Non-convergence Analysis of Probabilistic Direct Search

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Graduate Student Forum of ORSC Mathematical Programming Branch Chongqing, China, 2023

Department of Applied Mathematics The Hong Kong Polytechnic University 1. Preliminaries

What is derivative-free optimization and why Probabilistic direct search

- 2. Non-convergence analysis Motivation and basic idea Main results
- 3. Tightness of analysis
 - Almost zero gap
 - Tightness of assumptions
- 4. Conclusions

Preliminaries

Derivative-free optimization (DFO)

- \cdot A branch of optimization
- Do not use derivatives (only use function evaluations)

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- Problems are often noisy (finite difference?)
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Typical situation: black box $x \in \mathbb{R}^n \longrightarrow f: \mathbb{R}^n \to \mathbb{R} \longrightarrow f(x)$

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Nuclear Physics



Machine Learning



Cosmology

In this talk, we consider the unconstrained problem

 $\min_{x \in \mathbb{R}^n} f(x),$

where

- + ∇f is Lipschitz continuous, although it cannot be evaluated,
- \cdot f is bounded below.

Input: $x_0 \in \mathbb{R}^n$, $\alpha_0 \in (0, \infty)$, $0 < \theta < 1 < \gamma$.

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Input: x_0 \in \mathbb{R}^n, \alpha_0 \in (0, \infty), 0 < \theta < 1 < \gamma.
for k = 0, 1, \dots do
Select a finite set D_k \subset \mathbb{R}^n randomly.
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for k = 0, 1, ... do
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(In this talk, assume D_k is a set of unit vectors for simplicity.)
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Input: x_0 \in \mathbb{R}^n, \alpha_0 \in (0, \infty), 0 < \theta < 1 < \gamma.
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for k = 0, 1, ... do
Select a finite set D_k \subset \mathbb{R}^n randomly.
(In this talk, assume D_k is a set of unit vectors for simplicity.)
if f(x_k + \alpha_k d) < f(x_k) - \alpha_k^2 for some d \in D_k then
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if f(x_k + \alpha_k d) < f(x_k) - \alpha_k^2 for some d \in D_k then

Expand step size, and move to that point

Set \alpha_{k+1} = \gamma \alpha_k and x_{k+1} = x_k + \alpha_k d.

else

Shrink step size, and stand still
```

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Input: x_0 \in \mathbb{R}^n, \alpha_0 \in (0, \infty), 0 < \theta < 1 < \gamma.
for k = 0, 1, ... do
    Select a finite set D_k \subset \mathbb{R}^n randomly. How to select?
    (In this talk, assume D_k is a set of unit vectors for simplicity.)
    if f(x_k + \alpha_k d) < f(x_k) - \alpha_k^2 for some d \in D_k then
         Expand step size, and move to that point
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    else
         Shrink step size, and stand still
        Set \alpha_{k+1} = \theta \alpha_k and x_{k+1} = x_k.
```

Typical choice: $D_k = \{d_1, \ldots, d_m\}$, where $d_i \stackrel{\text{i.i.d.}}{\sim} \text{Unif}(\mathcal{S}^{n-1})$



























Convergence theory

Definition (Cosine measure)

Cosine measure for a finite set of nonzero vectors $D \subseteq \mathbb{R}^n$ w.r.t. a given vector $v \in \mathbb{R}^n$:

$$\operatorname{cm}(D, v) = \max_{d \in D} \frac{d^{\top} v}{\|d\| \|v\|}.$$

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Example



Measure the ability that "D approximates v"
Convergence theory

Definition (*p*-probabilistically κ-descent)

 $(D_k)_{k\geq 0}$ is said to be p-probabilistically κ -descent, if

 $\mathbb{P}\left(\operatorname{cm}(D_k,-g_k)\geq\kappa\mid D_0,\ldots,D_{k-1}\right)\ \geq\ p\quad\text{for each }k\geq0,$

where $g_k = \nabla f(x_k)$.

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Theorem (Gratton et al. 2015)

If $(D_k)_{k\geq 0}$ is *p*-probabilistically κ -descent with $\kappa > 0$ and

 $p = \log \theta / \log(\gamma^{-1}\theta),$

then PDS converges with probability 1.

Corollary (Gratton et al. 2015) If $D_k = \{d_1, \dots, d_m\}$, where $d_i \stackrel{i.i.d.}{\sim} Unif(S^{n-1})$, then PDS is convergent if $m > \log_2\left(1 - \frac{\log \theta}{\log \gamma}\right)$.

Corollary (Gratton et al. 2015)

If $D_k = \{d_1, \dots, d_m\}$, where $d_i \stackrel{i.i.d.}{\sim} \text{Unif}(S^{n-1})$, then PDS is convergent if $m > \log_2\left(1 - \frac{\log \theta}{\log \gamma}\right)$.

A natural question: what if

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Non-convergence analysis

Many well-known algorithms have non-convergence analysis.

- S. Reddi, S. Kale, and S. Kumar. On the convergence of Adam and beyond. In Y. Bengio, Y. LeCun, T. Sainath, I. Murray, M. Ranzato, and O. Vinyals, editors, *International Conference on Learning Representations (ICLR 2018)*. Curran Associates, Inc., 2018.
- C. Chen, B. He, Y. Ye, and X. Yuan. The direct extension of ADMM for multi-block convex minimization problems is not necessarily convergent. *Math. Program.*, 155:57-79, 2016.
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Recall *p*-probabilistically κ -descent:

 $\mathbb{P}\left(\operatorname{cm}\left(D_{k},-g_{k}\right)\geq\kappa\mid D_{0},\ldots,D_{k-1}\right)\geq p\quad\text{for each }k\geq0.$

Recall *p*-probabilistically κ -descent:

 $\mathbb{P}\left(\operatorname{cm}\left(D_{k},-g_{k}\right)\geq\kappa\mid D_{0},\ldots,D_{k-1}\right)\geq p\quad\text{for each }k\geq0.$

q-probabilistically ascent

 $\mathbb{P}\left(\operatorname{cm}\left(D_{k},-g_{k}\right)>0\mid D_{0},\ldots,D_{k-1}\right) \leq q \quad \text{for each } k\geq 0.$

q-probabilistically ascent

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 $(D_k)_{k\in\mathbb{N}} \text{ is } \\ q\text{-probabilistically ascent}$

 $(D_k)_{k\in\mathbb{N}} \text{ is } \\ q\text{-probabilistically ascent} \\ \clubsuit \\ \alpha_k \text{ shrinks with high probability} \\$







• Define indicator function $Y_k = \mathbb{1}_{\{\operatorname{cm}(D_k, -g_k) > 0\}}$ Indicator for "good" event

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$$\alpha_k \leq \alpha_0 \prod_{i=0}^{k-1} \gamma^{Y_i} \theta^{1-Y_i} =: \alpha_0 U_k$$

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• $\sum_{k=1}^{\infty} \alpha_k \le \alpha_0 \sum_{k=1}^{\infty} U_k$

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$$\alpha_k \leq \alpha_0 \prod_{i=0}^{k-1} \gamma^{Y_i} \theta^{1-Y_i} =: \alpha_0 U_k$$

• $\sum_{k=1}^{\infty} \alpha_k \leq \alpha_0 \sum_{k=1}^{\infty} U_k < \infty$ a.s. ?

Key to analysis

- Define indicator function $Y_k = \mathbb{1}_{\{\operatorname{cm}(D_k, -g_k) > 0\}}$ Indicator for "good" event
- $\alpha_{k+1} \leq \gamma^{Y_k} \theta^{1-Y_k} \alpha_k$, when f is convex k-1

•
$$\alpha_k \leq \alpha_0 \prod_{i=0}^{K} \gamma^{Y_i} \theta^{1-Y_i} =: \alpha_0 U_k$$

•
$$\sum_{k=1}^{\infty} \alpha_k \leq \alpha_0 \sum_{k=1}^{\infty} U_k < \infty$$
 a.s. ?

Under q-probabilistically ascent assumption, can we find a constant ζ such that

$$\mathbb{P}\left(\sum_{k=1}^{\infty} U_k < \zeta\right) > 0?$$

Assumption

 $\mathbb{P}\left(\operatorname{cm}\left(D_{k}, -g_{k}\right) \leq 0 \mid D_{0}, \dots, D_{k-1}\right) \geq q > q_{0} \quad \text{for each } k \geq 0,$ where $q_{0} = 1 - p_{0} = \log \gamma / \log(\theta^{-1}\gamma).$

Assumption

 $\mathbb{P}\left(Y_k = 0 \mid Y_0, \dots, Y_{k-1}\right) \ge q > q_0 \quad \text{for each } k \ge 0,$ where $q_0 = 1 - p_0 = \log \gamma / \log(\theta^{-1}\gamma).$

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Result

 $\mathbb{P}\left(\sum_{k=1}^{\infty} U_k < \infty\right) = 1$

 $\mathbb{P}\left(\sum_{k=1}^{\infty} U_k < \zeta\right) > 0 \quad \Longleftrightarrow \quad \zeta > \frac{\theta}{1-\theta}$

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Ζ		
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1.

Assumption

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Result

1.

$$\mathbb{P}\left(\sum_{k=1}^{\infty} U_k < \infty\right) = 1$$

2.

$$\mathbb{P}\left(\sum_{k=1}^{\infty} U_k < \zeta\right) > 0 \quad \Longleftrightarrow \quad \zeta > \frac{\theta}{1-\theta}$$

Note that
$$\sum_{k=1}^{\infty} U_k = \sum_{k=1}^{\infty} \prod_{i=0}^{k-1} \gamma^{Y_i} \theta^{1-Y_i} \ge \theta/(1-\theta)$$

Assumption

$$\mathbb{P}\left(Y_k = 0 \mid Y_0, \dots, Y_{k-1}\right) \geq q > q_0 \quad \text{for each } k \geq 0,$$

where $q_0 = 1 - p_0 = \log \gamma / \log(\theta^{-1} \gamma)$.

Result 1. $\mathbb{P}\left(\sum_{k=1}^{\infty} U_k < \infty\right) = 1$ 2. $\mathbb{P}\left(\sum_{k=1}^{\infty} U_k < \zeta\right) > 0 \iff \zeta > \frac{\theta}{1-\theta}$

Assumption

$$\liminf_{k \to \infty} \mathbb{P}\left(Y_k = 0 \mid Y_0, \dots, Y_{k-1}\right) > q_0,$$

where $q_0 = 1 - p_0 = \log \gamma / \log(\theta^{-1}\gamma)$.

Result

1.

$$\mathbb{P}\left(\sum_{k=1}^{\infty} U_k < \infty\right) = 1$$

2.



Tightness of analysis

Let $D_k = \{d_1, \ldots, d_m\}$, where $d_i \stackrel{\text{i.i.d.}}{\sim} \text{Unif}(\mathcal{S}^{n-1})$. Recall that PDS is convergent if

$$m > \log_2\left(1 - \frac{\log\theta}{\log\gamma}\right).$$

Let $D_k = \{d_1, \ldots, d_m\}$, where $d_i \stackrel{\text{i.i.d.}}{\sim} \text{Unif}(\mathcal{S}^{n-1})$. Recall that PDS is convergent if

$$m > \log_2\left(1 - \frac{\log \theta}{\log \gamma}\right).$$

With our non-convergence analysis, PDS is non-convergent if

$$m < \log_2\left(1 - \frac{\log\theta}{\log\gamma}\right).$$

Tightness of assumption

Natural question:

$$\mathbb{P}\left(\operatorname{cm}\left(D_{k},-g_{k}\right)\leq0\mid D_{0},\ldots,D_{k-1}\right)\geq q \geq q_{0},$$

Tightness of assumption

Natural question:

 $\mathbb{P}\left(\operatorname{cm}\left(D_k,-g_k\right) \leq 0 \mid D_0,\ldots,D_{k-1}\right) \geq q \ge q_0,$ Answer: NO

Tightness of assumption

Natural question:

 $\mathbb{P}\left(\operatorname{cm}\left(D_{k},-g_{k}\right)\leq0\mid D_{0},\ldots,D_{k-1}\right)\geq q\nearrow\geq q_{0},$ Answer: NO

Example

We assume

- $\cdot \ f: \mathbb{R}^n \rightarrow \mathbb{R}$ be gradient Lipschitz and strongly convex,
- + heta=1/2 and $\gamma=2$, $\Rightarrow q_0=1/2$
- $D_k = \{g_k / ||g_k||\}$ or $D_k = \{-g_k / ||g_k||\}$ with probability 1/2, respectively,

then we have

$$\mathbb{P}\left(\lim_{k \to \infty} \|g_k\| = 0\right) = 1.$$

Conclusions
In this talk

- Non-convergence analysis for probabilistic direct search
- Tightness of non-convergence analysis

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Future work

- Estimate the non-convergence probability
- Conduct non-convergence analysis for other frameworks

Thank you!

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