Non-convergence Analysis of Probabilistic Direct Search

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Preliminaries

What is derivative-free optimization and why

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Typical situation: black box

$$x \in \mathbb{R}^n \longrightarrow \boxed{f : \mathbb{R}^n \to \mathbb{R}} \longrightarrow f(x)$$

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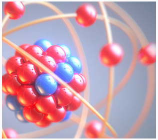

Nuclear Physics

Machine Learning

Cosmology

Basic assumptions

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,
- f is bounded below.

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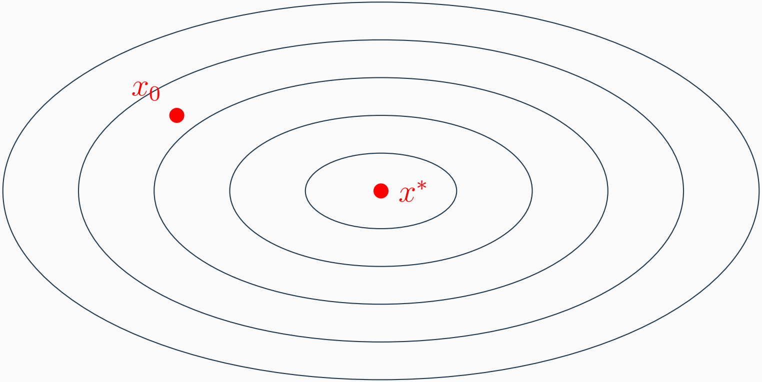
Typical choice: $D_k = \{d_1, \ldots, d_m\}$, where $d_i \overset{\text{i.i.d.}}{\sim} \text{Unif}(\mathcal{S}^{n-1})$

Illustration of how PDS works



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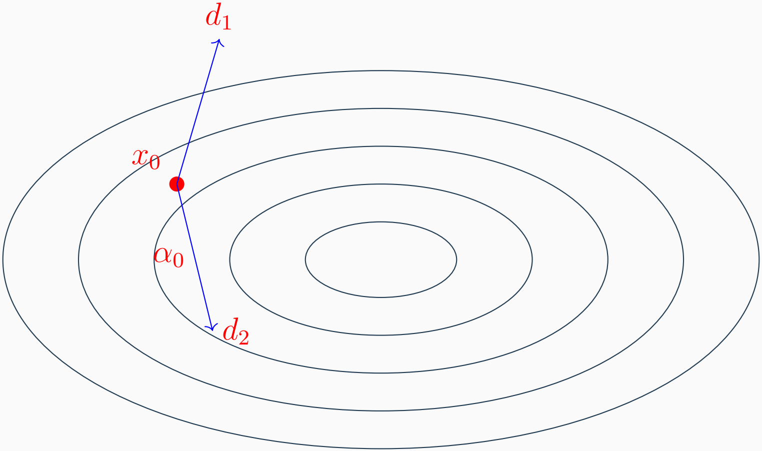

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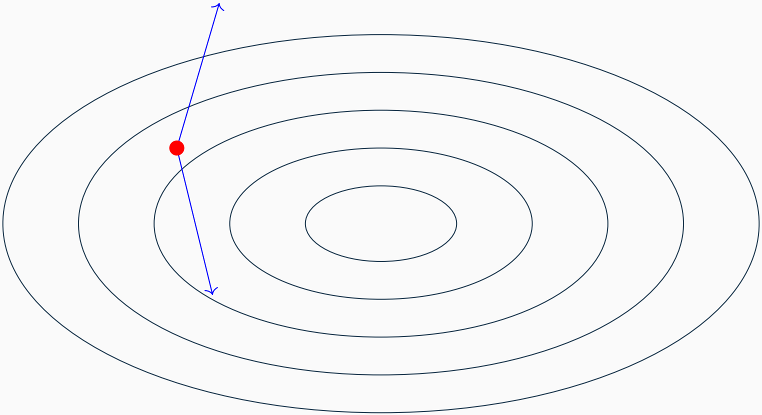

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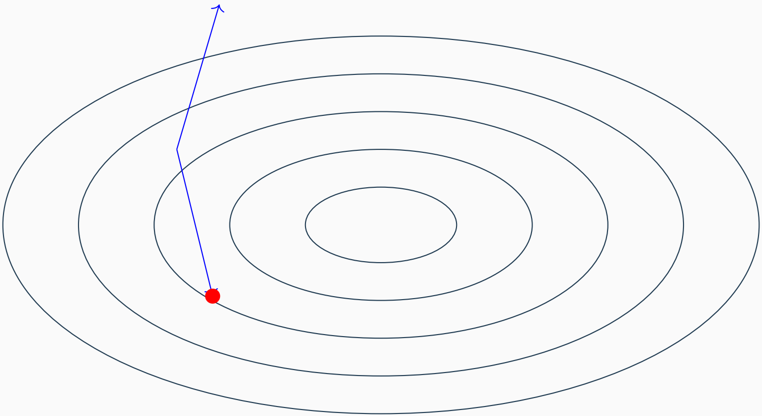

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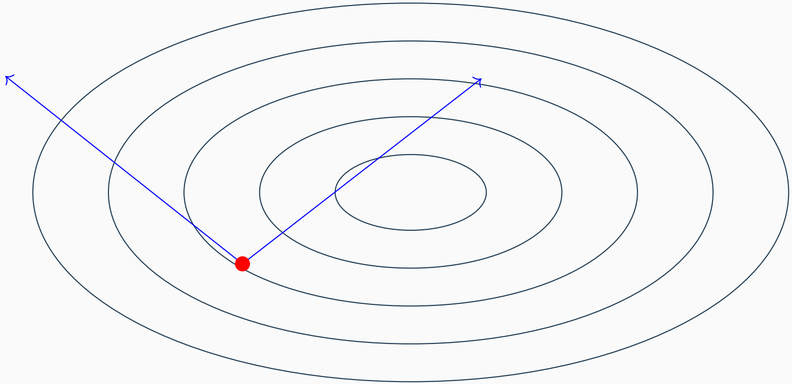

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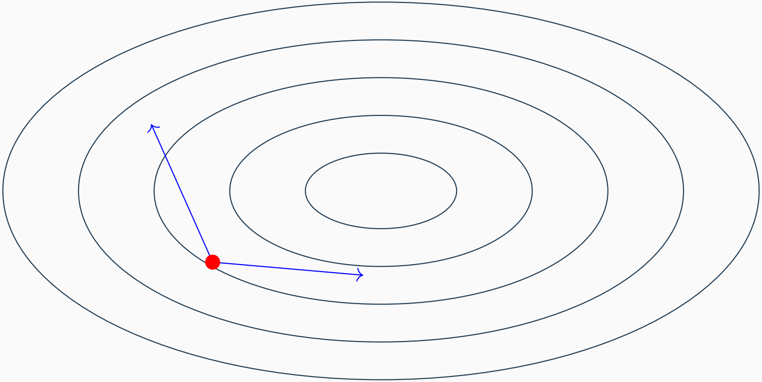

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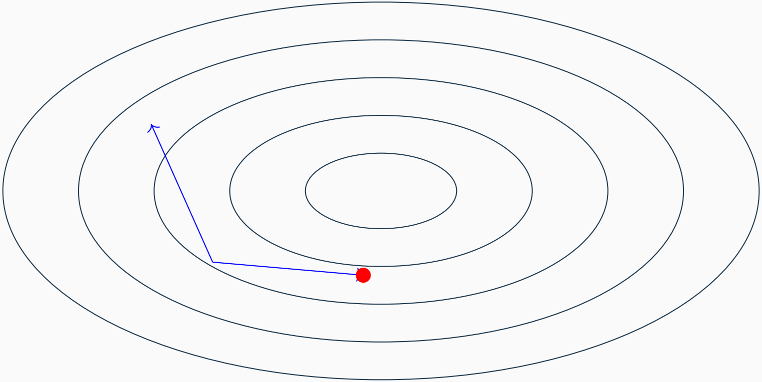

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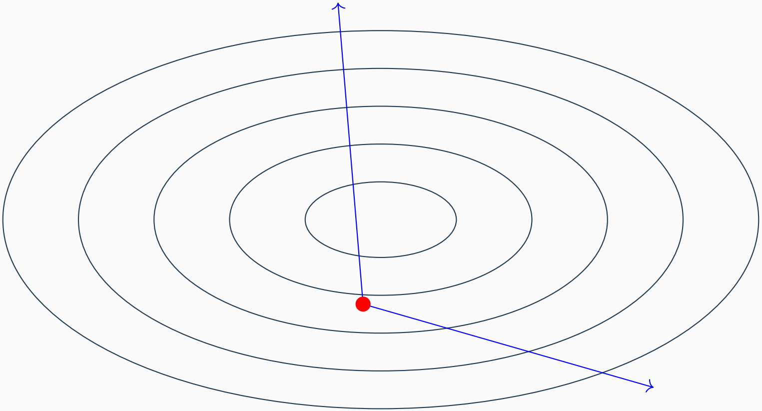

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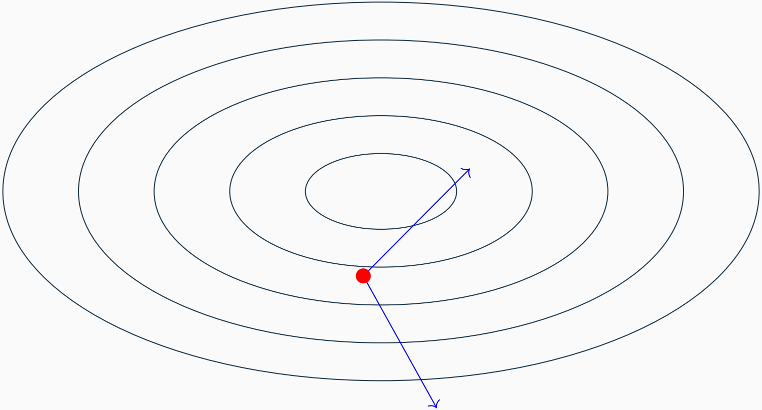

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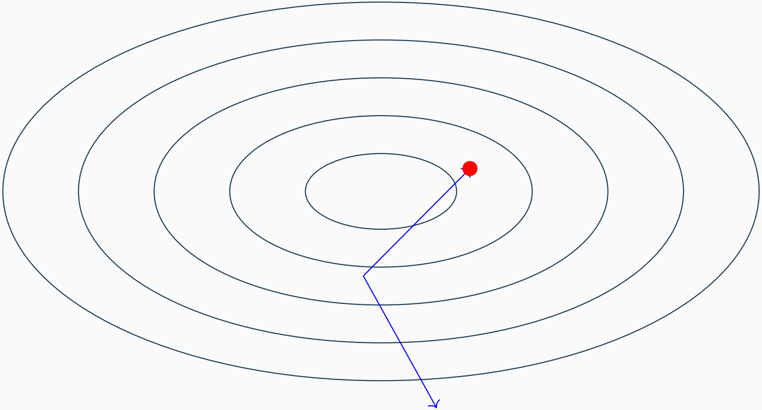

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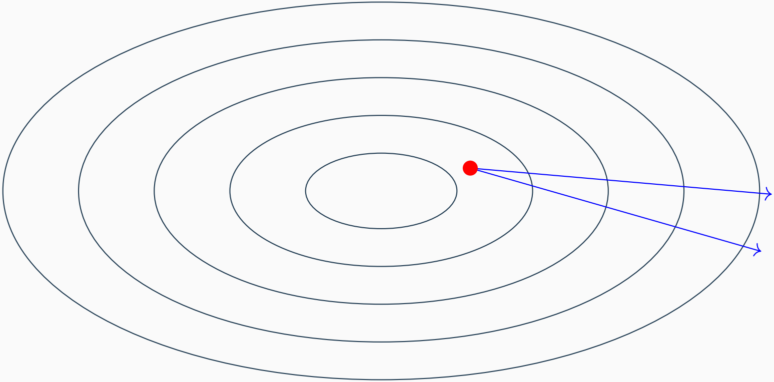

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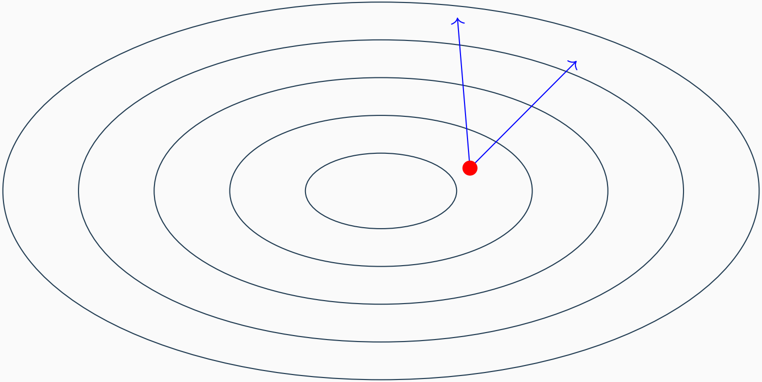

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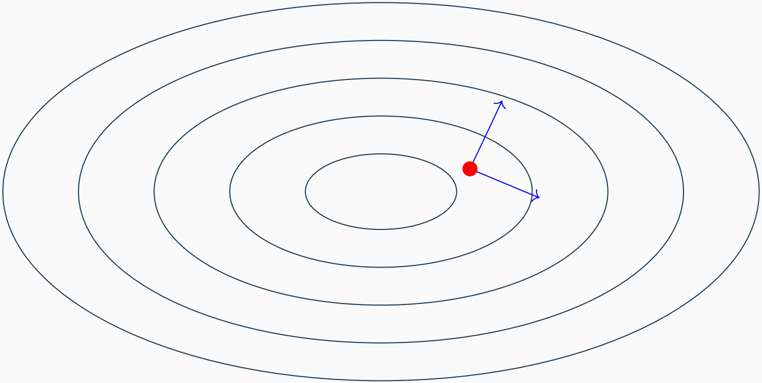

Definition (Cosine measure)

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

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

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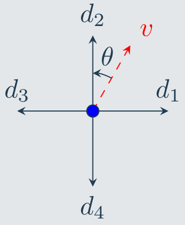
Example

$$\mathrm{cm}(D, v) \;=\; \cos\theta$$



Convergence theory

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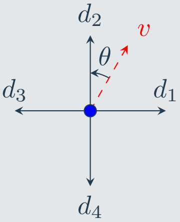

Measure the ability that "D approximates v"

Convergence theory

Definition (p-probabilistically κ-descent)

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

$$\mathbb{P}\left(\mathrm{cm}(D_k, -g_k) \geq \kappa \mid D_0, \ldots, D_{k-1}\right) \;\geq\; p \quad \text{for each } k \geq 0,$$

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.

Practical choice and natural question

Corollary (Gratton et al. 2015)

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

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

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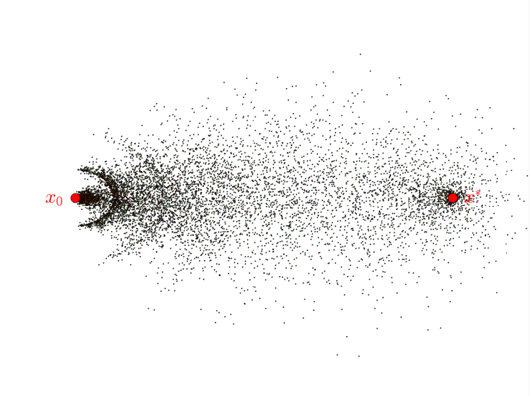

Non-convergence analysis

Motivation: non-convergence analysis matters

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.
- W. Mascarenhas. The divergence of the BFGS and Gauss Newton methods. *Math. Program.*, 147:253-276, 2014.
- ...

Naive idea of non-convergence

Recall p-probabilistically κ-descent:

$$\mathbb{P}\left(\mathrm{cm}\left(D_k, -g_k\right) \geq \kappa \mid D_0, \ldots, D_{k-1}\right) \geq p \quad \text{for each } k \geq 0.$$

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q-probabilistically ascent

$$\mathbb{P}\left(\mathrm{cm}\left(D_k, -g_k\right) > 0 \mid D_0, \ldots, D_{k-1}\right) \leq q \quad \text{for each } k \geq 0.$$

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$$\mathrm{cm}\left(D_k, -g_k\right) \leq 0 \longrightarrow \text{No descent direction}$$

$$\text{No descent direction} \xrightarrow{f \text{ convex}} f(x_k + \alpha_k d_k) \geq f(x_k) \; \forall d_k \in D_k$$

$$f(x_k + \alpha_k d_k) \geq f(x_k) \; \forall d_k \in D_k \longrightarrow \alpha_k \text{ shrinks}$$

Naive idea of non-convergence

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$$\begin{tikzcd}
 & \operatorname{cm}\left(D_k, -g_k\right) \leq 0 \arrow[r] & \text{No descent direction} \arrow[d, "f \text{ convex}"] \\
\alpha_k \text{ shrinks} & & f(x_k + \alpha_k d_k) \geq f(x_k)\ \forall d_k \in D_k \arrow[ll]
\end{tikzcd}$$

non-convergence for convex functions

$\Downarrow$

non-convergence in general

Establishment of non-convergence

$(D_k)_{k\in\mathbb{N}}$ is
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$$x_0 \; \notin \; \bar{\mathcal{B}}(x^*, \textstyle\sum_{k=0}^{\infty} \alpha_k)$$

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$\mathbb{P}\,$(Convergence) $\;<\; 1$

Key to analysis

- Define indicator function $Y_k = \mathbb{1}_{\{\mathrm{cm}(D_k, -g_k) > 0\}}$
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- $\sum_{k=1}^{\infty} \alpha_k \leq \alpha_0 \sum_{k=1}^{\infty} U_k$

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

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- $\alpha_k \le \alpha_0 \prod_{i=0}^{k-1} \gamma^{Y_i}\theta^{1-Y_i} =: \alpha_0 U_k$
- $\sum_{k=1}^{\infty} \alpha_k \le \alpha_0 \sum_{k=1}^{\infty} U_k < \infty$ a.s. ?

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

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

Main results

Assumption

$$\mathbb{P}\left(\mathrm{cm}\left(D_k, -g_k\right) \le 0 \mid D_0, \ldots, D_{k-1}\right) \;\ge\; q \;>\; q_0 \quad \text{for each } k \ge 0,$$

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

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Result

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

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

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Assumption

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

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

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

Main results

Assumption

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

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

Main results

Assumption

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

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

Result

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

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Tightness of analysis

Almost zero gap

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

Recall that PDS is convergent if

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

Almost zero gap

Let $D_k = \{d_1, \ldots, d_m\}$, where $d_i \overset{\text{i.i.d.}}{\sim}$ 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:

$$\mathbb{P}\left(\mathrm{cm}\left(D_k, -g_k\right) \leq 0 \mid D_0, \ldots, D_{k-1}\right) \;\geq\; q \cancel{>} \geq q_0,$$

Tightness of assumption

Natural question:

$$\mathbb{P}\left(\mathrm{cm}\left(D_k, -g_k\right) \leq 0 \mid D_0, \ldots, D_{k-1}\right) \;\geq\; q \cancel{>} \geq q_0,$$

Answer: NO

Tightness of assumption

Natural question:

$$\mathbb{P}\left(\mathrm{cm}\left(D_k, -g_k\right) \leq 0 \mid D_0, \ldots, D_{k-1}\right) \; \geq \; q \cancel{>} \geq q_0,$$

Answer: NO

Example

We assume

- $f : \mathbb{R}^n \to \mathbb{R}$ be gradient Lipschitz and strongly convex,
- $\theta = 1/2$ 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

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In this talk

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

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In this talk

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

Future work

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

Thank you!

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