5$.

ρ	Iteration	ℓ^2-distance	Function value
3.5	5415	188.54368262 ↓ 43.980512458	12.310134936 ↓ 4.7600200861
1.75	5064	↓ 24.909250731	↓ 3.3115891477
0.875	4099	↓ 10.893125123	↓ 2.0271413426
0.4375	4869	↓ 5.1289809138	↓ 0.88082043719
0.21875	3269	↓ 2.5698591962	↓ 0.34009221628
↓	↓	↓	↓
1.335144e-05	3340	1.5546421188e-04	1.2437651812e-05

4.3. A continuous but indifferentiable function

The last model is a 2 dimension variant of Dennis-Woods function [17, 23],

$$f(x) = \frac{1}{2}\max\{\|x - c_1\|^2, \|x - c_2\|^2\}, \quad x = (x_1, x_2) \in \mathbb{R}^2, \tag{6}$$

where $c_1 = (1, -1)^T$, $c_2 = -c_1$, $\|\cdot\|$ denotes ℓ^2 norm. This objective function has a unique

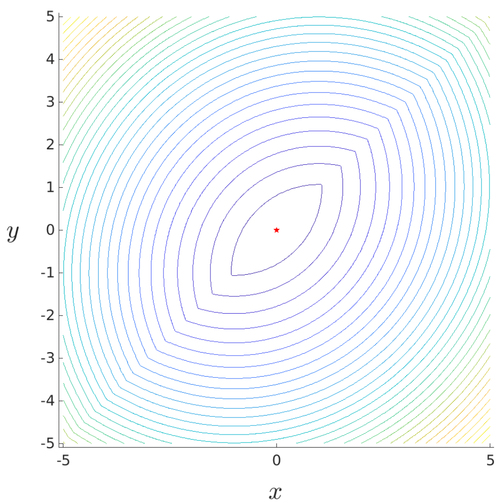


Figure 5: Contours of the variant of the Dennis-Woods function (6)

minimizer of 0, and $f(0, 0) = 1$, indicated by a red star in the contour plot of Fig. 5. The function is continuous and strictly convex everywhere, but its gradient is discontinuous along the line $x_1 = x_2$. It has been shown that the Nelder-Mead simplex algorithm fails to converge to the minimizer of Dennis-Woods function (6) in Ref. [23]. In this subsection, we will investigate the performance of our proposed method.

Firstly, we still examine the efficiency of the HiCS algorithm for the continuous but indifferentiable function. 30 numerical experiments are performed with random initial values generated in the space $[-5, 5]^2$. The search radius is fixed as $\rho = 0.5$ for these tests. Results demonstrate that the HiCS algorithm can find a neighbourhood of the minimizer 0 in each test no matter which initial value is used. The required iterations for convergence is shown in Fig. 6, while the

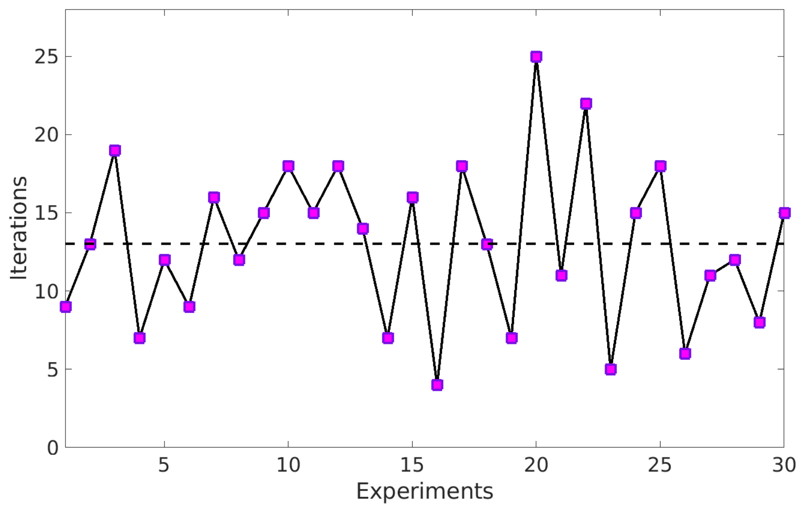


Figure 6: The iterations of convergence of the HiCS method to the Dennis-Woods function (6) in 30 test examples. Start points are randomly generated in the space $[-5, 5]^2$, and $\rho = 0.5$. The flat dashed line shows the average.

average iterations is about 13.

Subsequently, we will take an example to show the numerical behavior of the HiCS algorithm in detail. In particular, Tab. 6 gives the iterative information when the initial value is $x = (1.0, 1.5)$, and the search radius is fixed as $\rho = 0.5$. It can be found that the HiCS method

Table 6: The iterative information of optimizing Dennis-Woods function using HiCS algorithm with $\rho = 0.5$ and initial value $x = (3.2, 1.5)$

Iteration	m	ℓ^2-distance	Fun. Val.
1		3.5341194094	8.9450000000
↓	1	↓	↓
15		0.37927243150	1.1398729811
16	3	0.13421830119	1.1240707856
17	15	0.38930926651	1.0985484063
18	32	0.11218490755	1.0290602806

has a pronounced convergent behavior in 18 steps even for this indifferentiable function.

Finally we compare the performance of the HiCS algorithm with one of the standard directional direct-search methods, the coordinate-search (CS) method, for the Dennis-Woods function. Before we go further, a short introduction of the CS method is necessary. More details about the CS method can be found, for instance, in a recent monograph [5] or Ref. [17]. The CS method makes use of the positive bases $\mathcal{D}_\oplus$ which spans the $\mathbb{R}^2$ with positive coefficients. Let x_k be the current iterate and λ the current search step length. The CS method evaluates the function f at the points in the set

$$\mathcal{P}_k = \{x_k + \lambda d : d \in \mathcal{D}_\oplus\},$$

following some specified order, trying to find a point in $\mathcal{P}_k$ that decreases the objective function value. When that happens, the method defines a new iterate $x_{k+1} = x_k + \lambda d \in \mathcal{P}_k$ such that $f(x_{k+1}) < f(x_k)$. In such a case, one either leaves the parameter λ unchanged, or increases it, or decreases it. Here we will change λ during the iterative procedure. If none of the points in $\mathcal{P}_k$ leads to a decrease in f, then the parameter λ is reduced (here by a factor of $1/2$) and the next iteration at the same point ($x_{k+1} = x_k$). The algorithm is terminated when the λ is smaller than a given tolerance.

Like the CS method, the HiCS algorithm has similar algorithmic steps to update iterates and change the search radius. Unlike the CS method, however, the HiCS method does not predetermine the search directions, such as $\mathcal{D}_\oplus$ in the CS scheme. In k iteration, the HiCS method evaluates functions on the search surface $O(x_k, \rho)$, and compares them with $f(x_k)$. In practice, the search surface $O(x_k, \rho)$ is dynamically sampled as presented in Algorithm 3. From another perspective, the HiCS algorithm provides an adaptive mechanism to adjust the search directions according to objective function.

In the following numerical tests, the initial value is $x_0 = (1.1, 0.9)$, the initial search radius is $\rho = 1.0$. In the HiCS algorithm, the maximum sample points $N_{\max}$ of $O(x_k, \rho)$ is 8. In the CS method, the positive bases is $\mathcal{D}_\oplus = \{(1,0),(0,1),(-1,0),(0,-1)\}$ of standard choice. The control factor of adjusting search radius $\eta = 0.5$ in both methods.

Fig. 7 shows the error of $|f(x_k) - f(x^*)|$ against the number of function evaluations for both HiCS and CS methods. As observed in Fig. 7 the CS method stalls at the error of $O(10^{-2})$, however, the HiCS method can continue to reduce error. The reason is that when the iterate approaches to the minimizer, the CS method can not detect a sufficient decrease, even no decrease, along the predetermined search directions in $\mathcal{D}_\oplus$. This results in the stagnation phenomenon. However, the mechanism of detecting smaller values in the HiCS algorithm is dependent on the feature of $f(x_k)$ rather than along predetermined directions. It yields the efficient and flexible performance of the HiCS method when approximating the minimizer.

4.4. Sphere function

$$f(x) = \sum_{i=1}^{n} x_i^2 \tag{7}$$

The Sphere function has n local minima except for the global one $x = (0, 0, \ldots, 0)$ with $f = 0$. It is continuous, convex and unimodal.

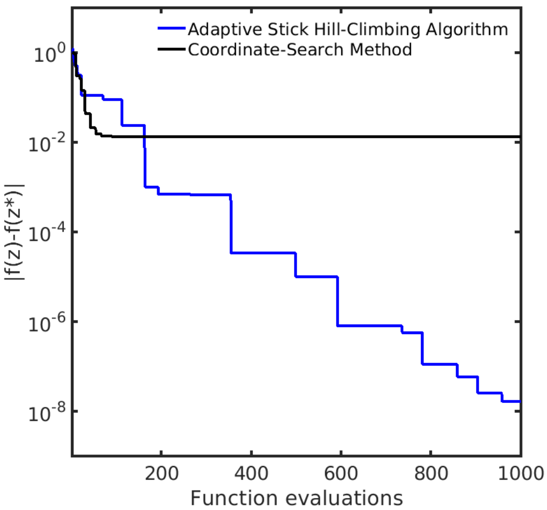


Figure 7: Application of the HiCS method ($N_{\max} = 8$) and the CS (with predetermined search directions $\mathcal{D}_{\oplus}$) methods to the Dennis-Woods function starting from $x_0 = (1.1, 0.9)$. In the HiCS algorithm, the initial search radius $\rho = 1.0$, and in the CS approach the initial search step length $\lambda = 1.0$. The control factor $\eta = 0.5$ in both methods. $f(x^*)$ is the global minimizer.

4.5. Powell function

$$F(x) = \sum_{i=1}^{n/4} [(x_{4i-3} + 10x_{4i-2})^2 + 5(x_{4i-1} - x_{4i})^2 + (x_{4i-2} - 2x_{4i-1})^4 + 10(x_{4i-3} - x_{4i})^4] \tag{8}$$

The function is usually evaluated on the hypercube $x_i \in [-4, 5]$ for all $i = 1, \ldots, n$.

available

4.6. ARWHEAD function

$$F(x) = \sum_{i=1}^{n-1} [(x_i^2 + x_n^2)^2 - 4x_i + 3] \tag{9}$$

The least value of F is zero, which occurs when the variables take the values $x_j = 1$, $j = 1, 2, \ldots, n-1$ and $x_n = 0$. The starting vector is given by $x_j^{(0)} = 1$, $j = 1, 2, \ldots, n$, as Powell done in Ref. [26].

available

4.7. CHROSEN function

$$F(x) = \sum_{i=1}^{n-1} [(4(x_i - x_{i+1}^2)^2 + (1 - x_{i+1})^2] \tag{10}$$

The least value of F is zero, which occurs when the variables take the values $x_j = 1$, $j = 1, 2, \ldots, n$. The starting vector is given by $x_j^{(0)} = -1$, $j = 1, 2, \ldots, n$, as Powell done in Ref. [26].

Hard

4.8. *Woods function [24, 25]*

The Woods function is a large and difficult problem in the CUTE test set [24]. The specified expression is

$$F(x) = \sum_{i=1}^{n/4} \Big[100(x_{4i-2} - x_{4i-3}^2)^2 + (1 - x_{4i-3})^2 + 90(x_{4i} - x_{4i-1})^2 + (1 - x_{4i-1})^2 + 10(x_{4i-2} + x_{4i} - 2)^2 + 0.1(x_{4i-2} - x_{4i})^2\Big]. \tag{11}$$

The global minimizer is $(1, 1, \ldots, 1)$ with $f = 0$. Here we choose the hard initial value [], i.e., $x_j^{(0)} = -3.0$ if j is even, and $x_j^{(0)} = -1.0$ if j odd, to test our proposed method HiCS with n variables. The choices of n are 4, 20, 80, 320, 1280, 2000.

Table 7: : Iteration information

ρ	Iter.	ℓ^2-distance	$F(x)$
5.0	111	2.0269797302e+01	1.9462281448e+04
2.5	21	2.1446697698e+01	1.7213410433e+04
1.25	38	2.3007762412e+01	1.4027762445e+04
0.625	49	2.1442322133e+01	9.2058823364e+03
0.3125	558	1.8950544937e+01	2.3646230729e+03
0.15625	634	1.6684359010e+01	1.2099516621e+03
0.078125	2502	1.2212940331e+01	2.9382990538e+02
$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$
1.907349e-05	114180	4.4027298178e-02	7.0921802110e-04

It costs 48665367 function evaluations.

We can further apply AHiCS approach ($\eta = 0.5$) to approximating the minimizer of Woods functions based on the above convergent results. Here we take $n = 80$ as an example to demonstrate the iteration procedure.

5. Discussion

Inspired by the hill-climbing behavior of the blind, we has proposed a new derivative-free method to unconstrained optimization problems in our previous work [1]. In this paper, we built a rigorous mathematical theory of HiCS algorithm which theoretically ensures finite-step convergence under mild conditions. Numerical results also have demonstrated this great property. In practice, the computational complexity of HiCS algorithm mainly depends on the sampling strategy which determines the function valuations. In our previous work, the number of sampling points increases exponentially with the dimension of problems. It limits the application to high-dimensional optimization. To deal with high-dimensional problems, we proposed a new strategy

Table 8: : Iteration information

ρ	Iter.	ℓ^2-distance	$F(x)$
5.0	111	2.0269797302e+01	1.9462281448e+04
2.5	21	2.1446697698e+01	1.7213410433e+04
1.25	38	2.3007762412e+01	1.4027762445e+04
0.625	49	2.1442322133e+01	9.2058823364e+03
0.3125	558	1.8950544937e+01	2.3646230729e+03
0.15625	634	1.6684359010e+01	1.2099516621e+03
0.078125	2502	1.2212940331e+01	2.9382990538e+02
$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$
1.907349e-05	114180	4.4027298178e-02	7.0921802110e-04

It costs 48665367 function evaluations.

of simplex sampling method to save computational amount. Using the new sampling strategy, the number of function valuations is linear dependent on the dimension of problems. Taking Ackley function as an example, it allows us to solve up to 2500 dimension function within a few hours.

Acknowledgments

[1] Huang, Yunqing and Jiang, Kai, Hill-Climbing Algorithm with a Stick for Unconstrained Optimization Problems, Advances in Applied Mathematics and Mechanics, 2017, 9: 307–323.

[2] W. Y. Sun and Y. Yuan, Optimization theory and methods: nonlinear programming, New York: Springer, 2006.

[3] A. R. Conn, N. I. M. Gould and P. L. Toint, Trust region methods, Philadelphia: SIAM, 2000.

[4] J. Nocedal and S. J. Wright, Numerical optimization, Berlin: Springer-Verlag, 2nd ed., 2006.

[5] A. R. Conn, K. Scheinberg and L. N. Vicente, Introduction to derivative-free optimization, Philadelphia: SIAM, 2009.

[6] L. M. Rios and N. V. Sahinidis, Derivative-free optimization: a review of algorithms and comparison of software implementations. J. Global Optim., 2013, 56: 1247–1293.

[7] M. J. D. Powell, UOBYQA: unconstrained optimization by quadratic approximation, Technical Report DAMTP NA2000/14, CMS, University of Cambridge, 2000.

[8] M. J. D. Powell, On trust region methods for unconstrained minimization without derivatives, Technical Report DAMTP NA2002/NA02, CMS, University of Cambridge, February 2002.

[9] T. Wu, Y. Yang, L. Sun, and H. Shao, A heuristic iterated-subspace minimization method with pattern search for unconstrained optimization, Comput. Math. Appl., 2009, 58: 2051-2059.

[10] Z. Zhang, Sobolev seminorm of quadratic functions with applications to derivative-free optimization, Math. Program., 2014, 146: 77-96.

[11] Z. Michalewicz and D. B. Fogel, How to solve it: modern heuristics, Springer, 2004.

[12] Y. LeCun, Bengio, Y. Hinton, G. Hinton, Deep learning, Nature, 2015, 521: 521-436.

[13] R. Hooke and T. A. Jeeves, "Direct search" solution of numerical and statistical problems, J. ACM, 1961, 8: 212–229.

[14] R. M. Lewis, V. Torczon and M. W. Trosset, Direct search methods: then and now, J. Comput. Appl. Math., 2000, 124: 191–207.

[15] J. A. Nelder and R. Mead, A simplex method for function minimization, Comput. J., 1965, 7: 308–313.

[16] V. Torczon, On the convergence of pattern search algorithms, SIAM J. Optim., 1997, 7: 1–25.

[17] T. G. Kolda, R. W. Lewis and V. Torczon, Optimization by direct search: new perspectives on some classical and modern methods, SIAM Rev., 2003, 45: 385–482.

[18] J. E. Jr Dennis and V. Torczon, Direct search methods on parallel machines, SIAM J. Optim., 1991, 1: 448–474.

[19] J. M. Dieterich and B. Hartke, Empirical review of standard benchmark functions using evolutionary global optimization, Appl. Math. 2012, 3: 1552–1564.
[20] S. Gratton, C. W. Royer, L. N. Vicente, Z. Zhang, Direct search based on probabilistic descent, SIAM J. Optim., 2015, 25:1515-1541.
[21] S. J. Russell and P. Norvig, Artificial intelligence: a modern approach, 3rd ed., Prentice Hall, 2010.
[22] T. Bäck, Evolutionary algorithms in theory and practice: evolution strategies, evolutionary programming, genetic algorithms, Oxford University Press, 1996.
[23] J. E. Jr Dennis and D. J. Woods, Optimization on microcomputers: The Nelder-Mead simplex algorithm. In: New computing environments: microcomputers in large-scale computing, A. Wouk ed., Philadelphia: SIAM, 1987.
[24] L. Lukšan, C. Matonoha, J. Vlcek, Modified CUTE problems for sparse unconstrained optimization, Techical Report, 2010, 1081.
[25] https://pythonhosted.org/algopy/index.html
[26] M. J. D. Powell, The NEWUOA software for unconstrained optimization without derivative, in Large-Scale Nonlinear Optimization , eds. G. Di Pillo and M. Roma, Springer (New York), 2006, 255 297.
[27] N. Andrei, An unconstrained optimization test functions collection, Adv. Model. Optim., 2008, 10: 147–161.