

# Propriétés probabilistes dans les algorithmes d'optimisation sans et avec dérivées

Clément Royer - University of Wisconsin-Madison

Séminaire SPOC  
Institut de Mathématiques de Bourgogne

12 avril 2017

*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.

*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 Analysis

- Estimate the **convergence rate** of a given criterion.
- Provide worst-case **bounds** on algorithmic behavior.
- With randomness: **results in expectation/probability**.

## Using complexity

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

## Main track

- 1 Introduce random aspects in derivative-free frameworks.
- 2 Provide theoretical guarantees (especially complexity).
- 3 Compare complexity results with numerical behavior.

## Main track

- 1 Introduce random aspects in derivative-free frameworks.
  - 2 Provide theoretical guarantees (especially complexity).
  - 3 Compare complexity results with numerical behavior.
- In this talk: focus on **direct-search** methods;
  - Apply to other frameworks, like **trust-region**.

- 1 Deterministic direct search
- 2 Direct search based on probabilistic descent
- 3 Extension to bound and linearly constrained problems
- 4 Probabilistic properties in derivative-based algorithms

- 1 **Deterministic direct search**
  - Derivative-free optimization
  - Direct search
- 2 Direct search based on probabilistic descent
- 3 Extension to bound and linearly constrained problems
- 4 Probabilistic properties in derivative-based algorithms



We consider an unconstrained smooth problem:

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

## Assumptions on $f$

- $f$  bounded from below, a priori not convex.
- $f$  continuously differentiable,  $\nabla f$  Lipschitz continuous.

We consider an unconstrained smooth problem:

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

## Assumptions on $f$

- $f$  bounded from below, a priori not convex.
- $f$  continuously differentiable,  $\nabla f$  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**

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

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, medicine,...

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, medicine,...

**Performance indicator:** Number of function evaluations.

## 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**.

## Stochastic DFO

- Typically **global optimization** methods:
    - Ex) Evolution Strategies, Genetic Algorithms.
  - No deterministic variant.
- 
- This talk does 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.

- 1 **Deterministic direct search**
  - Derivative-free optimization
  - **Direct search**
- 2 Direct search based on probabilistic descent
- 3 Extension to bound and linearly constrained problems
- 4 Probabilistic properties in derivative-based algorithms

- 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).



① **Initialization:** Set  $x_0 \in \mathbb{R}^n$ ,  $\alpha_0 > 0$ ,  $0 < \theta < 1 \leq \gamma$ .

② **For**  $k = 0, 1, 2, \dots$

- Choose a set  $D_k$  of  $r$  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  $\alpha_{k+1} := \theta \alpha_k$ .

① **Initialization:** Set  $x_0 \in \mathbb{R}^n$ ,  $\alpha_0 > 0$ ,  $0 < \theta < 1 \leq \gamma$ .

② **For**  $k = 0, 1, 2, \dots$

- Choose a set  $D_k$  of  $r$  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  $\alpha_{k+1} := \theta \alpha_k$ .

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

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

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

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

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

- When  $\text{cm}(D) > 0$ , 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  $x$ .

We would like to have  $\text{cm}(D) > 0$ .

## Positive Spanning Sets (PSS)

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

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

We would like to have  $\text{cm}(D) > 0$ .

## Positive Spanning Sets (PSS)

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

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

## Example

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

$$\text{cm}(D_{\oplus}) = \frac{1}{\sqrt{n}}.$$

## Lemma

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

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

## Lemma

*Independently of  $\{D_k\}$ ,*

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



# Convergence for deterministic direct search

## Lemma

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

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

## Lemma

Independently of  $\{D_k\}$ ,

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

## Convergence Theorem

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

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

## Theorem

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

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

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

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

- 1 Deterministic direct search
- 2 Direct search based on probabilistic descent
  - Probabilistic descent
  - Convergence and complexity analysis
  - Probabilistic descent in practice
- 3 Extension to bound and linearly constrained problems
- 4 Probabilistic properties in derivative-based algorithms

Idea (Gratton and Vicente, 2013)

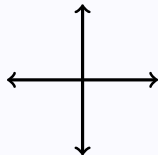
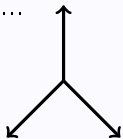
Randomly independently generate polling sets, possibly with **less than  $n + 1$  vectors!**

# Introducing randomness

Idea (Gratton and Vicente, 2013)

Randomly independently generate polling sets, possibly with *less than  $n + 1$  vectors!*

From PSS...



...to random sets

# Numerical motivations

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

Problem	$D_{\oplus}$	$Q D_{\oplus}$	$2n$	$n+1$	$n/2$	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	–
engval1	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,  $n = 40$ )

## 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:  $\alpha_k = A_k(\omega)$ .

1 **Initialization:** Set  $x_0 \in \mathbb{R}^n$ ,  $\alpha_0 > 0$ ,  $0 < \theta < 1 \leq \gamma$ .

2 **For**  $k = 0, 1, 2, \dots$ ,

- Choose a set  $\mathfrak{D}_k$  of  $r$  **independent random** vectors.
- If it exists  $\mathfrak{d}_k \in \mathfrak{D}_k$  so that

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

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  $A_{k+1} := \theta A_k$ .

- 1 Deterministic direct search
- 2 Direct search based on probabilistic descent
  - Probabilistic descent
  - **Convergence and complexity analysis**
  - Probabilistic descent in practice
- 3 Extension to bound and linearly constrained problems
- 4 Probabilistic properties in derivative-based algorithms



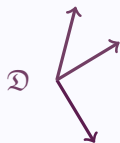
# First step: What is a good random polling set ?

$\mathcal{D}$  is not a PSS...

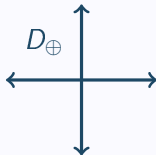


# First step: What is a good random polling set ?

$\mathcal{D}$  is not a PSS...

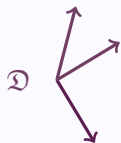


... $D_{\oplus}$  is...

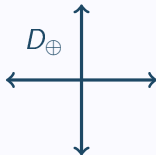


# First step: What is a good random polling set ?

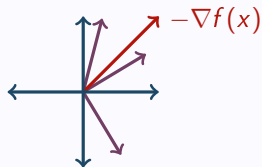
$\mathcal{D}$  is not a PSS...



... $D_{\oplus}$  is...



...but here  $-\nabla f(x)$  is closer to  $\mathcal{D}$ !



*Is being close to the negative gradient a sign of quality ?*

## Set assumption in the deterministic case

- We required

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

- What we really need is

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

- 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

Deterministic/For all realizations



With probability 1/Almost-sure



With a given probability.

## Submartingale

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

$$\mathbb{E}(V_k | V_0, V_1, \dots, V_{k-1}) \geq V_{k-1}.$$

- We want to look at

$$\mathbb{P}(\text{cm}(\mathfrak{D}_k, -\nabla f(X_k)) \geq \kappa).$$

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

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

- We want to look at

$$\mathbb{P}(\text{cm}(\mathfrak{D}_k, -\nabla f(X_k)) \geq \kappa).$$

where  $X_k$  depends on  $\mathfrak{D}_0, \dots, \mathfrak{D}_{k-1}$  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  $(\rho, \kappa)$ -descent if:

$$\begin{aligned} \mathbb{P}(\text{cm}(\mathfrak{D}_0, -\nabla f(x_0)) \geq \kappa) &\geq \rho \\ \forall k \geq 1, \quad \mathbb{P}(\text{cm}(\mathfrak{D}_k, -\nabla f(X_k)) \geq \kappa \mid \mathfrak{D}_0, \dots, \mathfrak{D}_{k-1}) &\geq \rho, \end{aligned}$$

## Lemma

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

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

## Lemma

If  $k$  is an unsuccessful iteration; then

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

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



## Convergence results (2)

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

### Proposition

Consider

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

- 1 If  $\liminf_k \|\nabla f(X_k)\| > 0$ , then  $S_k \rightarrow -\infty$ .
- 2 If  $p > p_0$ ,  $\{S_k\}$  is a **submartingale** and  $\mathbb{P}(\limsup S_k = \infty) = 1$ .

## Convergence results (2)

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

### Proposition

Consider

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

- 1 If  $\liminf_k \|\nabla f(X_k)\| > 0$ , then  $S_k \rightarrow -\infty$ .
- 2 If  $p > p_0$ ,  $\{S_k\}$  is a **submartingale** and  $\mathbb{P}(\limsup S_k = \infty) = 1$ .

### Almost-sure Convergence Theorem

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

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

## Intuitive idea

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

- If  $Z_k = 1$  and  $k$  unsuccessful, then  $\kappa \|G_k\| < \mathcal{O}(A_k) \dots$

## Intuitive idea

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

- If  $Z_k = 1$  and  $k$  unsuccessful, then  $\kappa \|G_k\| < \mathcal{O}(A_k)$ ...
- ... $A_k$  goes to zero...

## Intuitive idea

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

- If  $Z_k = 1$  and  $k$  unsuccessful, then  $\kappa \|G_k\| < \mathcal{O}(A_k)$ ...
- ... $A_k$  goes to zero...
- ...so if  $\inf_{0 \leq l \leq k} \|G_l\|$  has not decreased much,  $\sum_{l=0}^k Z_l$  should not be too high.

## Intuitive idea

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

- If  $Z_k = 1$  and  $k$  unsuccessful, then  $\kappa \|G_k\| < \mathcal{O}(A_k)$ ...
- ... $A_k$  goes to zero...
- ...so if  $\inf_{0 \leq l \leq k} \|G_l\|$  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  $\|\tilde{g}_k\| = \inf_{0 \leq l \leq k} \|g_l\|$ .

## WCC for probabilistic descent (2)

We use again  $Z_l = \mathbf{1}(\text{cm}(\mathcal{D}_l, -\nabla f(X_l)) \geq \kappa)$ .

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

A Chernoff-type probability result

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

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

## Probabilistic worst-case complexity

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

$$\mathbb{P} \left( N_\epsilon \leq \mathcal{O} \left( \frac{r(\kappa\epsilon)^{-2}}{\rho - \rho_0} \right) \right) \geq 1 - \exp \left( -\mathcal{O} \left( \frac{\rho - \rho_0}{\rho} (\kappa\epsilon)^{-2} \right) \right).$$



## Probabilistic worst-case complexity

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

$$\mathbb{P} \left( N_\epsilon \leq \mathcal{O} \left( \frac{r (\kappa \epsilon)^{-2}}{p - p_0} \right) \right) \geq 1 - \exp \left( -\mathcal{O} \left( \frac{p - p_0}{p} (\kappa \epsilon)^{-2} \right) \right).$$

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

- 1 Deterministic direct search
- 2 Direct search based on probabilistic descent
  - Probabilistic descent
  - Convergence and complexity analysis
  - Probabilistic descent in practice
- 3 Extension to bound and linearly constrained problems
- 4 Probabilistic properties in derivative-based algorithms

# A practical $(\rho, \kappa)$ -descent sequence

We must ensure

$$\rho > \rho_0 = \frac{\ln(\theta)}{\ln(\theta/\gamma)}$$

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

A practical example: uniform distribution over the unit sphere

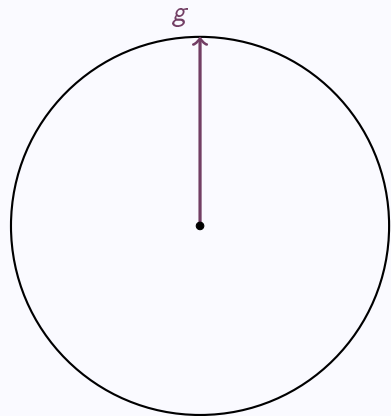
If

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

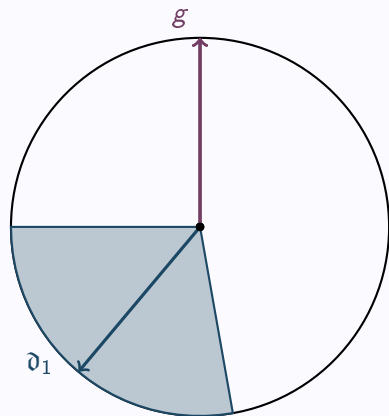
then there exist  $\rho$  and  $\tau$  independent of  $n$  such that the sequence  $\mathfrak{D}_k$  is  $(\rho, \tau/\sqrt{n})$ -descent, with  $\rho > \rho_0$ .

If  $\gamma = \theta^{-1} = 2$ , it suffices to choose  $r \geq 2$  to have  $\rho > \frac{1}{2}$ .

Two uniform directions are enough, one is not

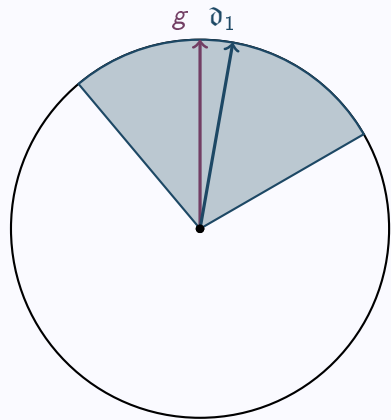


# Two uniform directions are enough, one is not



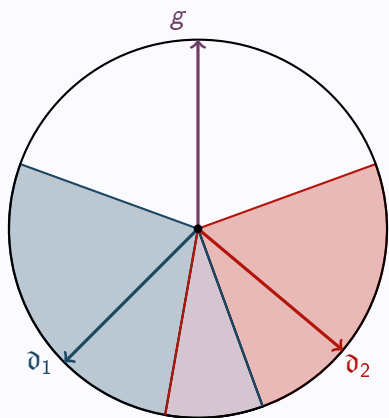
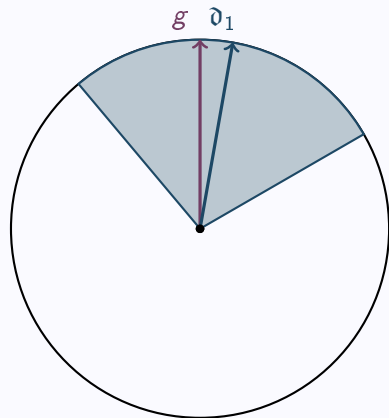
$$d_1 \sim \mathcal{U}(\mathbb{S}^1) \Rightarrow \forall \kappa \in (0, 1), \quad \mathbb{P}(\text{cm}(d_1, g) = d_1^\top g \geq \kappa) < 1/2.$$

# Two uniform directions are enough, one is not



$$\vartheta_1 \sim \mathcal{U}(\mathbb{S}^1) \Rightarrow \forall \kappa \in (0, 1), \quad \mathbb{P} \left( \text{cm}(\vartheta_1, g) = \vartheta_1^\top g \geq \kappa \right) < 1/2.$$

# Two uniform directions are enough, one is not



$$\vartheta_1 \sim \mathcal{U}(\mathbb{S}^1) \Rightarrow \forall \kappa \in (0, 1), \quad \mathbb{P}(\text{cm}(\vartheta_1, g) = \vartheta_1^\top g \geq \kappa) < 1/2.$$

$$\vartheta_1, \vartheta_2 \sim \mathcal{U}(\mathbb{S}^1) \Rightarrow \exists \kappa^* \in (0, 1), \quad \mathbb{P}(\text{cm}(\{\vartheta_1, \vartheta_2\}, g) \geq \kappa^*) > 1/2.$$

- 1 Deterministic direct search
- 2 Direct search based on probabilistic descent
- 3 Extension to bound and linearly constrained problems
- 4 Probabilistic properties in derivative-based algorithms



## Linear equality constraints

$$\begin{cases} \min_{x \in \mathbb{R}^n} & f(x) \\ \text{s.t.} & Ax = b. \end{cases}$$

- Equivalent to the **unconstrained** problem  $\min_{\tilde{x} \in \mathbb{R}^{n-m}} f(x_0 + W\tilde{x})$  with  $W \in \mathbb{R}^{n \times (n-m)}$  orthonormal basis for  $\text{null}(A)$  and  $Ax_0 = b$ .
- Deterministic and probabilistic analyses apply !

# Two linearly constrained problems

## Linear equality constraints

$$\begin{cases} \min_{x \in \mathbb{R}^n} & f(x) \\ \text{s.t.} & Ax = b. \end{cases}$$

- Equivalent to the **unconstrained** problem  $\min_{\tilde{x} \in \mathbb{R}^{n-m}} f(x_0 + W\tilde{x})$  with  $W \in \mathbb{R}^{n \times (n-m)}$  orthonormal basis for  $\text{null}(A)$  and  $Ax_0 = b$ .
- **Deterministic and probabilistic analyses apply !**

## Bound constrained case

$$\begin{cases} \min_{x \in \mathbb{R}^n} & f(x) \\ \text{s.t.} & l \leq x \leq u. \end{cases}$$

- **Deterministic practice:** Uses  $D_{\oplus} = \{e_1, \dots, e_n, -e_1, \dots, -e_n\}$  to guarantee convergence and moves **parallel to the constraints**.

# Algorithm (deterministic version)

① **Initialization:** Set  $x_0 \in \mathbb{R}^n$ ,  $\alpha_0 > 0$ ,  $0 < \theta < 1 \leq \gamma$ .

② **For**  $k = 0, 1, 2, \dots$

- Choose a set  $D_k$  of **at most**  $r$  vectors.
- If it exists  $d_k \in D_k$  so that  $x_k + \alpha_k d_k$  **is feasible** and

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

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  $\alpha_{k+1} := \theta \alpha_k$ .

- Feasible set:  $\mathcal{F} = \{l \leq x \leq u\}$ .

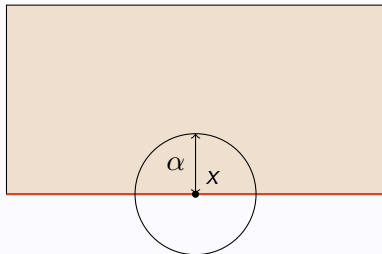
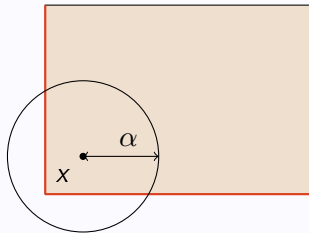
## Nearby constraints

The indexes

$$I_u(x, \alpha) = \{i : |u_i - [x]_i| \leq \alpha\}$$

$$I_l(x, \alpha) = \{i : |l_i - [x]_i| \leq \alpha\}$$

define the **nearby constraints** at  $x \in \mathcal{F}$  given  $\alpha > 0$ .

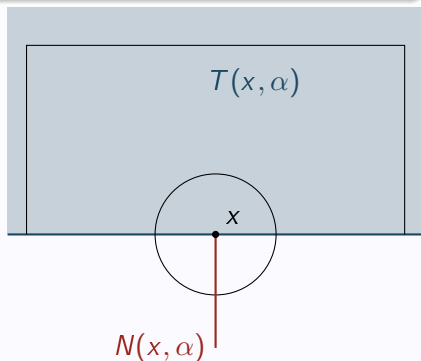
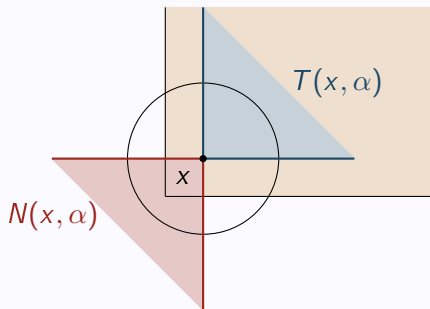


## Bound constraints (2)

- **Approximate normal cone**  $N(x, \alpha)$ : Positive span of

$$\{e_i\}_{i \in I_u(x, \alpha)} \cup \{-e_i\}_{i \in I_l(x, \alpha)}.$$

- **Approximate tangent cone**  $T(x, \alpha)$ : polar of  $N(x, \alpha)$ .



# Feasible descent property

- Recall the cosine measure that identifies descent directions

$$\text{cm}(D, -\nabla f(x)) = \max_{d \in D} \frac{d^\top [-\nabla f(x)]}{\|d\| \|\nabla f(x)\|}.$$

## Feasible descent property

$D$  is a  $\kappa$ -feasible descent set for  $T(x, \alpha)$  if  $D \subset T(x, \alpha)$  and

$$\text{cm}_{T(x, \alpha)}(D, -\nabla f(x)) = \max_{d \in D} \frac{d^\top [-\nabla f(x)]}{\|d\| \|P_{T(x, \alpha)}[-\nabla f(x)]\|} \geq \kappa.$$

## Feasible descent property

- Recall the cosine measure that identifies descent directions

$$\text{cm}(D, -\nabla f(x)) = \max_{d \in D} \frac{d^\top [-\nabla f(x)]}{\|d\| \|-\nabla f(x)\|}.$$

### Feasible descent property

$D$  is a  $\kappa$ -feasible descent set for  $T(x, \alpha)$  if  $D \subset T(x, \alpha)$  and

$$\text{cm}_{T(x, \alpha)}(D, -\nabla f(x)) = \max_{d \in D} \frac{d^\top [-\nabla f(x)]}{\|d\| \|P_{T(x, \alpha)}[-\nabla f(x)]\|} \geq \kappa.$$

- Using  $\kappa$ -feasible descent sets guarantee both convergence and complexity (similar analysis than unconstrained case).
- $D_\oplus \cap T(x, \alpha)$  is always  $\frac{1}{\sqrt{n}}$ -feasible descent.

## Definition

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

$$\begin{aligned} \mathbb{P}(\text{cm}_{T_0}(\mathfrak{D}_0, -\nabla f(x_0)) \geq \kappa) &\geq p \\ \forall k \geq 1, \quad \mathbb{P}(\text{cm}_{T_k}(\mathfrak{D}_k, -\nabla f(X_k)) \geq \kappa \mid \mathfrak{D}_0, \dots, \mathfrak{D}_{k-1}) &\geq p. \end{aligned}$$

where  $T_k = T(X_k, A_k)$ .

## Theoretical guarantees

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

- **Almost-sure convergence towards stationary point;**
- **Complexity bound for  $\epsilon$ -stationarity:**

$$\mathbb{P}\left(N_\epsilon \leq \mathcal{O}\left(\frac{r(\kappa\epsilon)^{-2}}{p - p_0}\right)\right) \geq 1 - \exp\left(-\mathcal{O}\left(\frac{p - p_0}{p}(\kappa\epsilon)^{-2}\right)\right).$$



## Main concerns

- How to define **probabilistic feasible descent sets** ?
- What are the orders of  $r$  and  $\kappa$  ?
- Can we use **less directions** than in the deterministic case ?

## Main concerns

- How to define **probabilistic feasible descent** sets ?
- What are the orders of  $r$  and  $\kappa$  ?
- Can we use **less directions** than in the deterministic case ?

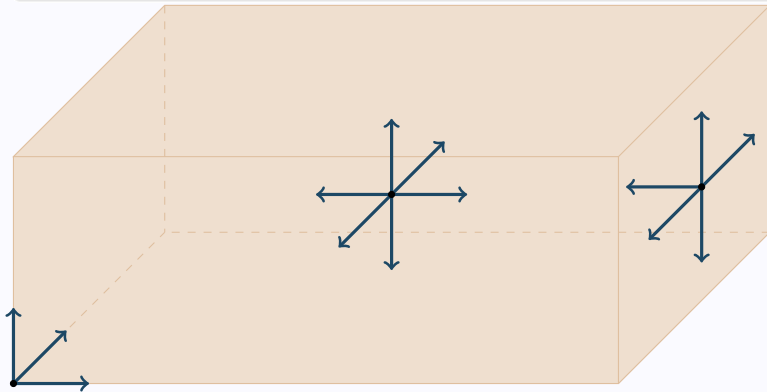
## Our approach

- Based on tangent cone generators;
- Choice of a random **feasible** polling set;
- **At worst as expensive as the deterministic case.**

# Possible direction generation techniques

## A random generator sampling approach

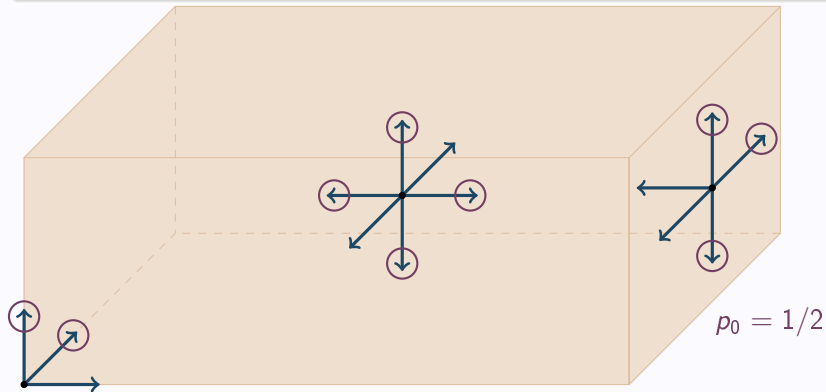
- 1 Compute a **deterministic** generating set  $V_k$  for  $T_k$ ;



# Possible direction generation techniques

## A random generator sampling approach

- 1 Compute a **deterministic** generating set  $V_k$  for  $T_k$ ;
- 2 Take a **random sample**  $\mathfrak{D}_k$  of  $V_k$  of size  $> |V_k|p_0$ ;
- 3  $\{\mathfrak{D}_k\}$  is  $(p, \kappa)$ -descent with  $p > p_0$ .



# Using fewer directions by exploiting subspaces

## Idea

- Unconstrained case: probabilistic descent can use less directions;
- Also for linear equalities: **unconstrained problem** in the null space of  $A$ ;
- **Benefit in exploiting unconstrained subspaces ?**

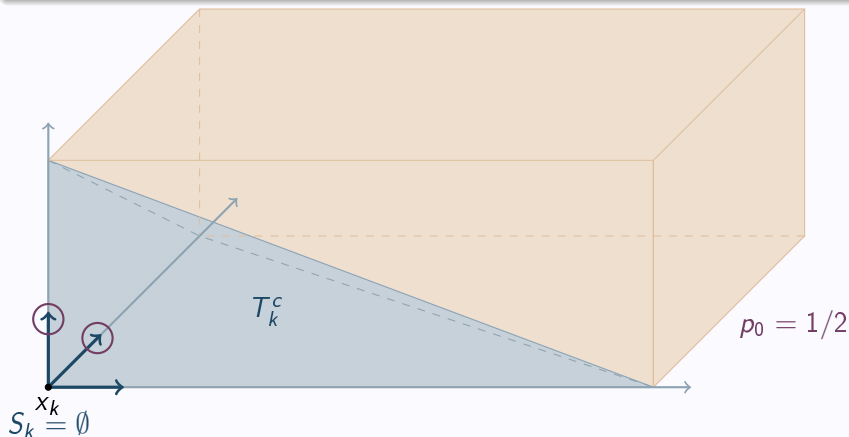
## Lemma

Let  $S_k$  be a linear subspace within a cone  $T_k$ . Then  $T_k = S_k + T_k^c$ , where  $T_k^c$  is a cone lying in  $S_k^\perp$ .

## Second technique: Illustration

### Two types of directions

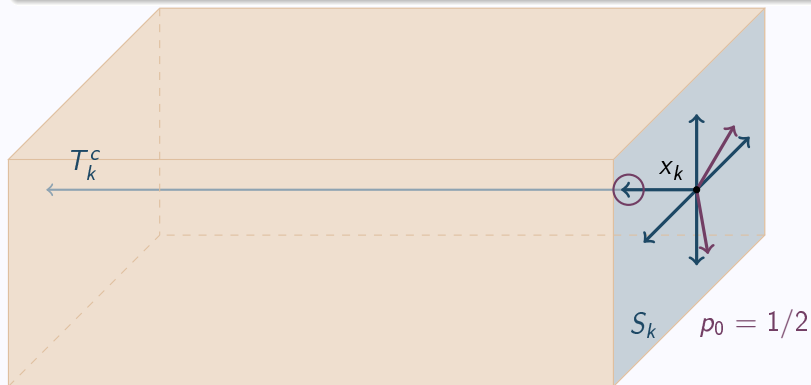
- Subspace  $S_k$ : Generate random directions;
- Orthogonal part  $T_k^c$ : Use a random subset of the generators.



## Second technique: Illustration

### Two types of directions

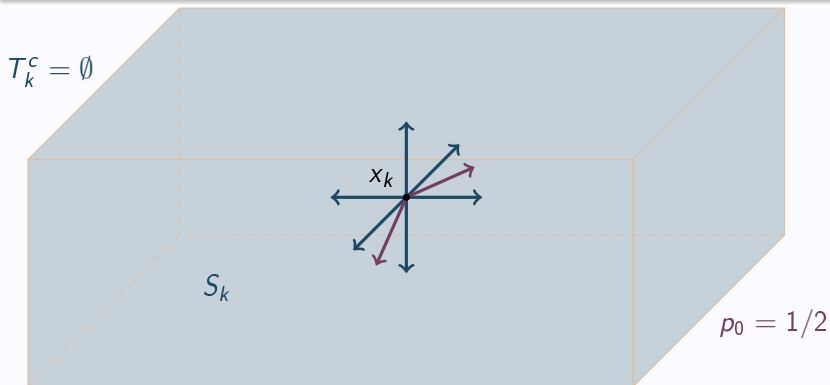
- Subspace  $S_k$ : Generate randomly directions;
- Orthogonal part  $T_k^c$ : Use a random subset of the generators.



## Second technique: Illustration

### Two types of directions

- Subspace  $S_k$ : Generate randomly directions;
- Orthogonal part  $T_k^c$ : Use a random subset of the generators.





- The general bound is  $\mathcal{O}(r\kappa^{-2}\epsilon^{-2})$ .

## Comparison of results - Linear constraints only

Method	$r$	$\kappa$	Bound
Determ.	$2(n - m)$	$\frac{1}{\sqrt{n-m}}$	$\mathcal{O}((n - m)^2\epsilon^{-2})$
Proba. 1	$\mathcal{O}(2(n - m)p_0)$	$\frac{1}{\sqrt{n-m}}$	$\mathcal{O}((n - m)^2\epsilon^{-2})$
Proba. 2 (subspace)	$\mathcal{O}(1)$	$\frac{\tau}{\sqrt{n-m}}$	$\mathcal{O}((n - m)\epsilon^{-2})$

## Comparison of results - Bounds on $n_b < n$ variables only

Method	$r$	$\kappa$	Bound
Determ.	$2n$	$\frac{1}{\sqrt{n}}$	$\mathcal{O}(n^2\epsilon^{-2})$
Proba. 1	$\mathcal{O}(2np_0)$	$\frac{1}{\sqrt{n}}$	$\mathcal{O}(n^2\epsilon^{-2})$
Proba. 2 (subspace)	$\mathcal{O}(1) + \mathcal{O}(n_b p_0)$	$\frac{1}{\sqrt{n}}$	$\mathcal{O}(n n_b \epsilon^{-2})$

# Numerical experiments-Bound constraints

- Comparison with MATLAB built-in `patternsearch` function.

## Four solvers

Name	Polling in $T(x_k, \alpha_k) = T_k = S_k + T_k^c$	Guarantees
<code>dspfd-0</code>	Shuffled $D_{\oplus} \cap T_k$	Deterministic
<code>dspfd-1</code>	Random subset of $D_{\oplus} \cap T_k$	Probabilistic
<code>dspfd-2</code>	Random vectors in $S_k$ /subset of $D_{\oplus} \cap T_k^c$	Probabilistic
<code>matlab</code>	$D_{\oplus} \cap T(x_k, t\alpha_k), t \in (0, 1)$	Deterministic

## Performance profiles

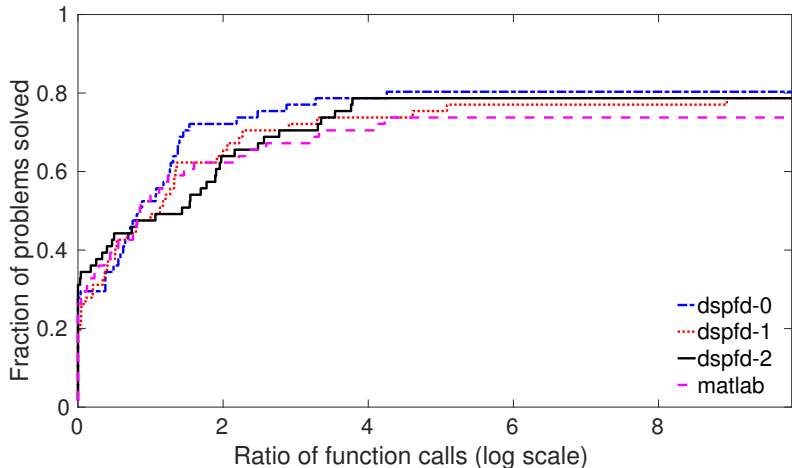
- Criterion: # of function evaluations (budget of  $2000n$ ) to satisfy

$$f(x_k) - f_{best} < 10^{-3}(f(x_0) - f_{best}).$$

- Benchmark: Problems from the CUTEst collection.

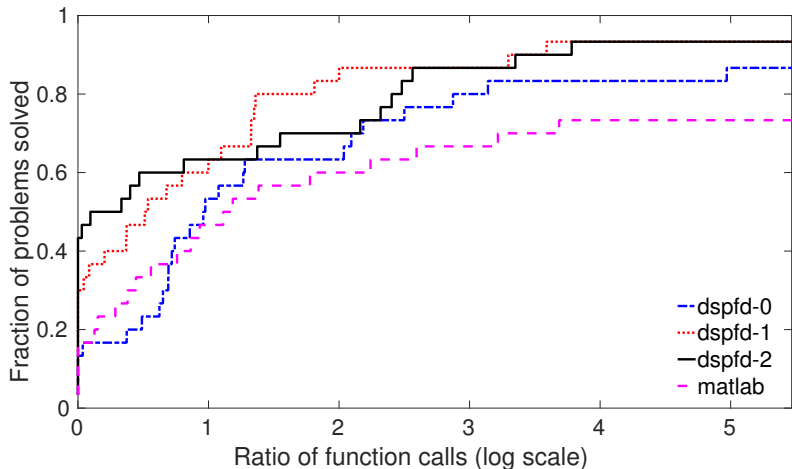
# Profiles for bound-constrained problems

- Performance on 63 problems with bounds, small dimensions:  
 $2 \leq n \leq 20$ .



## Profiles for bound-constrained problems (2)

- Performance on 31 problems with bounds constraints, **larger dimensions**:  $20 \leq n \leq 52$ .



- 1 Deterministic direct search
- 2 Direct search based on probabilistic descent
- 3 Extension to bound and linearly constrained problems
- 4 Probabilistic properties in derivative-based algorithms**

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

- $f$  twice continuously differentiable,
- $f$  typically nonconvex.

## From first to second-order algorithms

- Expensive to access the Hessian...
- ...or to perform associated procedures:
  - Eigenvectors;
  - Linear systems.

Can probabilistic properties come to the rescue ?

## Probabilistic analysis of linear algebra methods

With a *random start*...

- Power method finds an  $\epsilon$ -approximate eigenvector in  $\mathcal{O}(\epsilon^{-1})$  steps;
- Lanczos method finds an  $\epsilon$ -approximate eigenvector in  $\mathcal{O}(\epsilon^{-1/2})$  steps.

...with *high probability*.

## Uses

- Combined with *first-order methods*;
- For convex and *nonconvex* problems.

## Key points

- Escape saddle points;
- Detect **negative Hessian eigenvalues**;
- Use **negative curvature directions**;

The best methods in terms of complexity guarantee second-order convergence!



- Revisit practically efficient methods;
- Develop a full complexity analysis;
- Complete known observations.

## Tools

- Newton-Krylov (e.g. CG) methods:  
*Matrix-free, efficient.*
- Line search techniques and properties;
- Probabilistic analysis.

## For unconstrained problems

- Convergence results hold for probabilistic properties.
- Requires less evaluations in theory and practice.

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

## Bounds and linear constraints

- Using (probabilistic) **feasible descent** is the key.
- Random generation in “unconstrained” subspaces.
- Can improve complexity bounds, **practically efficient**.

***Direct search based on probabilistic feasible descent for bound and linearly constrained problems.*** Gratton, Royer, Vicente and Zhang, *Submitted*, 2017.

- In derivative-free
  - Nonlinear constraints;
  - Parallel setting.
- More generally
  - Complexity analysis;
  - **Negative curvature.**

- In derivative-free
  - Nonlinear constraints;
  - Parallel setting.
- More generally
  - Complexity analysis;
  - **Negative curvature.**

Thank you for your attention !

croyer2@wisc.edu