Derivative-Free Optimization Methods based on Probabilistic and Deterministic Properties: Complexity Analysis and Numerical Relevance

Clément W. Royer

Thesis defence - Soutenance de doctorat Université de Toulouse

4 novembre 2016

Supervisors S. Gratton (INPT-ENSEEIHT, Univ. Toulouse) L. N. Vicente (Univ. Coimbra, Portugal). Laboratory Institut de Recherche en Informatique de Toulouse. Funding Université Toulouse 3 Paul Sabatier.

A thesis in numerical optimization

Main topics:

- Introduction of random elements in derivative-free optimization.
- Complexity as a designing tool of optimization methods.

An Optimization Problem

- An objective function f(x) to be minimized or maximized.
- A set of values for x.

Goal: find the value(s) of x giving the best value of f.

Numerical Optimization

Obj: Develop algorithms to solve optimization problems.

- Theoretical analysis.
- Practical implementation.

Introduction: Randomness and optimization

Randomness has triggered significant recent advances in numerical optimization.

Multiple reasons:

- Large-scale setting: Classical methods too expensive.
- *Distributed computing:* Data not stored on a single computer/processor.
- Applications: Machine learning.

Introduction: Randomness and optimization

Randomness has triggered significant recent advances in numerical optimization.

Multiple reasons:

- Large-scale setting: Classical methods too expensive.
- *Distributed computing:* Data not stored on a single computer/processor.
- Applications: Machine learning.

Concerning randomness

- How does it affect the analysis of a method ?
- Improvement over deterministic ?
- Randomness in derivative-free methods ?

Complexity of optimization algorithms

Complexity Analysis

- Estimate the convergence rate of a given criterion.
- Provide worst-case bounds on algorithmic behavior.
- In presence of randomness: results in expectation.

Using complexity

- Guidance provided by complexity ?
- Practical relevance ?
- Importance for derivative-free methods ?

Main track

- Introduce random aspects in derivative-free frameworks.
- Provide theoretical guarantees (especially complexity).
- Compare complexity results with numerical behavior.
- Treat first-order and second-order aspects.

Main track

- Introduce random aspects in derivative-free frameworks.
- Provide theoretical guarantees (especially complexity).
- S Compare complexity results with numerical behavior.
- Treat first-order and second-order aspects.
- In this talk: focus on direct-search methods;
- In the thesis: direct-search and trust-region algorithms.

- Deterministic direct search
- 2 Direct search based on probabilistic descent
- 3 Deterministic and probabilistic second-order methods
- 4 Summary and conclusions

Deterministic direct search

- Derivative-free optimization
- Direct search

2 Direct search based on probabilistic descent

- 3 Deterministic and probabilistic second-order methods
- 4 Summary and conclusions

Introductory assumptions and definitions

We consider an unconstrained smooth problem:

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

Assumptions on f

- f bounded from below.
- f continuously differentiable, ∇f Lipschitz continuous.

Introductory assumptions and definitions

We consider an unconstrained smooth problem:

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

Assumptions on f

- f bounded from below.
- f continuously differentiable, ∇f Lipschitz continuous.

Solving the problem using the derivative

At $x \in \mathbb{R}^n$, moving along $-\nabla f(x)$ can decrease the function value !

- Basic paradigm of gradient-based methods.
- Goal: convergence towards a first-order stationary point

$$\liminf_{k\to\infty} \|\nabla f(x_k)\| = 0.$$

The gradient exists but cannot be used in an algorithm.

- Simulation code: gradient too expensive to be computed.
- Black-box objective function: no derivative code available.
- Automatic differentiation: inapplicable.

Examples: Weather forecasting, oil industry, biology,...

The gradient exists but cannot be used in an algorithm.

- Simulation code: gradient too expensive to be computed.
- Black-box objective function: no derivative code available.
- Automatic differentiation: inapplicable.

Examples: Weather forecasting, oil industry, biology,...

Performance indicator: Number of function evaluations.

Derivative-Free Optimization (DFO) algorithms

Deterministic DFO methods

- Model-based methods, e.g. Trust Region.
- Directional methods, e.g. Direct Search.
- Introduction to Derivative-Free Optimization A.R. Conn, K. Scheinberg, L.N. Vicente. (2009)
- Well-established: convergence theory (to local optima).
- Recent advances: complexity bounds/convergence rates.

Derivative-Free Optimization (DFO) 'ed

Stochastic DFO

- Typically global optimization methods:
 Ex) Evolution Strategies, Genetic Algorithms.
- Often use heuristics \Rightarrow No general proof of convergence.
- No deterministic variant.
- This thesis did NOT address those methods.
- Distinction: stochastic VS using probabilistic elements.

DFO methods based on probabilistic properties

- Developed from deterministic algorithms.
- Keep theoretical guarantees from deterministic.
- Improve performance with randomness.

Outline

Deterministic direct search

- Derivative-free optimization
- Direct search

2 Direct search based on probabilistic descent

3 Deterministic and probabilistic second-order methods

4 Summary and conclusions

- \bullet Directional methods \sim Steepest/Gradient Descent.
- Early appearance: 1960s, convergence theory: 1990s.
- Attractive: simplicity, parallel potential.

• Optimization by direct search: new perspectives on some classical and modern methods. Kolda, Lewis and Torczon (*SIAM Review*, 2003).

A basic framework for direct-search algorithms

- **1** Initialization: Set $x_0 \in \mathbb{R}^n, \alpha_0 > 0, 0 < \theta < 1 \leq \gamma$.
- **3** For k = 0, 1, 2, ...
 - Choose a set D_k of m vectors.
 - If it exists $d_k \in D_k$ so that

$$f(x_k + \alpha_k d_k) < f(x_k) - \alpha_k^2,$$

then declare k successful, set $x_{k+1} := x_k + \alpha_k d_k$ and update $\alpha_{k+1} := \gamma \alpha_k$.

• Otherwise declare k unsuccessful, set $x_{k+1} := x_k$ and update $\alpha_{k+1} := \theta \alpha_k$.

A basic framework for direct-search algorithms

- **1** Initialization: Set $x_0 \in \mathbb{R}^n, \alpha_0 > 0, 0 < \theta < 1 \leq \gamma$.
- **3** For k = 0, 1, 2, ...
 - Choose a set D_k of m vectors.
 - If it exists $d_k \in D_k$ so that

$$f(x_k + \alpha_k d_k) < f(x_k) - \alpha_k^2,$$

then declare k successful, set $x_{k+1} := x_k + \alpha_k d_k$ and update $\alpha_{k+1} := \gamma \alpha_k$.

• Otherwise declare k unsuccessful, set $x_{k+1} := x_k$ and update $\alpha_{k+1} := \theta \alpha_k$.

Polling choice in deterministic direct search

We would like to choose directions/polling sets D_k sufficiently good to ensure convergence.

Polling choice in deterministic direct search

We would like to choose directions/polling sets D_k sufficiently good to ensure convergence.

A measure of set quality

For a set of vectors D, the cosine measure of D is

$$\mathsf{cm}(D) = \min_{v \in \mathbb{R}^n \setminus \{0\}} \max_{d \in D} rac{d^{ op} v}{\|d\| \|v\|}.$$

We would like to choose directions/polling sets D_k sufficiently good to ensure convergence.

A measure of set quality

For a set of vectors D, the cosine measure of D is

$$\operatorname{cm}(D) = \min_{v \in \mathbb{R}^n \setminus \{0\}} \max_{d \in D} \frac{d^\top v}{\|d\| \|v\|}.$$

- When cm(D) > 0, any v makes an acute angle with some $d \in D$.
- If $v = -\nabla f(x) \neq 0$, D contains a descent direction for f at x.

Set quality

We would like to have cm(D) > 0.

Positive Spanning Sets (PSS)

D is a PSS if it generates \mathbb{R}^n by nonnegative linear combinations.

- D is a PSS iff cm(D) > 0.
- A PSS contains at least n + 1 vectors.

Set quality

We would like to have cm(D) > 0.

Positive Spanning Sets (PSS)

D is a PSS if it generates \mathbb{R}^n by nonnegative linear combinations.

- D is a PSS iff cm(D) > 0.
- A PSS contains at least n + 1 vectors.

Example

$$D_{\oplus} = \{e_1, \ldots, e_n, -e_1, \ldots, -e_n\}$$
 is a PSS with

$$\mathsf{cm}\left(D_\oplus
ight) \;=\; rac{1}{\sqrt{n}}.$$

DFO Methods based on Probabilistic and Deterministic Properties 17 / 46

Convergence for deterministic direct search

Lemma

Independently of $\{D_k\}$,

$$\lim_{k \to \infty} \alpha_k = 0.$$

Lemma

If the k-th iteration is unsuccessful and $\operatorname{cm}(D_k) \geq \kappa > 0$, then

 $\kappa \|\nabla f(x_k)\| \leq \mathcal{O}(\alpha_k).$

Convergence for deterministic direct search

Lemma

Independently of $\{D_k\}$,

$$\lim_{k \to \infty} \alpha_k = 0.$$

Lemma

If the k-th iteration is unsuccessful and $cm(D_k) \ge \kappa > 0$, then

 $\kappa \left\| \nabla f(x_k) \right\| \leq \mathcal{O}(\alpha_k).$

Convergence Theorem

If $\forall k$, $\operatorname{cm}(D_k) \geq \kappa$, we have

$$\liminf_{k\to\infty} \|\nabla f(x_k)\| = 0.$$

Worst-case complexity in deterministic direct search

Theorem (Vicente 2013)

Let $\epsilon \in (0, 1)$ and N_{ϵ} be the number of function evaluations needed to reach an point such that $\inf_{0 \le l \le k} \|\nabla f(x_l)\| < \epsilon$. Then,

 $N_{\epsilon} \leq \mathcal{O}\left(m(\kappa \epsilon)^{-2}\right).$

Choosing $D_k=D_\oplus$, one has $\kappa=1/\sqrt{n},\,m=2n$, and the bound becomes

$$N_{\epsilon} \leq \mathcal{O}\left(n^2 \epsilon^{-2}\right).$$

Deterministic direct search

Direct search based on probabilistic descent

- Probabilistic descent
- Convergence and complexity analysis
- Probabilistic descent in practice

3 Deterministic and probabilistic second-order methods

4 Summary and conclusions

Introducing randomness

Idea from Gratton and Vicente (2013)

Randomly independently generate polling sets, possibly of less than n + 1 vectors!



Numerical motivations

- Convergence test: $f(x_k) < f_{low} + 10^{-3} (f(x_0) f_{low});$
- Budget: 2000 *n* evaluations.

Problem	D_\oplus	QD_\oplus	2 n	n+1	<i>n</i> /2	2	1
	Deterministic		Probabilistic				
arglina	3.42	16.67	10.30	6.01	3.21	1.00	-
arglinb	20.50	11.38	7.38	2.81	2.35	1.00	2.04
broydn3d	4.33	11.22	6.54	3.59	2.04	1.00	-
dqrtic	7.16	19.50	9.10	4.56	2.77	1.00	-
engva 1	10.53	23.96	11.90	6.48	3.55	1.00	2.08
freuroth	56.00	1.33	1.00	1.67	1.33	1.00	4.00
integreq	16.04	18.85	12.44	6.76	3.52	1.00	-
nondquar	6.90	17.36	7.56	4.23	2.76	1.00	-
sinquad	-	2.12	1.31	1.00	1.60	1.23	-
vardim	1.00	3.30	1.80	2.40	2.30	1.80	4.30

Table : Relative number of function evaluations for different types of polling (mean on 10 runs,n = 40)

A probabilistic direct-search algorithm

From deterministic to probabilistic notations

- Polling sets/directions: $D_k = \mathfrak{D}_k(\omega)$, $d_k = \mathfrak{d}_k(\omega)$;
- Iterates: $x_k = X_k(\omega)$;
- Step sizes: $\alpha_k = \mathcal{A}_k(\omega)$.
- **1** Initialization: Set $x_0 \in \mathbb{R}^n$, $\alpha_0 > 0$, $0 < \theta < 1 \le \gamma$.
- **3** For k = 0, 1, 2, ...,
 - Choose a set \mathfrak{D}_k of *m* independent random vectors.
 - If it exists $\mathfrak{d}_k \in \mathfrak{D}_k$ so that

$$f(X_k + \mathcal{A}_k \mathfrak{d}_k) < f(X_k) - \mathcal{A}_k^2$$

then declare k successful, set $X_{k+1} := X_k + A_k \mathfrak{d}_k$ and update $A_{k+1} := \gamma A_k$.

• Otherwise, declare k unsuccessful, set $X_{k+1} := X_k$ and update $\mathcal{A}_{k+1} := \theta \mathcal{A}_k$.

Deterministic direct search

Direct search based on probabilistic descent

- Probabilistic descent
- Convergence and complexity analysis
- Probabilistic descent in practice

3 Deterministic and probabilistic second-order methods

4 Summary and conclusions

First step: What is a good random polling set ?

D is not a PSS...



First step: What is a good random polling set ?

D is not a PSS...

...*D*⊕ is...





First step: What is a good random polling set ?



Is being close to the negative gradient a sign of quality ?
Set assumption in the deterministic case

• We required

$$\operatorname{cm}(D_k) = \min_{v \neq 0} \max_{d \in D_k} \frac{d^\top v}{\|d\| \|v\|} \geq \kappa.$$

• What we really need is

$$\mathsf{cm}\left(D_k, -\nabla f(x_k)\right) = \max_{d \in D_k} \frac{d^\top (-\nabla f(x_k))}{\|d\| \|\nabla f(x_k)\|} \geq \kappa.$$

• In the random case, the second one might happen with some probability.

• Can we find adequate probabilistic tools to express this fact ?

Several types of results

Submartingale

A submartingale is a sequence of random variables $\{V_k\}$ such that $\mathbb{E}\left[|V_k|\right] < \infty$ and

$$\mathbb{E}\left(V_k | \sigma\left(V_0, V_1, \ldots, V_{k-1}\right)\right) \geq V_{k-1}.$$

We want to look at

$$\mathbb{P}\left(\operatorname{cm}\left(\mathfrak{D}_{k},-\nabla f(X_{k})\right)\geq\kappa\right).$$

where X_k depends on $\mathfrak{D}_0, \ldots, \mathfrak{D}_{k-1}$ but not on \mathfrak{D}_k .

• A solution is to use conditional probabilities/conditioning to the past.

We want to look at

$$\mathbb{P}\left(\operatorname{cm}\left(\mathfrak{D}_{k},-\nabla f(X_{k})\right)\geq\kappa\right).$$

where X_k depends on $\mathfrak{D}_0, \ldots, \mathfrak{D}_{k-1}$ but not on \mathfrak{D}_k .

• A solution is to use conditional probabilities/conditioning to the past.

Probabilistic descent property

A random set sequence $\{\mathfrak{D}_k\}$ is said to be (p,κ) -descent if:

$$\mathbb{P}\left(\operatorname{cm}\left(\mathfrak{D}_{0},-\nabla f(x_{0})\right)\geq\kappa\right) \geq \rho$$

$$\forall k\geq 1, \quad \mathbb{P}\left(\operatorname{cm}\left(\mathfrak{D}_{k},-\nabla f(X_{k})\right)\geq\kappa \mid \mathfrak{S}_{k-1}^{\mathfrak{D}}\right) \geq \rho,$$

where $\mathfrak{S}_{k-1}^{\mathfrak{D}} = \sigma(\mathfrak{D}_0, \dots, \mathfrak{D}_{k-1}).$

Lemma

For all realizations $\{\alpha_k\}$ of $\{\mathcal{A}_k\}$, independently of $\{\mathfrak{D}_k\}$,

 $\lim_{k\to\infty}\alpha_k=0.$

Lemma

If k is an unsuccessful iteration; then

$$\{\operatorname{cm}(\mathfrak{D}_k, -\nabla f(X_k)) \geq \kappa\} \subset \{\kappa \| \nabla f(X_k) \| \leq \mathcal{O}(\mathcal{A}_k) \}.$$

We need to show that $\{\operatorname{cm}(\mathfrak{D}_k, -\nabla f(X_k)) \ge \kappa\}$ happens sufficiently often.

Convergence results (2)

Let $\{\mathfrak{D}_k\}$ (p,κ) -descent and $Z_k = \mathbf{1} (\operatorname{cm} (\mathfrak{D}_k, -\nabla f(X_k)) \geq \kappa)$.

Proposition

Consider

$$S_k = \sum_{i=0}^{k-1} \left[Z_i - p_0
ight], \quad p_0 = rac{\ln heta}{\ln \left(heta / \gamma
ight)}.$$

Convergence results (2)

Let $\{\mathfrak{D}_k\}$ (p,κ) -descent and $Z_k = \mathbf{1} (\operatorname{cm} (\mathfrak{D}_k, -\nabla f(X_k)) \geq \kappa)$.

Proposition

Consider

$$S_k = \sum_{i=0}^{k-1} \left[Z_i - p_0 \right], \quad p_0 = \frac{\ln \theta}{\ln(\theta/\gamma)}.$$

Almost-sure Convergence Theorem

If
$$\{\mathfrak{D}_k\}$$
 is (p,κ) -descent with $p > p_0$, then

$$\mathbb{P}\left(\liminf_{k\to\infty}\|\nabla f(X_k)\|=0\right)=1.$$

Probabilistic worst-case complexity

Let $\{\mathfrak{D}_k\}$ be (p,κ) -descent, $\epsilon \in (0,1)$ and N_{ϵ} the number of function evaluations needed to have $\inf_{0 \le l \le k} \|\nabla f(X_l)\| \le \epsilon$. Then

$$\mathbb{P}\left(N_{\epsilon} \leq \mathcal{O}\left(\frac{m(\kappa\epsilon)^{-2}}{p-p_{0}}\right)\right) \geq 1 - \exp\left(-\mathcal{O}\left(\frac{p-p_{0}}{p}(\kappa\epsilon)^{-2}\right)\right).$$

Probabilistic worst-case complexity

Let $\{\mathfrak{D}_k\}$ be (p,κ) -descent, $\epsilon \in (0,1)$ and N_{ϵ} the number of function evaluations needed to have $\inf_{0 \le l \le k} \|\nabla f(X_l)\| \le \epsilon$. Then

$$\mathbb{P}\left(N_{\epsilon} \leq \mathcal{O}\left(\frac{m(\kappa\epsilon)^{-2}}{p-p_{0}}\right)\right) \geq 1 - \exp\left(-\mathcal{O}\left(\frac{p-p_{0}}{p}(\kappa\epsilon)^{-2}\right)\right).$$

- Deterministic: $\mathcal{O}(n^2 \epsilon^{-2})$.
- Probabilistic: $\mathcal{O}(m n \epsilon^{-2})$ in probability $\Rightarrow \mathcal{O}(n \epsilon^{-2})$ when m = 2 !
- Improvement with high probability using few directions ?

Deterministic direct search

Direct search based on probabilistic descent

- Probabilistic descent
- Convergence and complexity analysis
- Probabilistic descent in practice

3 Deterministic and probabilistic second-order methods

4 Summary and conclusions

We must ensure

$$p > p_0 = rac{\ln(heta)}{\ln(heta/\gamma)}$$

with the minimum $m = |\mathfrak{D}_k|$ possible.

A practical example: uniform distribution over the unit sphere

lf

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

then there exist p and τ independent of n such that the sequence \mathfrak{D}_k is $(p, \tau/\sqrt{n})$ -descent, with $p > p_0$.

If $\gamma = \theta^{-1} = 2$, it suffices to choose $m \ge 2$ to have $p > \frac{1}{2}$.





$$\mathfrak{d}_1 \sim \mathcal{U}(\mathbb{S}^1) \Rightarrow orall \kappa \in (0,1), \quad \mathbb{P}\left(\mathsf{cm}\left(\mathfrak{d}_1, g
ight) = \mathfrak{d}_1^ op g \geq \kappa
ight) < 1/2.$$



$$\mathfrak{d}_1 \sim \mathcal{U}(\mathbb{S}^1) \Rightarrow orall \kappa \in (0,1), \quad \mathbb{P}\left(\mathsf{cm}\left(\mathfrak{d}_1, g
ight) = \mathfrak{d}_1^ op g \geq \kappa
ight) < 1/2.$$



$$\mathfrak{d}_1 \sim \mathcal{U}(\mathbb{S}^1) \Rightarrow orall \kappa \in (0,1), \quad \mathbb{P}\left(\mathsf{cm}\left(\mathfrak{d}_1, g\right) = \mathfrak{d}_1^\top g \ge \kappa\right) < 1/2.$$

 $\mathfrak{d}_1, \mathfrak{d}_2 \sim \mathcal{U}(\mathbb{S}^1) \Rightarrow \exists \kappa^* \in (0,1), \quad \mathbb{P}\left(\mathsf{cm}\left(\left\{\mathfrak{d}_1, \mathfrak{d}_2\right\}, g\right) \ge \kappa^*\right) > 1/2.$

Deterministic direct search

2 Direct search based on probabilistic descent

Oeterministic and probabilistic second-order methods

- Second-order optimality and DFO
- Probabilistic concepts and second order

4 Summary and conclusions

- Previous analysis was concerned with first-order aspects.
- We improved the deterministic case and saved function values.
- Second-order considerations can come into play.
- Usually at a higher expense in evaluations, especially in DFO.

Assumption

- f twice continuously differentiable, ∇f and $\nabla^2 f$ Lipschitz continuous.
- f typically nonconvex.

Second-order methods

- Exploit (negative) curvature information given by $abla^2 f$.
- Converge towards second-order stationary points:

$$\liminf_{k} \max \left\{ \|\nabla f(x)\|, -\lambda_{\min} \left(\nabla^2 f(x) \right) \right\} = 0.$$

A new deterministic second-order direct search

Objective

- Introduce second order in our framework.
- Guarantees at the iteration level.
- Complexity analysis.

Key features

- A PSS D_k, as before.
- A linear basis B_k used to gather curvature information.
- Polling sets are of size $\mathcal{O}(n^2)$.
- Function decrease: α_k^3 .

Second-order convergence

Arguments

- We still have $\alpha_k \to 0$.
- On unsuccessful iterations:
 - D_k is a PSS $\Rightarrow \|\nabla f(x_k)\| \leq \mathcal{O}(\alpha_k)$
 - B_k well conditioned $\Rightarrow -\lambda_{\min} (\nabla^2 f(x_k)) \leq \mathcal{O} (\alpha_k).$

Theorem

If there exist $\kappa, \sigma \in (0,1)$ such that

$$\forall k, \quad \operatorname{cm}(D_k) \geq \kappa \quad \& \quad \sigma_{\min}(B_k) \geq \sigma,$$

then

$$\liminf_{k\to\infty} \max\left\{\|\nabla f(x_k)\|, -\lambda_{\min}\left(\nabla^2 f(x_k)\right)\right\} = 0.$$

Complexity of second-order direct search

Theorem

For $(\epsilon_g,\epsilon_H)\in (0,1)^2$, the number of evaluations of f needed to achieve

$$\begin{cases} \inf_{0 \le l \le k} \|\nabla f(x_k)\| < \epsilon_g \\ \sup_{0 \le l \le k} \lambda_{\min} \left(\nabla^2 f(x_k) \right) > -\epsilon_H \end{cases}$$

is of order

$$\mathcal{O}\left(\mathbf{n^{5}} \max\left\{\epsilon_{g}^{-3}, \epsilon_{H}^{-3}
ight\}
ight).$$

Theorem

For $(\epsilon_{g},\epsilon_{H})\in(0,1)^{2}$, the number of evaluations of f needed to achieve

$$\begin{cases} \inf_{0 \le l \le k} \|\nabla f(x_k)\| < \epsilon_g \\ \sup_{0 \le l \le k} \lambda_{\min} \left(\nabla^2 f(x_k)\right) > -\epsilon_H \end{cases}$$

is of order

$$\mathcal{O}\left(n^{5} \max\left\{\epsilon_{g}^{-3}, \epsilon_{H}^{-3}\right\}\right).$$

- Second-order expense (much) higher than first-order: Power of tolerances + $O(n^2)$ evaluations per iteration.
- Reflects on practice:
 - Second order more robust...
 - ...but more expensive.

From deterministic to probabilistic second-order methods

What we have

- Second-order convergent deterministic method.
- First-order convergent probabilistic method.

What we would like

- Incorporate randomness in the second-order method.
- Improve its worst-case cost.

On the "first-order" directions

- We can satisfy $\operatorname{cm}(D_k, -\nabla f(x_k)) \geq \kappa$ in probability...
- ...with deterministic B_k !

On the "second-order" directions

- Focus on ensuring $\mathbb{P}(\sigma_{\min}(B_k) \geq \sigma)$;
- Use results from random linear algebra.

On the "first-order" directions

- We can satisfy $\operatorname{cm}(D_k, -\nabla f(x_k)) \geq \kappa$ in probability...
- ...with deterministic B_k !

On the "second-order" directions

- Focus on ensuring $\mathbb{P}(\sigma_{\min}(B_k) \geq \sigma)$;
- Use results from random linear algebra.
- Both converge almost surely.
- Still $\mathcal{O}(n^2)$ evaluations per iteration.
- Challenge: Get rid of B_k in probability.

- Deterministic direct search
- 2 Direct search based on probabilistic descent
- 3 Deterministic and probabilistic second-order methods
- 4 Summary and conclusions

Main conclusions and contributions

- Derivative-free optimization can be combined with probabilistic tools.
- Convergence can be maintained.
- Practical performance is enhanced in the direct-search case.
- Complexity confirms the numerical observations.

Direct search based on probabilistic descent Gratton, Royer, Vicente and Zhang, SIAM J. Optim., 2015.

Main conclusions and contributions

- Derivative-free optimization can be combined with probabilistic tools.
- Convergence can be maintained.
- Practical performance is enhanced in the direct-search case.
- Complexity confirms the numerical observations.

Direct search based on probabilistic descent Gratton, Royer, Vicente and Zhang, SIAM J. Optim., 2015.

- Second-order convergence can be ensured in the deterministic case.
- First complexity result for second order in DFO.
- Reveals worst-case cost of such guarantees.

A second-order globally convergent direct-search method and its worst-case complexity

Gratton, Royer and Vicente, Optimization, 2016.

Short-term perspectives of the manuscript

- MATLAB implementation of direct search using probabilistic descent Probabilistic treatment of bounds and linear constraints.
- De-coupled techniques for second-order convergent methods Ease the introduction of random aspects.

Challenges

- Probabilistic second-order properties in DFO.
- Probabilistic second-order derivative-based methods.

Thank you for your attention !

Thank you for your attention !

Intuitive idea

Let
$$G_k = \nabla f(X_k)$$
, so $Z_k = \mathbf{1} (\operatorname{cm}(\mathfrak{D}_k, -G_k) \ge \kappa)$.

• If
$$Z_k = 1$$
 and k unsuccessful, then $\kappa \|G_k\| < \mathcal{O}(\mathcal{A}_k)$...

Intuitive idea

Let
$$G_k = \nabla f(X_k)$$
, so $Z_k = \mathbf{1}(\operatorname{cm}(\mathfrak{D}_k, -G_k) \ge \kappa)$.

- If $Z_k = 1$ and k unsuccessful, then $\kappa \| \mathcal{G}_k \| < \mathcal{O}(\mathcal{A}_k)...$
- ...so if $\inf_{0 \le l \le k} ||G_l||$ has not decreased much, $\sum_{l=0}^{k} Z_l$ should not be too high.

Intuitive idea

Let
$$G_k =
abla f(X_k)$$
, so $Z_k = 1 \left(\operatorname{cm}(\mathfrak{D}_k, -G_k) \geq \kappa \right)$.

- If $Z_k = 1$ and k unsuccessful, then $\kappa \| \mathcal{G}_k \| < \mathcal{O}(\mathcal{A}_k)...$
- ...so if $\inf_{0 \le l \le k} ||G_l||$ has not decreased much, $\sum_{l=0}^{k} Z_l$ should not be too high.

A useful bound

For all realizations of the algorithm, one has

$$\sum_{l=0}^k z_l \leq \mathcal{O}\left(\frac{1}{\kappa^2 \|\tilde{g}_k\|^2}\right) + p_0 k,$$

with $\|\tilde{g}_k\| = \inf_{0 \le l \le k} \|g_l\|$.

We use again
$$Z_l = \mathbf{1} \left(\mathsf{cm}(\mathfrak{D}_l, -
abla f(X_l) \geq \kappa)
ight)$$

An inclusion argument

$$\left\{\inf_{0\leq l\leq k} \|\nabla f(X_k)\|\geq \epsilon\right\} \subset \left\{\sum_{l=0}^k Z_l \leq \lambda k\right\}$$

with
$$\lambda = \mathcal{O}\left(rac{1}{k \kappa^2 \epsilon^{-2}} \right) + p_0.$$

A Chernoff-type probability result

For any $\lambda \in (0, p)$,

$$\mathbb{P}\left(\sum_{I=0}^{k-1} Z_I \leq \lambda k\right) \leq \exp\left[-\frac{(p-\lambda)^2}{2p}k\right].$$

Probabilistic worst-case complexity

Let $\{\mathfrak{D}_k\}$ be (p,κ) -descent, $\epsilon \in (0,1)$ and N_{ϵ} the number of function evaluations needed to have $\inf_{0 \le l \le k} \|\nabla f(X_l)\| \le \epsilon$. Then

$$\mathbb{P}\left(N_{\epsilon} \leq \mathcal{O}\left(\frac{m(\kappa\epsilon)^{-2}}{p-p_{0}}\right)\right) \geq 1 - \exp\left(-\mathcal{O}\left(\frac{p-p_{0}}{p}\kappa^{-2}\epsilon^{-2}\right)\right).$$

Corollary

Using 2 uniformly distributed directions at every iteration, with $\gamma=\theta^{-1}=$ 2, one has

$$\mathbb{P}\left(N_{\epsilon} \leq \frac{32}{3}\left(f(x_{0}) - f_{\text{low}} + \frac{\alpha_{0}^{2}}{2}\right)\frac{(2+\nu)^{2}}{(2p-1)\tau^{2}} n\epsilon^{-2}\right) \\ \geq 1 - \exp\left[-\frac{1}{6}\left(f(x_{0}) - f_{\text{low}} + \frac{\alpha_{0}^{2}}{2}\right)\frac{(2p-1)(2+\nu)^{2}}{p\tau^{2}} n\epsilon^{-2}\right]$$
Looking at the second-order Taylor model

Let x such that $\|\nabla f(x)\| \neq 0$, $\lambda_{\min}(\nabla^2 f(x)) < 0$, and $\alpha > 0$.

Problem

Characterize the directions $d \in \mathbb{R}^n, \|d\| = 1$ for which the quadratic Taylor expansion

$$\alpha \nabla f(x)^{\top} d + \frac{\alpha^2}{2} d^{\top} \nabla^2 f(x) d$$

gives information on $\lambda = \lambda_{\min} \left(\nabla^2 f(x) \right)$.

$$\mathbb{P}\left(c_1 \, \alpha \, \nabla f(x)^\top \, d + \frac{\alpha^2}{2} d^\top \, \nabla^2 f(x) \, d \leq c_2 \frac{\alpha^2}{2} \, \lambda + c_3 \, \alpha^3\right) \geq p.$$

Looking for d satisfying:

$$\mathbb{P}\left(\qquad \qquad \frac{\alpha^2}{2}d^{\top}\nabla^2 f(x)\,d \ \leq \ c_2\frac{\alpha^2}{2}\,\lambda \qquad \right) \geq p.$$

• $c_1 = c_3 = 0, c_2 \in (0, 1)$ (Negative curvature direction) Gets harder as $\lambda \nearrow 0$.

$$\mathbb{P}\left(\frac{\alpha^2}{2}d^{\top}\nabla^2 f(x) d \leq c_2 \frac{\alpha^2}{2}\lambda + c_3 \alpha^3 \right) \geq p.$$

- $c_1 = c_3 = 0, c_2 \in (0, 1)$ (Negative curvature direction) Gets harder as $\lambda \nearrow 0$.
- $c_1 = 0, c_2 \in (0, 1), c_3 > 0$ (Approx. Negative curvature direction) Ok but expensive.

$$\mathbb{P}\left(c_1 \, \alpha \, \nabla f(x)^\top \, d + \frac{\alpha^2}{2} d^\top \, \nabla^2 f(x) \, d \leq c_2 \frac{\alpha^2}{2} \, \lambda + c_3 \, \alpha^3\right) \geq p.$$

- $c_1 = c_3 = 0, c_2 \in (0, 1)$ (Negative curvature direction) Gets harder as $\lambda \nearrow 0$.
- $c_1 = 0, c_2 \in (0, 1), c_3 > 0$ (Approx. Negative curvature direction) Ok but expensive.
- $c_1, c_2 \in (0, 1), c_3 > 0$ (Approx. second-order direction) Cheap but depends on α .

$$\mathbb{P}\left(c_1 \, \alpha \, \nabla f(x)^\top \, d + \frac{\alpha^2}{2} d^\top \, \nabla^2 f(x) \, d \leq c_2 \frac{\alpha^2}{2} \, \lambda + c_3 \, \alpha^3\right) \geq p.$$

- $c_1 = c_3 = 0, c_2 \in (0, 1)$ (Negative curvature direction) Gets harder as $\lambda \nearrow 0$.
- $c_1 = 0, c_2 \in (0, 1), c_3 > 0$ (Approx. Negative curvature direction) Ok but expensive.
- $c_1, c_2 \in (0, 1), c_3 > 0$ (Approx. second-order direction) Cheap but depends on α .