# Non-convergence Analysis of Probabilistic Direct Search

The 25th International Symposium on Mathematical Programming

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Cunxin Huang

Joint work with Zaikun Zhang

Montréal, Canada July 26, 2024

The Hong Kong Polytechnic University

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# PRIMA and my gratitude

libprima.net

PRIMA is an acronym for

"Reference Implementation for Powell's Methods
with Modernization and Amelioration".

- Number of lines: > 100,000.
- The total time I spent on PRIMA:

$$\geq\ 3 \text{ years} \times 300 \text{ days per year} \times 10 \text{ hours per day} \ = \ 9,000 \text{ hours}.$$

In the past years, due to the gap in my publication record while working on PRIMA, I needed a lot of support from the community. **Thank you** for the help and support, explicit or implicit, known or unknown to me. Without your support, I would not have survived.

# Non-convergence analysis: What?

Consider an algorithm

$$\mathscr{A} \ : \ \Xi \times \mathbb{F} \times \mathcal{X} \to \mathcal{X}^{\infty}, \quad (\xi,\ f,\ x_0) \mapsto \{x_k\}.$$

- $\xi$ represents algorithmic parameters.
- $f$ is the objective function.
- $x_0$ is the starting point.

When $\mathscr{A}$ is deterministic:

- (Global) Convergence analysis: For all $(\xi, f, x_0) \in \hat{\Xi} \times \hat{\mathbb{F}} \times \mathcal{X}$, prove

$$\{x_k\} \text{ achieves stationarity asymptotically.}$$

- Non-convergence analysis: For all $(\xi, f, x_0) \in \tilde{\Xi} \times \tilde{\mathbb{F}} \times \tilde{\mathcal{X}}$, prove

$$\{x_k\} \text{ fails to achieve stationarity asymptotically.}$$

# Non-convergence analysis: What?

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When $\mathscr{A}$ is random:

- (Global) Convergence analysis: For all $(\xi, f, x_0) \in \hat{\Xi} \times \hat{\mathbb{F}} \times \mathcal{X}$, prove

$$\mathbb{P}\left(\{x_k\} \text{ achieves stationarity asymptotically}\right) \;=\; 1.$$

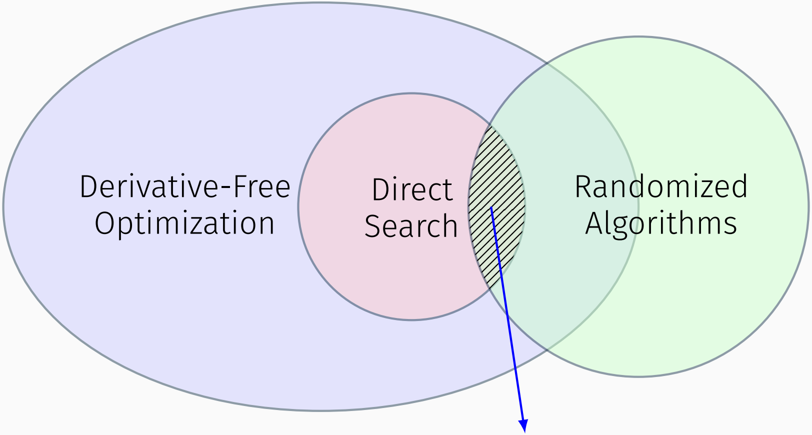
- Non-convergence analysis: For all $(\xi, f, x_0) \in \tilde{\Xi} \times \tilde{\mathbb{F}} \times \tilde{\mathcal{X}}$, prove

$$\mathbb{P}\left(\{x_k\} \text{ fails to achieve stationarity asymptotically}\right) \;>\; 0.$$

# Non-convergence analysis: Why?

- Sharpen our knowledge about the algorithm.
- Deepen our understanding about the convergence analysis.
- Guide the selection of algorithmic parameters.
- Provide new perspectives on convergence analysis.

# Probabilistic Direct Search (PDS)




The algorithm we consider in this talk:
Probabilistic Direct Search
(Gratton, Royer, Vicente, and Zhang 2015)

# Derivative-Free Optimization (DFO)

## Derivative-Free Optimization

- Do not use derivatives (first-order info.), only use function values
- Closely related: zeroth-order/black-box optimization ...

Derivatives are often not available in applications

Quantum Computing

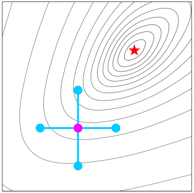

Machine Learning

Circuit Design

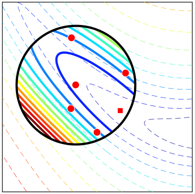
# Direct-search methods and model-based methods

How to determine iterates?

- Direct-search methods: “simple” comparison of function values
- Model-based methods: build a surrogate of the objective function



Direct-search methods[1]



Model-based methods[2]

[1]Source: Kolda, Lewis, and Torczon 2003
[2]Source: Larson, Menickelly, and Wild 2019

# PDS: a simplified framework

**Algorithm 1:** Direct Search based on sufficient decrease

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(Move and expand step size)

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Typical choice of $\{\mathcal{D}_k\}$ (GRVZ 2015): $\mathcal{D}_k = \{d_1, \ldots, d_m\}$ with $d_\ell \overset{\text{i.i.d.}}{\sim} \mathrm{U}(\mathcal{S}^{n-1})$

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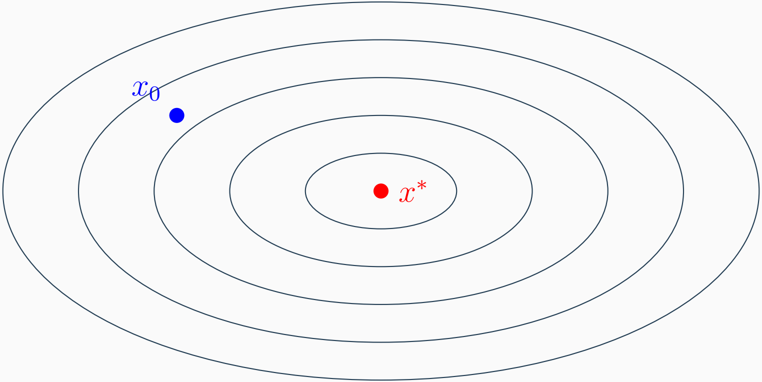
N.B.: typical choice in the deterministic case is $\{\pm e_i\}_{i=1}^n$, Coordinate Search (CS)

# Illustration of how PDS works

$\mathcal{D}_k = \{d_1, d_2\}$, where $d_\ell \overset{\text{i.i.d.}}{\sim} \mathsf{U}(\mathcal{S}^1)$



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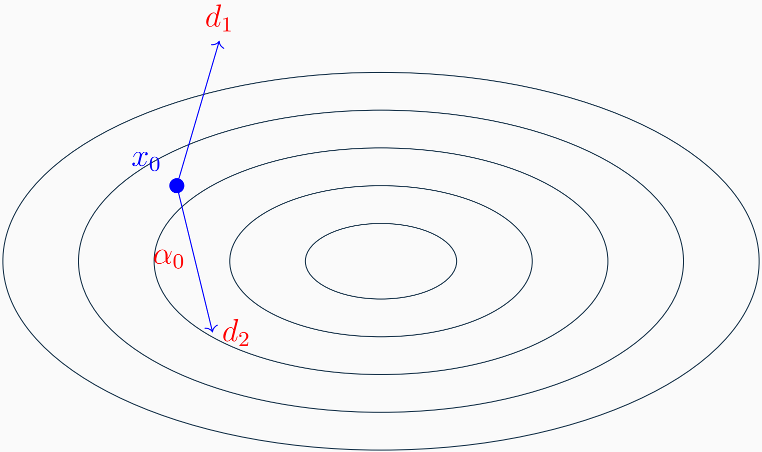

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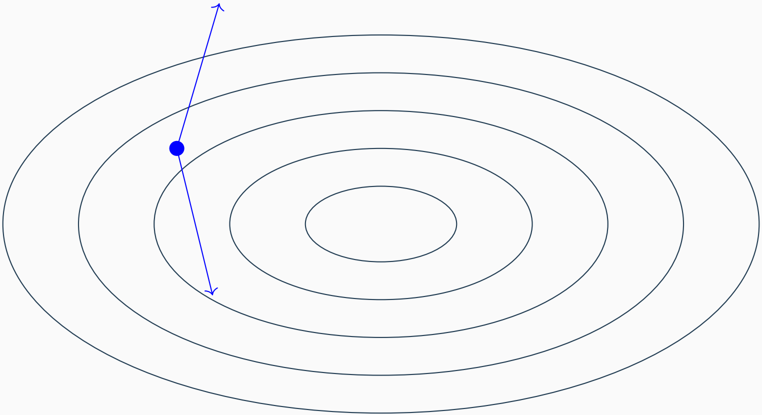

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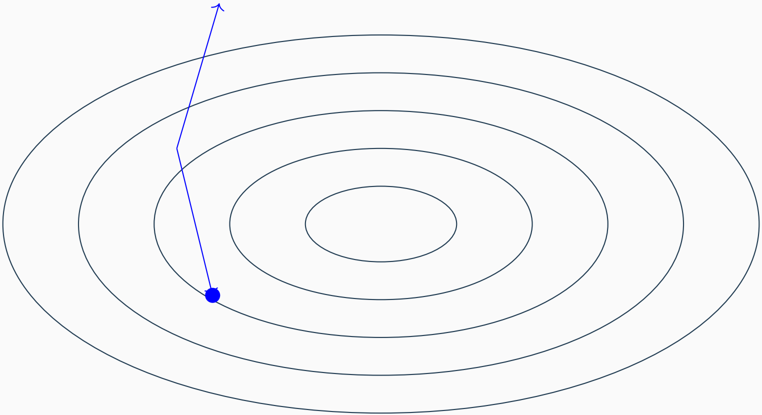

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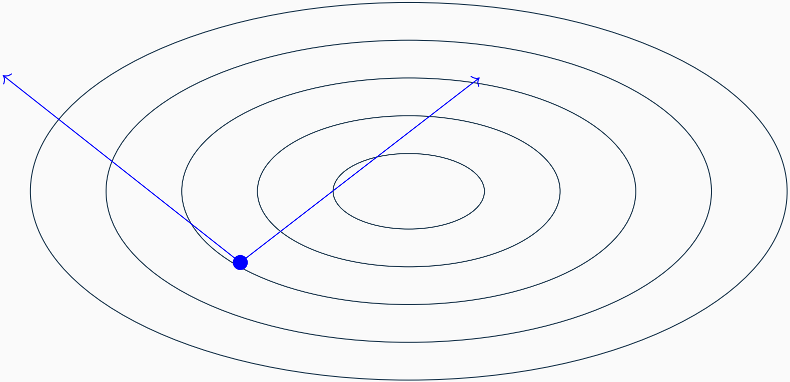

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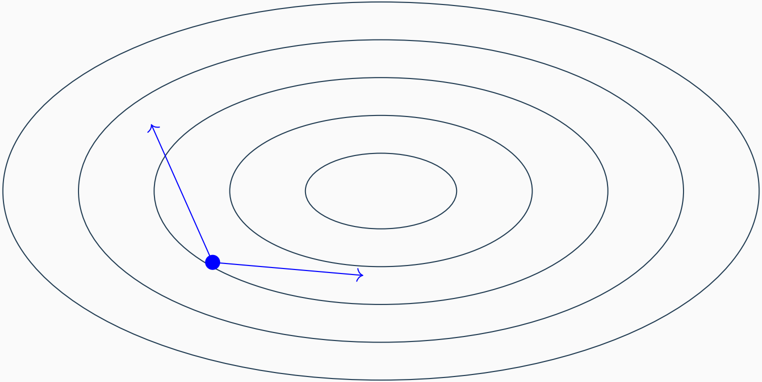

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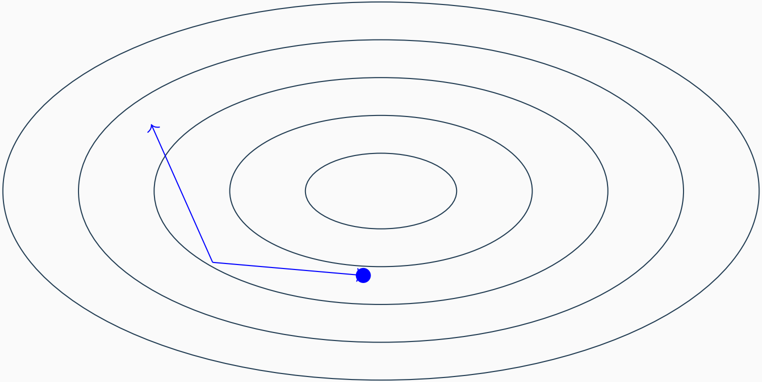

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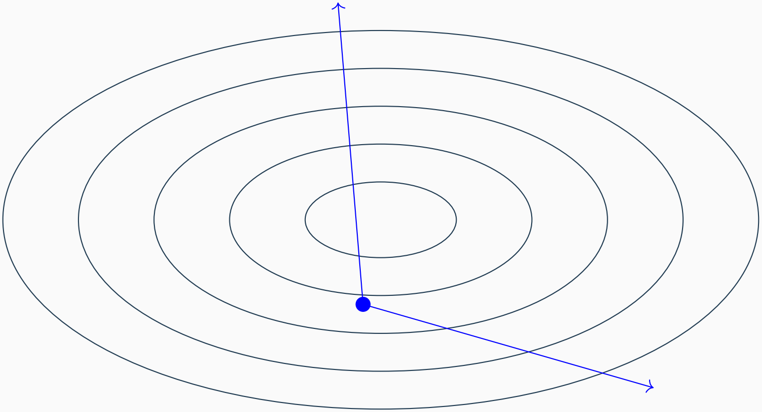

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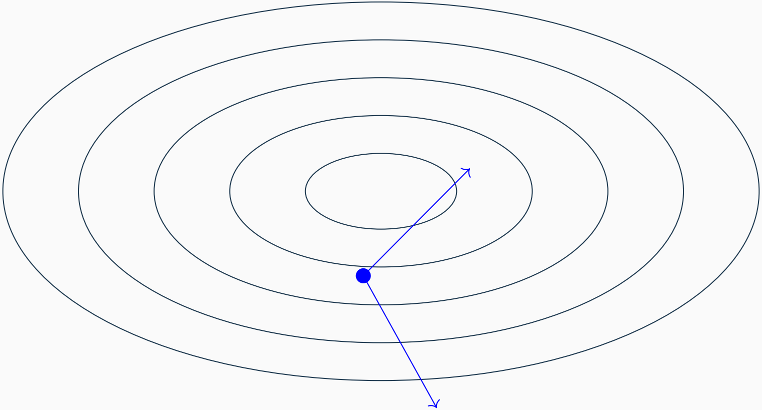

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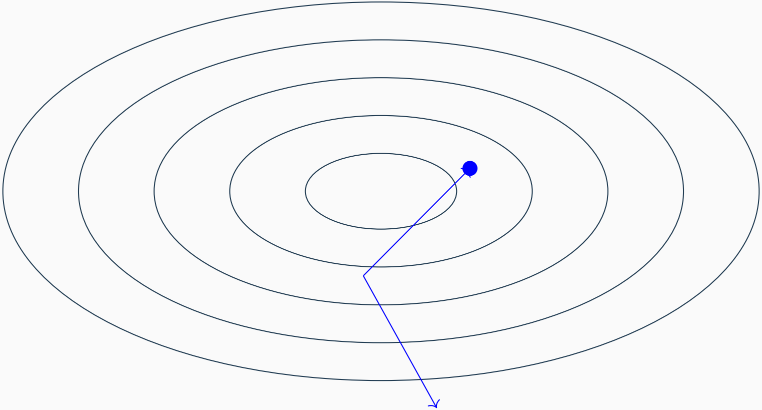

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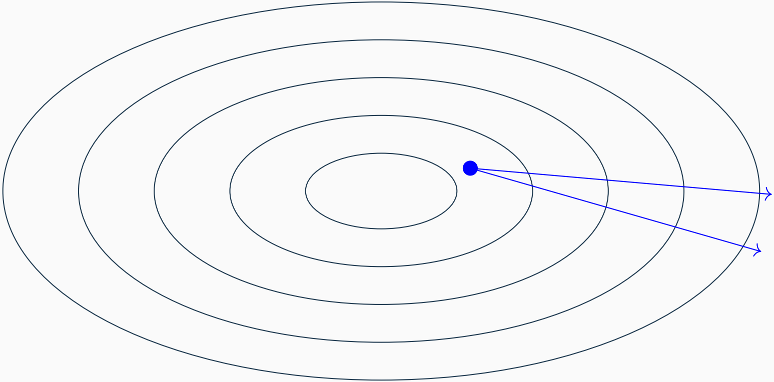

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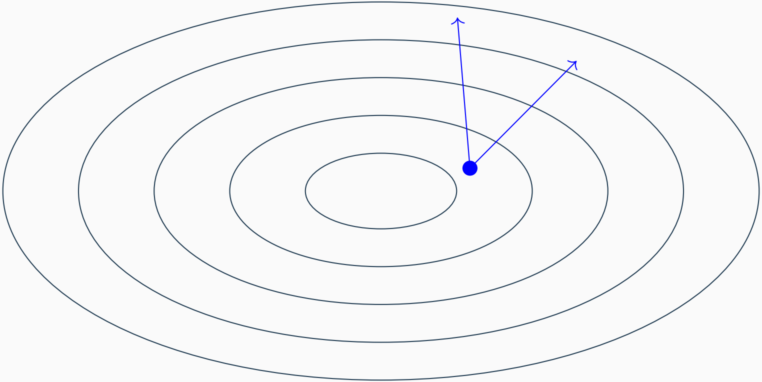

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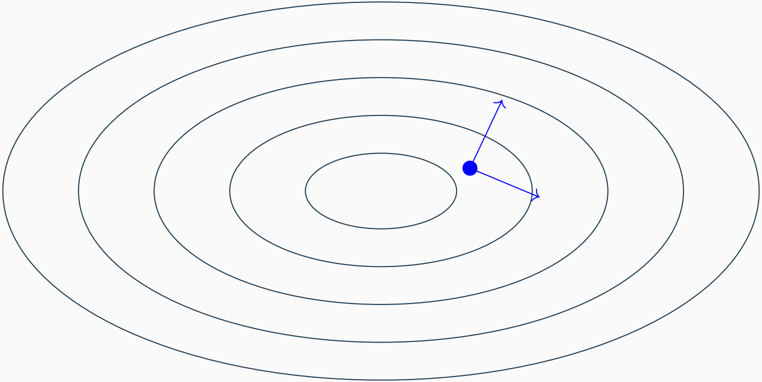
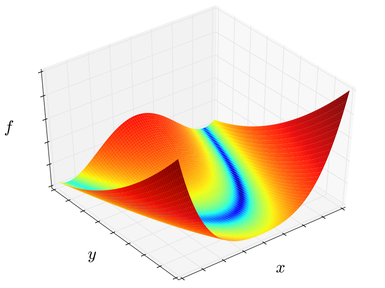
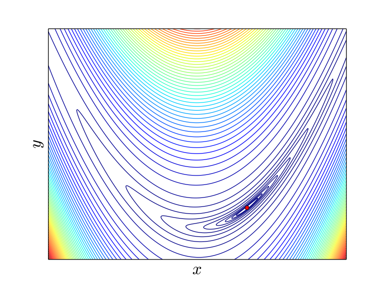


# A numerical example: CS v.s. PDS with $2$ directions

Rosenbrock "banana" function:

$$f(x) = \sum_{i=1}^{n-1} \left[(1 - x_i)^2 + 100(x_{i+1} - x_i^2)^2\right]$$



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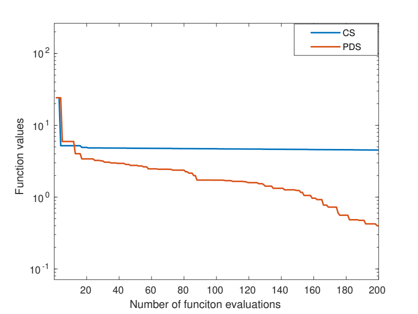
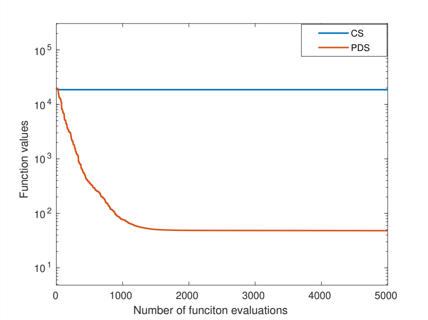



$n = 2$




$n = 50$

Function value v.s. number of function evaluations

**Worst case complexity of function evaluations** (GRVZ 2015)

$\mathcal{O}(n^2\epsilon^{-2})$ for CS while $\mathcal{O}(n\epsilon^{-2})$ for PDS

# Cosine measure

## Definition (Cosine measure w.r.t. a vector)

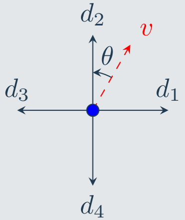
Given a finite set $\mathcal{D} \subseteq \mathbb{R}^n \setminus \{0\}$ and a vector $v \in \mathbb{R}^n \setminus \{0\}$, define

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

which is the cosine measure of $\mathcal{D}$ with respect to $v$.

## Example

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



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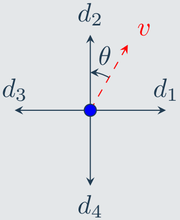


$\mathrm{cm}(\mathcal{D}, v)$ measures the ability of $\mathcal{D}$ to “approximate” $v$

# Convergence theory

## Definition ($p$-probabilistically $\kappa$-descent)

$\{\mathcal{D}_k\}$ is said to be $p$-probabilistically $\kappa$-descent, if

$$\mathbb{P}\left(\mathrm{cm}(\mathcal{D}_k, -g_k) \geq \kappa \mid \mathcal{D}_0, \ldots, \mathcal{D}_{k-1}\right) \;\geq\; p \quad \text{for each } k \geq 0,$$

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

## Intuitive meaning of $p$-probabilistically $\kappa$-descent

Each $\mathcal{D}_k$ is "good enough" with probability at least $p$
no matter what has happened in the history

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**Theorem (GRVZ 2015)**

*If $\{\mathcal{D}_k\}$ is $p_0$-probabilistically $\kappa$-descent with $\kappa > 0$ and*

$$p_0 \;=\; \frac{\log\theta}{\log(\gamma^{-1}\theta)},$$

*then PDS converges w.p.1 when $f$ is $L$-smooth and lower-bounded.*

# Practical choice and natural questions

**Corollary (GRVZ 2015)**

*If* $\mathcal{D}_k = \{d_1, \ldots, d_m\}$*, where* $d_\ell \overset{\text{i.i.d.}}{\sim} U(\mathcal{S}^{n-1})$*, then PDS converges w.p.1 if*

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

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## Questions:

- Is $p_0$-probabilistically $\kappa$-descent an essential assumption or a technical one? (Such supermartingale-like assumptions are ubiquitous in the convergence analysis of randomized methods!)
- What will happen if

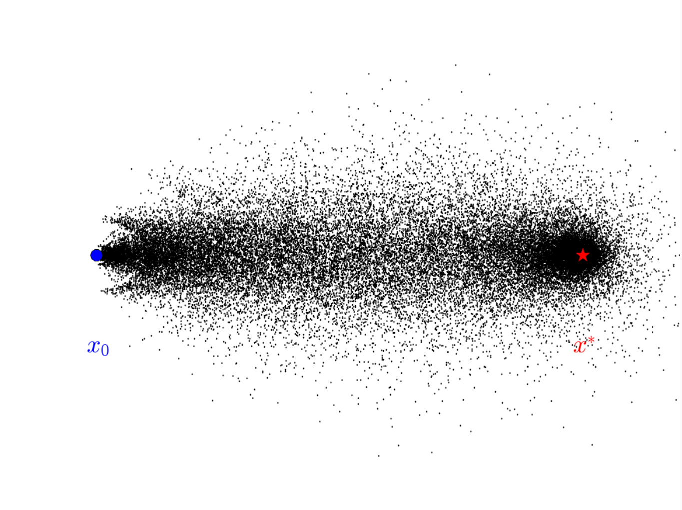
$$m \leq \log_2\left(1 - \frac{\log\theta}{\log\gamma}\right)?$$

# A simple test

- Objective function: $f(x) = x^{\mathsf{T}} x/2$
- Initial point: $x_0 = (-10, 0)^{\mathsf{T}}$
- Stopping criterion: $\alpha_k \leq$ machine epsilon
- Number of experiments: $100,000$
- Parameters of PDS: $\alpha_0 = 1$, $\theta = 0.25$, $\gamma = 1.5$, $m = 2$, which render

$$m = 2 < 2.143 \approx \log_2 \left( 1 - \frac{\log \theta}{\log \gamma} \right)$$

# A simple test (Cont'd)




Note: each **black dot** represents the **output point** of one run of PDS.

# Non-convergence study is not rare

Many well-known algorithms have non-convergence examples

- Powell, On search directions for minimization algorithms, 1973.
- Yuan, An example of non-convergence of trust region algorithms, 1998.
- Reddi, Kale, and Kumar, On the convergence of Adam and beyond, 2018.
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**Instead of finding a non-convergence example,**
**can we develop a theorem?**

# An overview of our theory

We assume that $f$ is smooth and convex (explained later).

We denote the optimal solution set of $f$ by $\mathcal{S}^*$.

We will establish the following.

Under some assumption on $\{\mathcal{D}_k\}$ and algorithmic parameters, there exist choices of $x_0$ such that

$$\mathbb{P}\left(\liminf_{k\to\infty} \operatorname{dist}(x_k, \mathcal{S}^*) > 0\right) > 0.$$

Differences from a non-convergence example:

| | | |
|---|---|---|
| one function | v.s. | some function class |
| special parameters | v.s. | conditions for parameters |
| a specific initial point | v.s. | a region for initial points |

# Assumption on $\{\mathcal{D}_k\}$: probabilistic ascent

Recall $p$-probabilistically $\kappa$-descent

$$\mathbb{P}\left(\mathrm{cm}\left(\mathcal{D}_k, -g_k\right) \geq \kappa \mid \mathcal{D}_0, \ldots, \mathcal{D}_{k-1}\right) \geq p \quad \text{for each } k \geq 0.$$

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**$q$-probabilistically ascent**

$$\mathbb{P}\left(\mathrm{cm}\left(\mathcal{D}_k, -g_k\right) \leq 0 \mid \mathcal{D}_0, \ldots, \mathcal{D}_{k-1}\right) \geq q \quad \text{for each } k \geq 0.$$

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**Note**

If $\mathrm{cm}\left(\mathcal{D}_k, -g_k\right) \leq 0$, then $\mathcal{D}_k$ is "bad" (no descent direction).

# Why assuming convexity?

$$\begin{tikzcd}
\operatorname{cm}(\mathcal{D}_k, -g_k) \le 0 \arrow[r] & \text{No descent direction} \arrow[d, "f \text{ convex}"] \\
\alpha_k \text{ shrinks} & f(x_k + \alpha_k d) \ge f(x_k)\ \forall d \in \mathcal{D}_k \arrow[l]
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- Convexity connects $\operatorname{cm}\left(\mathcal{D}_k, -g_k\right) \le 0$ and shrinking of step size
- $\{\mathcal{D}_k\}$ is probabilistic ascent implies $\alpha_k$ “often” shrinks

# From probabilistic ascent to non-convergence: How?

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$\Downarrow$

$\mathbb{P}\,(\text{non-convergence}) > 0$ if $\mathrm{dist}(x_0, \mathcal{S}^*)$ is "large"?

## Key ingredients of the analysis

- Define the indicator function for "bad $\mathcal{D}_k$":

$$Y_k = \mathbb{1}(\mathrm{cm}\left(\mathcal{D}_k, -g_k\right) \leq 0)$$

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$$\alpha_{k+1} \;\le\; \begin{cases} \gamma\alpha_k, & \text{if } Y_k = 0 \\ \theta\alpha_k, & \text{if } Y_k = 1 \end{cases} \;=\; \gamma^{1-Y_k}\theta^{Y_k}\alpha_k$$

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- Get an upper bound of the series of step sizes:

$$\sum_{k=1}^{\infty} \alpha_k \le \alpha_0 \sum_{k=1}^{\infty} \prod_{\ell=0}^{k-1} \gamma^{1-Y_\ell}\theta^{Y_\ell} =: \alpha_0 S$$

- Analyze the behavior of the random series $S$

# A closer look at the random series $S$

Recall that

$$S = \sum_{k=1}^{\infty} \prod_{\ell=0}^{k-1} \gamma^{1-Y_\ell} \theta^{Y_\ell},$$

where $Y_\ell = \mathbb{1}(\mathrm{cm}\,(\mathcal{D}_\ell, -g_\ell) \leq 0)$.

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## Two questions

- (Q1) Does there exist a constant $\zeta$ such that

$$\mathbb{P}\,(S < \zeta) \;>\; 0?$$

- (Q2) Moreover, can we specify the value of $\zeta$?

# Answer to Q1 and Q2

## Proposition

If $\{\mathcal{D}_k\}$ is $q$-probabilistically ascent with $q > q_0$, where

$$q_0 \;=\; 1 - p_0 \;=\; \frac{\log \gamma}{\log(\theta^{-1}\gamma)},$$

then

1. $$\mathbb{P}\left(S < \infty\right) \;=\; 1,$$

2. $$\mathbb{P}\left(S < \zeta\right) \;>\; 0 \quad \iff \quad \zeta > \frac{\theta}{1-\theta}.$$

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## Note

- $\mathbb{P}(S < \infty) = 1$ already implies the existence of a $\zeta$ but not its value.
- The lower bound in 2 is tight, as $S = \sum_{k=1}^{\infty} \prod_{\ell=0}^{k-1} \gamma^{1-Y_\ell} \theta^{Y_\ell} \geq \dfrac{\theta}{1-\theta}$.

# Non-convergence of PDS

**Theorem**

*Under aforementioned assumptions on $f$, if the sequence $\{\mathcal{D}_k\}$ in PDS is $q$-probabilistically ascent with $q > q_0$, then*

$$\mathbb{P}\left(\liminf_{k\to\infty} \operatorname{dist}(x_k, \mathcal{S}^*) > 0\right) \; > \; 0,$$

*provided that $\operatorname{dist}(x_0, \mathcal{S}^*) > \alpha_0/(1-\theta)$.*

# What happens in the typical implementation of PDS?

Let $\mathcal{D}_k = \{d_1, \ldots, d_m\}$, where $d_\ell \overset{\text{i.i.d.}}{\sim} \mathsf{U}(\mathcal{S}^{n-1})$.

Recall that PDS is convergent if

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

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

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which is equivalent to

$$\left(\frac{1}{2}\right)^m \ > \ q_0 \ = \ \frac{\log\gamma}{\log(\theta^{-1}\gamma)},$$

or, equivalently,

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

# Tightness of our assumption on $\{\mathcal{D}_k\}$

Our assumption on $\{\mathcal{D}_k\}$:

$q$-probabilistically ascent with $q > q_0$.

Natural question:

Is it sufficient to require $q \geq q_0$?

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Natural question:

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Answer: NO!

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Natural question:

$$\text{Is it sufficient to require } q \geq q_0?$$

Answer: NO!

**Example**

We assume

- $\theta = 1/2$ and $\gamma = 2$, which implies $q_0 = 1/2$;
- $\mathcal{D}_k = \{g_k/\|g_k\|\}$ or $\{-g_k/\|g_k\|\}$ with probability $1/2$, respectively.

Then PDS converges w.p.1.

# Convergence results inspired by non-convergence analysis

Consider the series

$$S(\kappa) \;=\; \sum_{k=1}^{\infty} \prod_{\ell=0}^{k-1} \gamma^{1-Y_\ell(\kappa)} \theta^{Y_\ell(\kappa)},$$

where $Y_\ell(\kappa) = \mathbb{1}(\mathrm{cm}\,(\mathcal{D}_\ell, -g_\ell) \leq \kappa)$.

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**Theorem**

*If there exists a $\kappa > 0$ such that $S(\kappa) = \infty$, then DS converges.*

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*If there exists a $\kappa > 0$ such that $S(\kappa) = \infty$, then DS converges.*

**Relation with existing result in [GRVZ 2015]**

$$p_0\text{-probabilistically } \kappa\text{-descent} \quad \Longrightarrow \quad S(\kappa) = \infty \text{ w.p.1}$$

# Take away

In this talk, we

- theoretically explain the non-convergence phenomenon of PDS,
- find out the behavior of PDS is closely related to the random series

$$S = \sum_{k=1}^{\infty} \prod_{\ell=0}^{k-1} \gamma^{1-Y_\ell} \theta^{Y_\ell}.$$

Non-convergence analysis can

- sharpen our knowledge about the algorithm,
- deepen our understanding about the convergence analysis,
- guide the selection of algorithmic parameters, and
- provide new perspectives on convergence analysis.

Thank you!

# One more thing: OptiProfiler

github.com/optiprofiler

OptiProfiler (joint work with Cunxin Huang and Tom M. Ragonneau) is

a benchmarking platform for DFO solvers.

Our goal: fair, convenient, and uniform benchmarking.

- Creating performance profiles, data profiles, and log-ratio profiles [Moré, Wild 2009; Shi, Xuan, Oztoprak, and Nocedal 2023]
- Providing multiple types of tests
  noisy function, unrelaxable constraints, randomized initial point ...
- Implemented in Python and MATLAB
- Default problem set: S2MPJ [Gratton, Toint 2024]

# One more thing: OptiProfiler

Example (MATLAB):

```
benchmark({@bds, @fminsearch}, "noisy")
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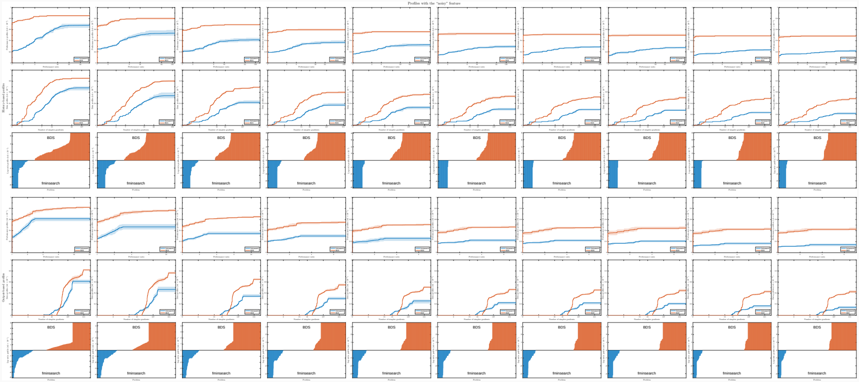


N.B.: Separate profiles can also be generated.

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