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

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joint work with Kai Jiang

June 2019

Outline

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Unconstrained optimization

$$\min_{x} f(x), \quad \text{where} \quad f : \mathbb{R}^n \mapsto \mathbb{R}.$$

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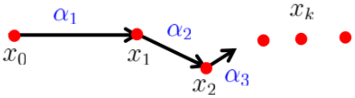
- Directional search method: direction + step length



Unconstrained optimization

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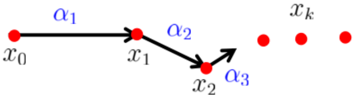
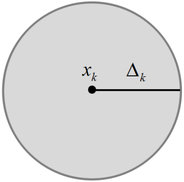


- Trust region method



$$\min_d f_k + g_k^T d + \frac{1}{2} d^T G_k d$$
$$\text{s.t. } \|d\| \le \Delta_k$$

Motivation

- The blind climbs mountains

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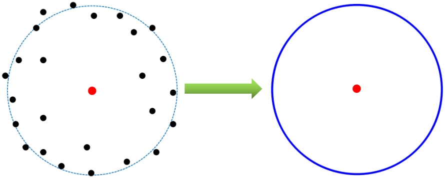
- Boundary search: no direction, "no step length"



Outline

Suspected minimum point

Definition (Suspected minimum point)

For a given function $f(x)$, $\tilde{x}$ is a suspected minimum point (SMP) if $f(\tilde{x}) \leq f(x)$ for $\forall x \in \partial U(\tilde{x}, \rho)$, where $\partial U(\tilde{x}, \rho) = \{y : \|y - \tilde{x}\| = \rho\}$ is the boundary of a neighborhood $U(\tilde{x}, \rho)$ of $\tilde{x}$.

- A minimizer $\Rightarrow$ A SMP
- A minimizer $\not\Leftarrow$ A SMP
- There exists, at least, a minimizer in $U(\tilde{x}, \rho)$ if f is continuous
- The distance of the SMP and a minimizer is smaller than ρ.

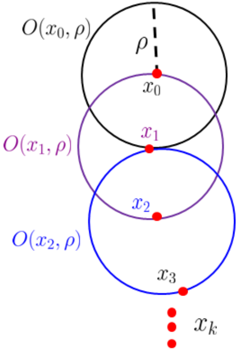
Hill-Climbing method with a Stick (**HiCS**)

- Consider the unconstrained optimization problem

$$\min_x f(x), \quad \text{where} \quad f : \mathbb{R}^n \mapsto \mathbb{R}.$$

Algorithm 1 HiCS

1: **Initialization:** given x_0 and ρ.
2: **for** $k = 0, 1, 2, \ldots$
   Find $\bar{x} = \mathrm{argmin}_{y \in O(x_k, \rho)} f(y)$
   If $f(\bar{x}) < f(x_k)$, then set $x_{k+1} = \bar{x}$.
   Otherwise, a SMP is found, and declare the iteration successful.



Finite-Step Convergence

Theorem (Finite-step convergence)

Suppose 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 $|x_* - x^*| = \rho$ such that $f(x^*) = f(x_*)$, Then HiCS algorithm converges in finite steps.

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Sketch of proof.

- The HiCS algorithm produces $\{x_n, f(x_n)\}_{n=0}^{\infty}$.
- From the assumption, $f(x)$ is bounded, then the decreasing sequence $\{f(x_n)\}$ is convergent. Assume that $f(x_n) \to A$.
- Exists a convergent subsequence $\{x_{n_k}\} \subset \{x_n\}$, s.t. $x_{n_k} \to x^*$.
- We have a bounded subsequence $\{x_{n_k-1}\} \subset \{x_n\}$ which satisfies $|x_{n_k} - x_{n_k-1}| = \rho$. Obviously, $f(x_{n_k-1}) \to A$.
- $\{x_{n_k-1}\}$ has a convergent subsequence $\{x_{n_m}\}$, s.t. $x_{n_m} \to x_*$.
- From $\{x_{n_m}\}$, we have a subsequence $\{x_{n_m+1}\} \subset \{x_{n_k}\}$ satisfying $|x_{n_m} - x_{n_m+1}| = \rho$, and $x_{n_m+1} \to x^*$.
- We have $|x^* - x_*| = \rho$, but $f(x^*) = f(x_*) = A$. This implies that x^* and x_* are both SMP.

Finite-Step Convergence

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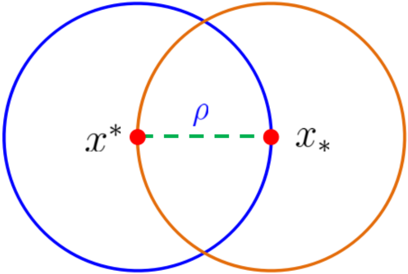
Suppose that objective function $f(x)$ is continuous and the search domain Ω is a compact set. If there are not two SMPs x_* and x^* satisfying $|x_* - x^*| = \rho$ such that $f(x^*) = f(x_*)$, Then HiCS algorithm converges in finite steps.



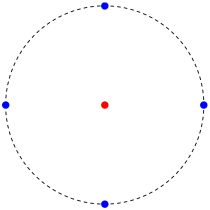
$O(x_k, \rho) \to O_h(x_k, \rho)$

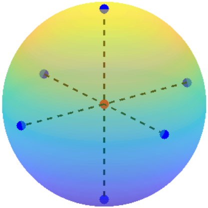
The principles of sampling $O(x_k, \rho)$ *without a priori information of objective function*

- Symmetry
- Uniform distribution
- As few points as possible

$O(x_k, \rho) \to O_h(x_k, \rho)$

- Cartesian coordinate axes





- Sampling points: $2n$

$O(x_k, \rho) \to O_h(x_k, \rho)$: Regular Simplex

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

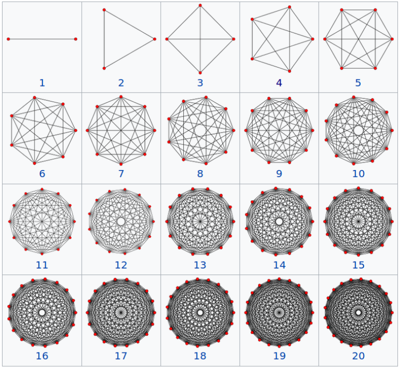


Figure 1: cited from wiki

Refinement Strategy

- Principle: No-repeat, Uniform distribution

Refinement Strategy

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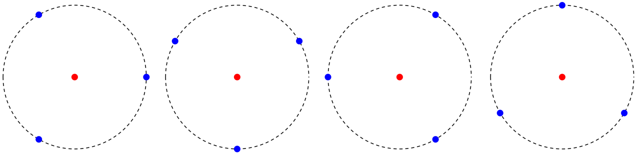
- Strategy: Rotation

Refinement Strategy

- Principle: No-repeat, Uniform distribution
- Strategy: Rotation
- Simplex: rotation matrices can be obtained through Euler angles
  1. 2D case:



  2. 3D case: Movie: Iteration procedure
  3. Computational complexity: $m(n+1)$

- In practice, the HiCS algorithm can be given as follows

Algorithm 2 HiCS

Input x_0, ρ, and $m_{\max}$
for $k = 0, 1, 2, \cdots$ **do**
  Set $m = 0$
  if $m \leq m_{\max}$ **then**
    Discretize $O(x_k, \rho)$ to obtain $O_h^m(x_k, \rho)$
    $\bar{x} = \{x : f(x) = \min\{f(x_h), x_h \in O_h^m(x_k, \rho)\}\}$
    if $f(\bar{x}) < f(x_k)$ **then**
      Set $x_{k+1} = \bar{x}$, and $m = m_{\max} + 1$
    else
      Set $m = m + 1$
    end if
  else
    Declare that find a SMP, end program
  end if
end for

Adaptive HiCS (AHiCS): adjust ρ

- We can repeat HiCS algorithm through changing ρ

Algorithm 3 AHiCS

Input x_0, ρ, $m_{\max}$, ε and $\eta < 1$
if $\rho > \varepsilon$ **then**
    for $k = 0, 1, 2, \cdots$ **do**
        Set $m = 0$
        if $m \leq m_{\max}$ **then**
            Discretize $O(x_k, \rho)$ to obtain $O_h^m(x_k, \rho)$
            $\bar{x} = \{x : f(x) = \min\{f(x_h), x_h \in O_h^m(x_k, \rho)\}\}$
            if $f(\bar{x}) < f(x_k)$ **then**
                Set $x_{k+1} = \bar{x}$, and $m = m_{\max} + 1$
            else
                Set $m = m + 1$
            end if
        else
            Set $\rho = \eta\rho$
        end if
        Set $k = k + 1$
    end for
end if

- The restart mechanism can be obtained by set $\eta > 1$

Outline

Gauss Function

$$f(x) = -20 \exp\left(-\sum_{i=1}^{n} x_i^2\right).$$

- A unique global minimum 0 with $f(0) = -20$.

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- A unique global minimum 0 with $f(0) = -20$.
- Apply HiCS to 2D Gauss function with $x_0 = (0.57, -0.6)$, $\rho = 0.3$, $m_{max} = 4$. $(\|x\|_{\ell^2} = (\sum_{i=1}^{n} x_i^2)^{1/2})$

Iter.	ℓ^2-distance	Fun. Val.
1	8.27587e-01	-1.00828e+01
1	5.40491e-01	-1.49334e+01
1	2.81712e-01	-1.84741e+01
1	2.15853e-01	-1.90895e+01
4	8.58004e-02	-1.98533e+01

Gauss Function

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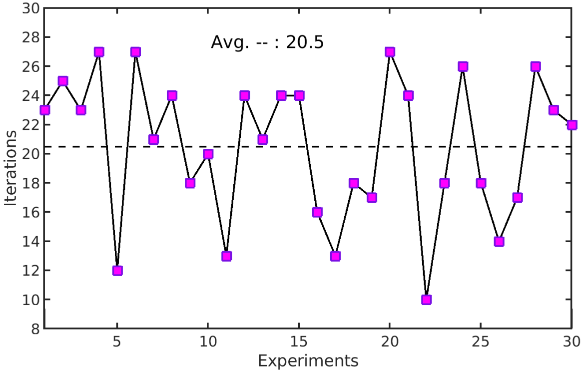
- We can further apply AHiCS approach $(\eta = 0.5)$ to this case.

Movie: Iteration procedure

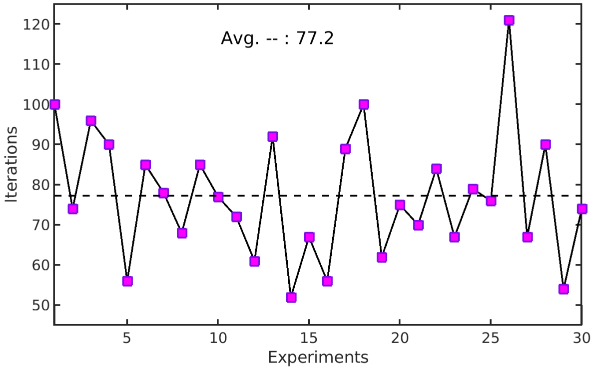
10D Gauss Function: finite-step convergence

- HiCS can capture the global minimizer within finite-step iterations
- The iterations of convergence of the HiCS with constant $\rho = 0.3$ for 10D Gauss function. The initial values were randomly generated in $[-1, 1]^2$.



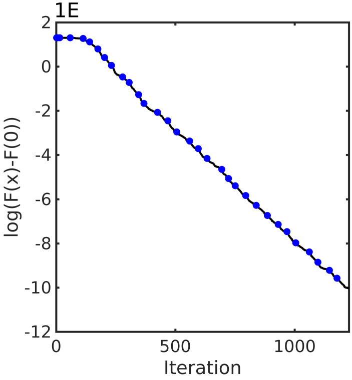
10D Gauss Function: finite-step convergence

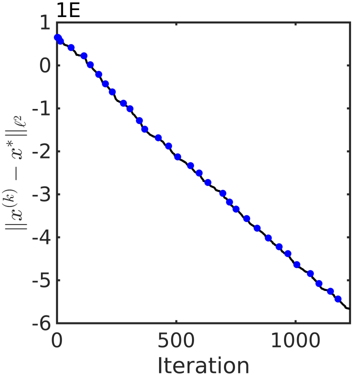
- Decreasing ρ to 0.1 for 10D Gauss function. The initial values were randomly generated in $[-1, 1]^2$.



50D Gauss Function: AHiCS

- Apply the AHiCS method to approximate the minimizer
- Setup: $\rho_0 = 10.0$, $m_{\max} = 32$, $\eta = (\sqrt{5} - 1)/2$, initial position is randomly generated.





Dennis-Woods Function

$$f(z) = \frac{1}{2}\max\{\|z - c_1\|^2, \|z - c_2\|^2\}, \qquad z = (x, y),$$

where $c_1 = (1, -1)^T$, $c_2 = -c_1$, $\|\cdot\|$ denotes ℓ^2-norm.

- continuous, strictly convex, but its gradient is discontinuous along the line $x = y$

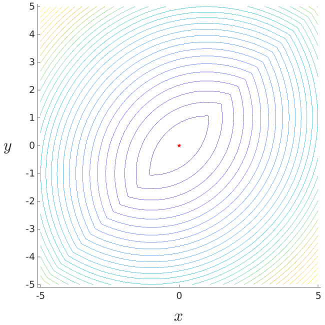


Figure 2: Contours of the variant of the Dennis-Woods function

Dennis-Woods Function

- HiCS can capture the minimizer within finite-step iterations

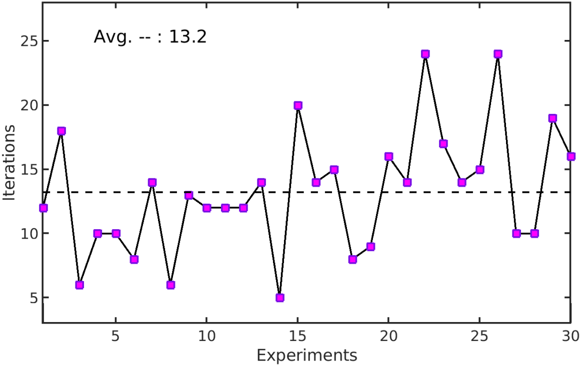


Figure 3: The iterations of convergence of the HiCS with constant $\rho = 0.5$ for 2D Dennis-Woods function. The initial values were randomly generated in $[-5, 5]^2$.

Dennis-Woods Function

- HiCS: initial value $x_0 = (3.2, 1.5)$, $\rho = 0.5$, $m_{max} = 32$.

Iter.	ℓ^2-distance	Fun. Val.
1 (1-15)	3.53412 $\downarrow$ 3.79272e-01	8.94500 $\downarrow$ 1.13987
3	1.34218e-01	1.12407
15	3.89309e-01	1.09854
32	1.12185e-01	1.02906

Dennis-Woods Function

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Movie: Iteration procedure

Dennis-Woods Function: Comparison

- The popular Nelder-Mead simplex algorithm fails
- The coordinate-search (CS) method (with predetermined search directions $\mathcal{D}_{\oplus}$) stalls

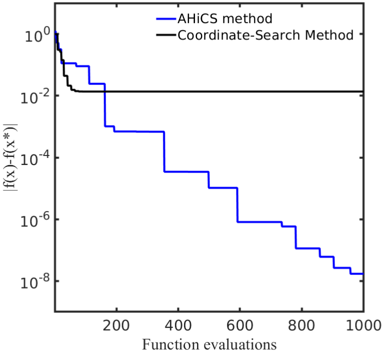


Figure 4 Application of the AHiCS method ($m_{\max} = 8$) and the CS method with $\mathcal{D}_{\oplus} = \{(1,0),(0,1),(-1,0),(0,-1)\}$, starting from $x_0 = (1.1, 0.9)$. The initial search radii are both $\rho_0 = 1.0$, the control factor $\eta = 0.5$.

Ackley Function

- Many local minima and a unique global minimum 0 with $f(0) = 0$.
- Non-convex

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

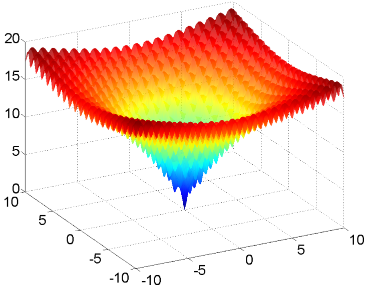


Figure 5: 2D Ackley function

Ackley Function: 2D

- HiCS method has potential to capture different minimizer
- Initial value $x_0 = (4.1, 3.4)$
- $\rho = 0.9$: global minimizer

Movie: Iteration procedure

- $\rho = 0.55$: a local minimizer

Movie: Iteration procedure

Ackley Function: 2D

- Has potential to distinguish different minima

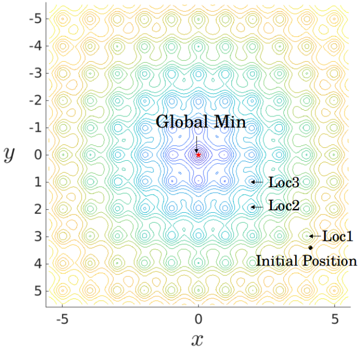


Table 1: The convergent results and required iterations with differently constant ρ starting from the initial state $(x_0, y_0) = (4.1, 3.4)$.

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

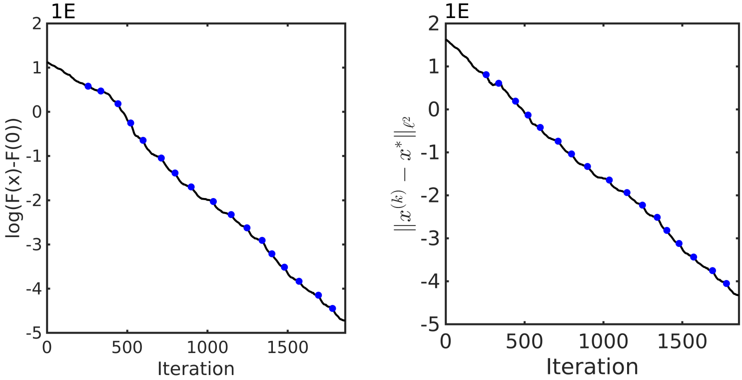
Ackley Function: 100D

- We apply HiCS to 100D Ackley with constant $\rho_0 = 2$. The initial value is randomly generated in $[-10, 10]^{100}$. $m_{\max} = 32$.

Iter.	ℓ^2-distance	Fun. Val.
1 (1-353)	43.76984 $\downarrow$ 5.67057	13.40276 $\downarrow$ 3.65003
3	5.76768	3.64961
5	5.84103	3.64579
5	5.75717	3.63706
1	5.72732	3.63154
1	5.68106	3.63021
6	5.67458	3.60655
12	5.76181	3.60569
5	5.84496	3.59674
1	5.76528	3.59377
1	5.71754	3.59277
2	5.90908	3.59054
32 (m_{max})	5.93767	3.58252

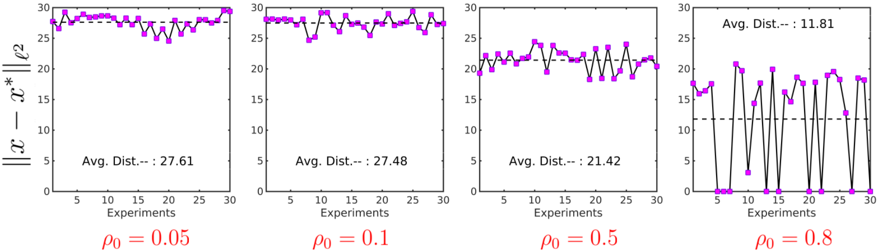
Ackley Function: 100D

- We can continue to apply AHiCS ($\eta = 0.5$) to 100D Ackley.



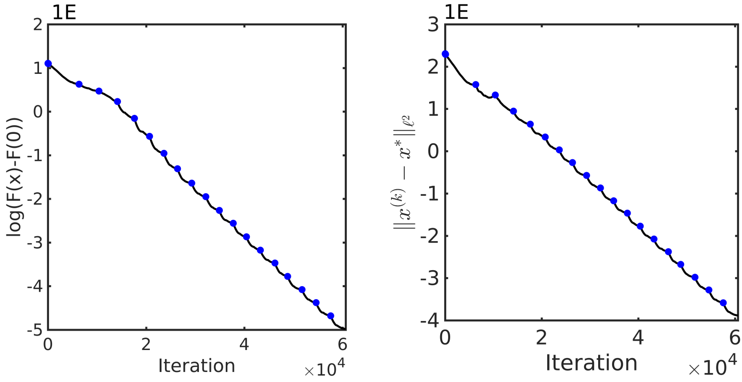
Ackley Function: 100D

- AHiCS can capture different minima with different ρ_0.
- Setup: x_0 is randomly generated in $[-5,5]^{100}$, $m_{\max} = 32$, $\eta = 0.5$ and $\rho < 10^{-14}$.
- x^* is the global minimizer.



Ackley Function: 2500D

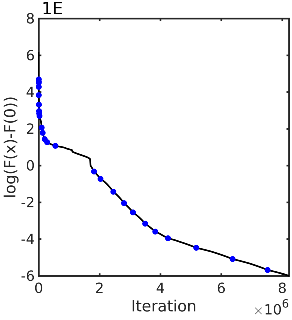
- Apply AHiCS algorithm ($\eta = 0.5$) to 2500D Ackley function with random initial value in $[-10, 10]^{2500}$ and $\rho_0 = 3.5$, $m_{max} = 16$.

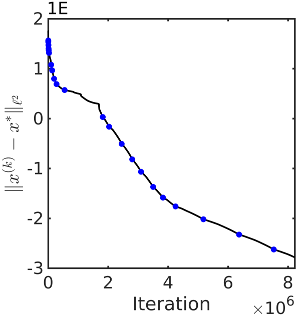


Woods Function (CUTE)

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

The global minimizer is $(1, 1, \ldots, 1)$ with $f = 0$. The initial value $x_j^{(0)} = -3.0$ if j is even, and $x_j^{(0)} = -1.0$ if j odd. We apply AHiCS algorithm to 320D Woods functions with $\rho_0 = 5$ and $m_{\max} = 8$.

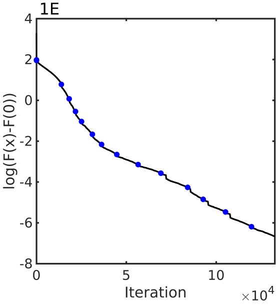


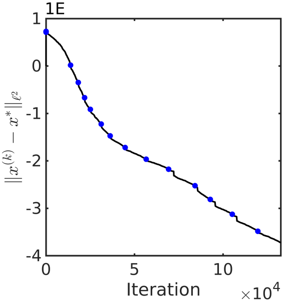


ARWHEAD Function

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

The least value of F is zero, which occurs when the variables take the values $x_j = 1$, $j = 1, 2, \dots, n-1$ and $x_n = 0$. We apply AHiCS method ($\eta = 0.5$) to 640D ARWHEAD function. The starting vector is given by $x_j^{(0)} = 1$, $j = 1, 2, \dots, n$, as Powell (2006) done. The search radius $\rho_0 = 3$ and $m_{\max} = 32$.

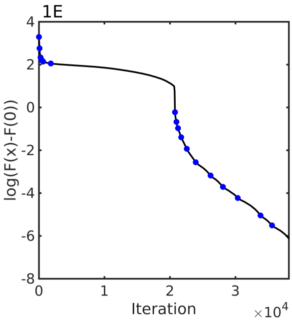


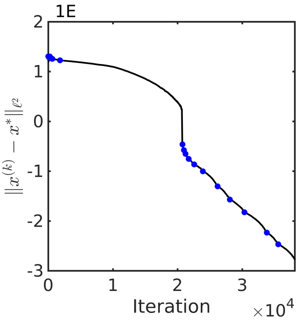


CHROSEN Function

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

The least value of F is zero, which occurs when the variables take the values $x_j = 1$, $j = 1, 2, \ldots, n$. We apply AHiCS method ($\eta = 0.5$) to 100D CHROSEN function. The starting vector is given by $x_j^{(0)} = -1$, $j = 1, 2, \ldots, n$, as Powell (2006) done. The search radius $\rho_0 = 5$ and $m_{\max} = 32$.





Outline

Summary

- Propose a Hill-Climbing method with a Stick (**HiCS**)
- Theory: Finite-step convergence
- An efficient method of obtaining $O_h(x_k, \rho)$: Simplex
- Be able to implement to high dimension optimization
- Other properties:
  - Only one parameter ρ
  - Capture the neighborhood of a minimizer
  - Has potential to approximate the global minimizer

Thanks for Your Attention !