Are we Pushing Direct Search to its Limit?

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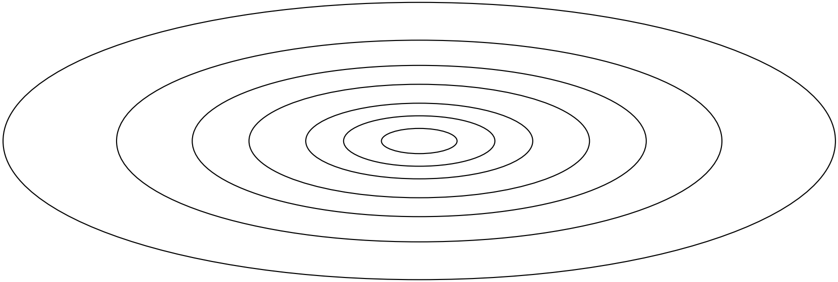
- Direct search of directional type: Achieve descent by using positive spanning sets and moving in the directions of the best points.
- Direct search of simplicial type: e.g., Nelder-Mead based methods.

Coordinate search (poll step & simple decrease)



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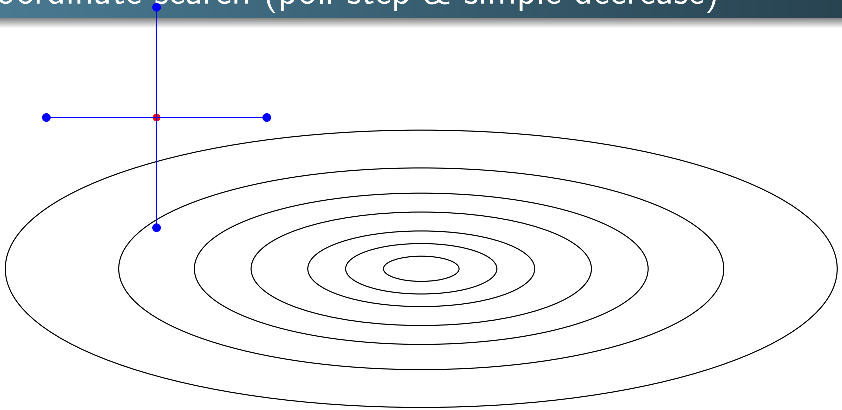

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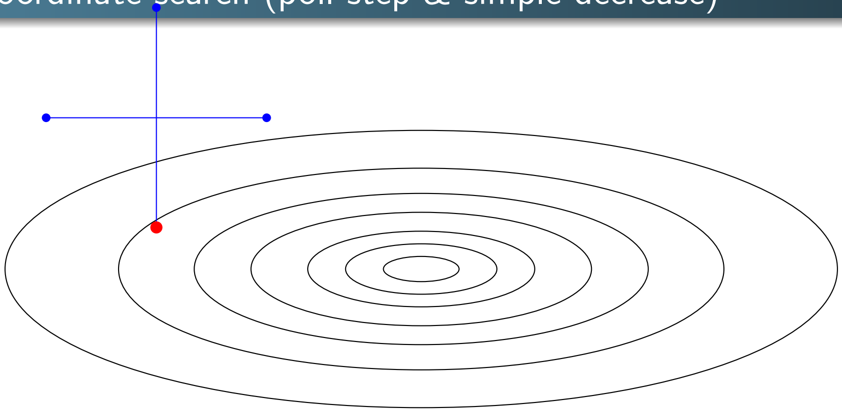

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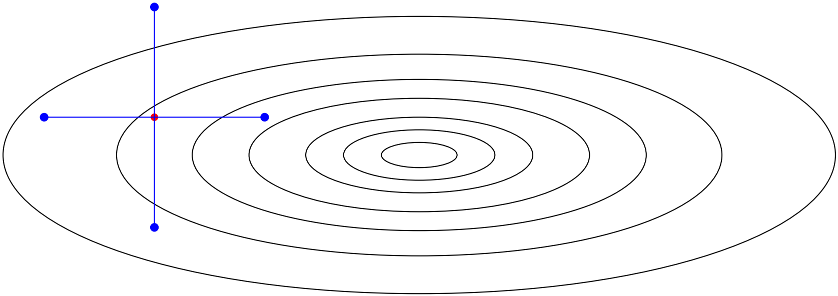

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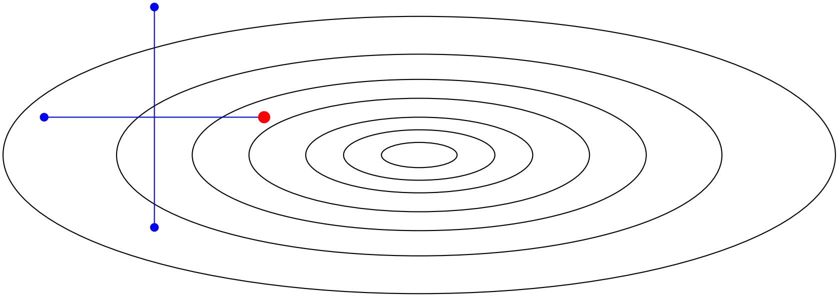

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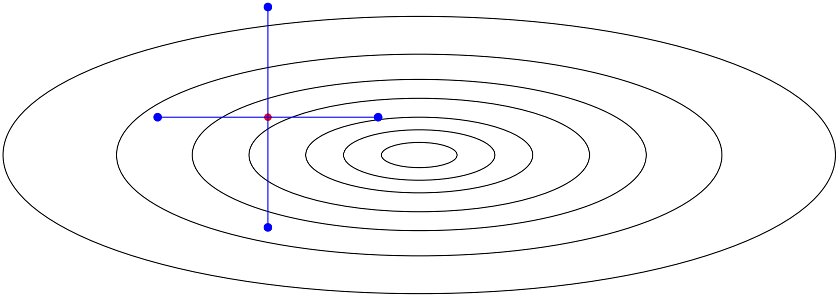

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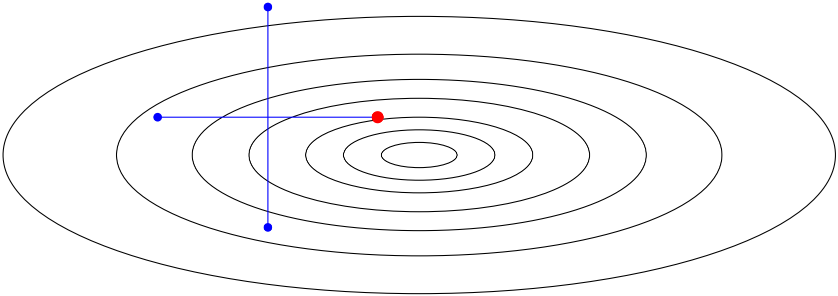

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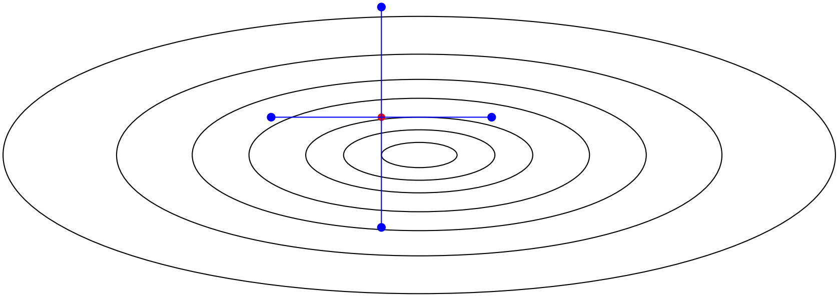

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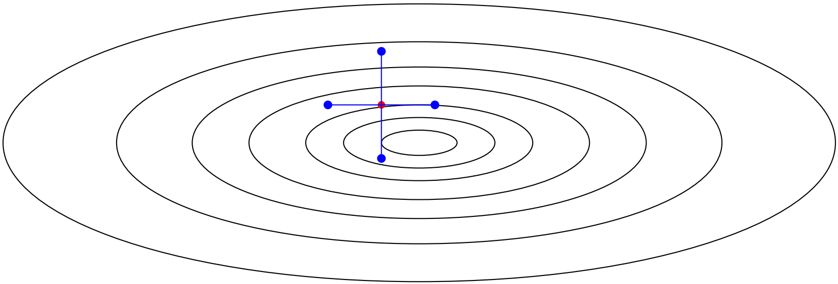

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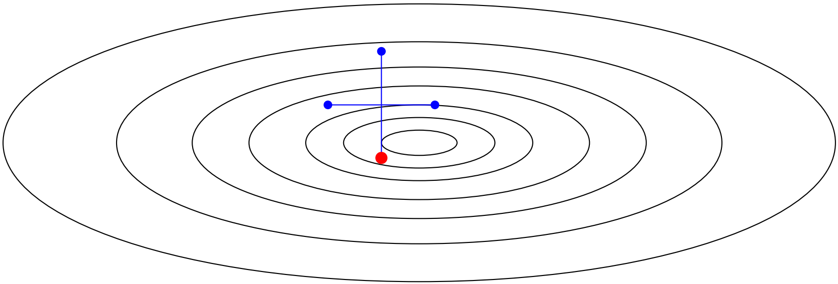

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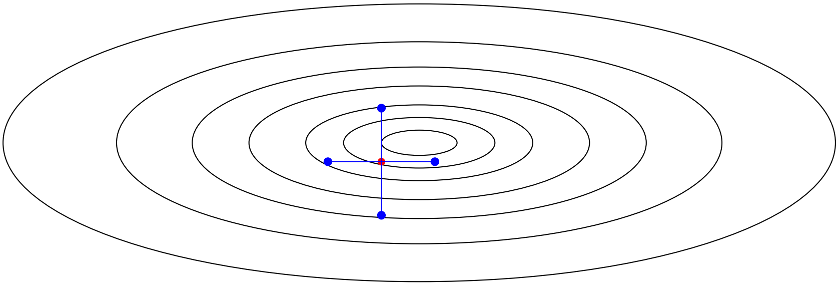

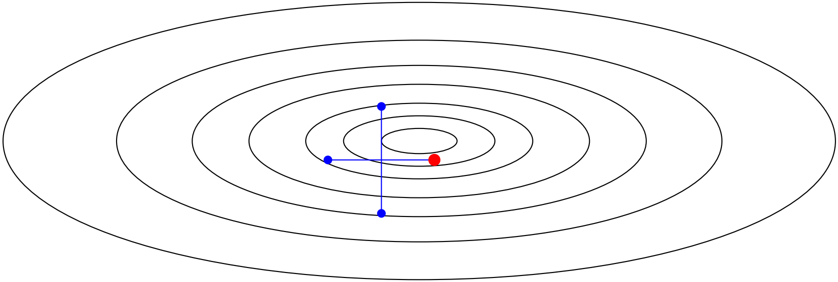

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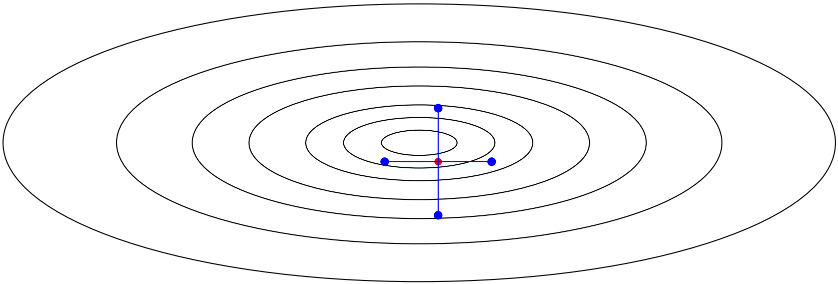

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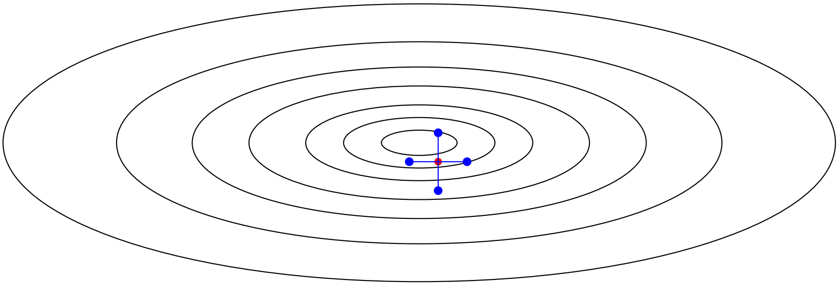

Problem setting and extreme barrier

In this talk, we consider a constrained minimization problem:

$$\begin{aligned} \min \quad & f(x), \\ \text{s.t.} \quad & x \in \Omega, \end{aligned}$$

where $f : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is nonsmooth and extended-real-valued and where $\Omega \subseteq \mathbb{R}^n$.

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We will make use of the extreme barrier function:

$$f_\Omega(x) = \begin{cases} f(x) & \text{if } x \in \Omega, \\ +\infty & \text{otherwise.} \end{cases}$$

Forcing function

A forcing function $\rho(\cdot)$ is continuous, positive, and satisfies

$$\lim_{t \longrightarrow 0^+} \frac{\rho(t)}{t} = 0 \qquad \text{and} \qquad \rho(t_1) \leq \rho(t_2) \quad \text{if} \quad t_1 < t_2.$$

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We will use $\bar{\rho}(\cdot)$ for either $\rho(\cdot)$ above or $\rho(\cdot) = 0$.

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Includes Coordinate Search, GPS or GSS, and MADS ...

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For $k = 0, 1, 2, \ldots$

(1) Search step (optional): Try to compute a point x with

$$f_\Omega(x) < f(x_k) - \bar{\rho}(\alpha_k)$$

by evaluating the function f at a finite number of points.

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If such a point is found then set $x_{k+1} = x$, declare the iteration and the search step successful, and skip the poll step.

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Order $P_k = \{x_k + \alpha_k d : \, d \in D_k\}$ and start evaluating f_Ω following the chosen order.

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If a point $x_k + \alpha_k d_k$ is found such that

$$f_\Omega(x_k + \alpha_k d_k) < f(x_k) - \bar{\rho}(\alpha_k)$$

then stop polling, set $x_{k+1} = x_k + \alpha_k d_k$, and declare the iteration and the poll step successful.

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Otherwise declare the iteration (and the poll step) unsuccessful and set $x_{k+1} = x_k$.

(3) Step size update: If the iteration was successful then maintain or increase the step size parameter: $\alpha_{k+1} \in [\alpha_k, \gamma\alpha_k]$.

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The parameters are chosen at initialization: $0 < \beta_1 \leq \beta_2 < 1$, and $\gamma \geq 1$

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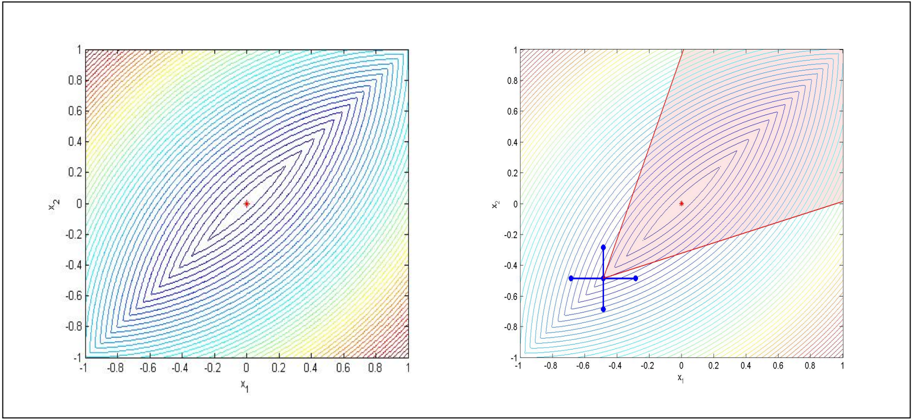
Polling can be opportunistic (like before) or complete (all the poll points are evaluated and the best is taken if better than the current iterate).

Finite directions in the nonsmooth case



The cone of descent directions at the poll center is shaded.

Need for infinitely many directions

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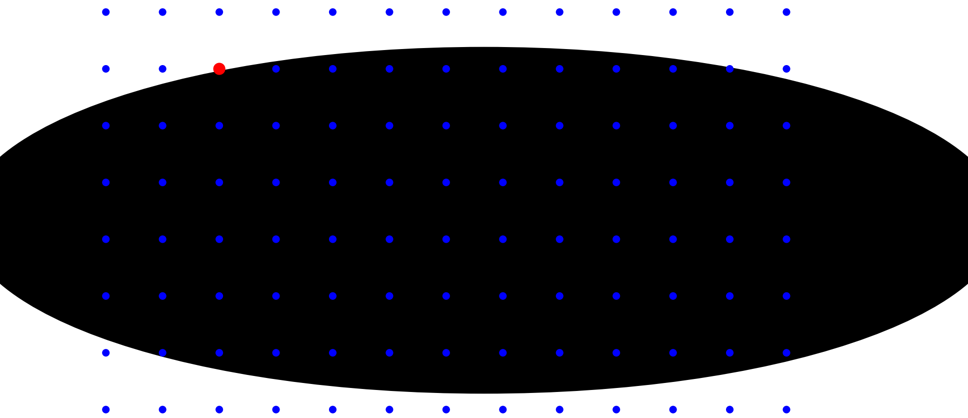
(1) Using integer lattices and simple decrease:

$\longrightarrow$ directions must be extracted from a finite set with integer/rational properties

$\longrightarrow$ search step must be restricted to the lattice (and the step size update must also follow integer/rational requirements).

(MADS by Audet and Dennis, 2006)

Integer lattice requirements (when using simple decrease)



$$L(x_0) = \{x \in \mathbb{R}^n : \ f(x) \leq f(x_0)\}$$

The intersection of $L(x_0)$ with the underlying lattice must be finite.

Need for infinitely many directions (suff. decrease)

(2) Using sufficient decrease:

$\longrightarrow$ directions can be randomly generated.

(like in GSS — see the 2003 SIAM Review paper of Kolda, Lewis, and Torczon)

Conditions on the directions

In both cases, one must also have:

Condition

The distance between x_k and the point $x_k + \alpha_k d_k$ tends to zero if and only if α_k does:

$$\lim_{k \in K} \alpha_k \|d_k\| \; = \; 0 \iff \lim_{k \in K} \alpha_k \; = \; 0,$$

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and

Condition

The set of refining directions at a limit point (associated with any refining subsequence) is dense is the unit sphere.

Behavior of the step size parameter

Assumption

The level set $L(x_0) = \{x \in \Omega : \ f(x) \leq f(x_0)\}$ *is bounded. The function* f *is bounded below in* $L(x_0)$.

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Lemma

If one uses (1) MADS or (2) suff. decrease, then $\exists$ *a subsequence* K *of unsuccessful iterations:*

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The proof goes back to Torczon 1997 (and was adapted to MADS later by Audet and Dennis, 2003 and 2006).

The case of suff. decrease is trivial (see IDFO book or the SIAM Rev. paper).

Refining subsequence and refining direction

This shows the existence of:

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($x_k + \alpha_k d_k$ must be in Ω for sufficiently large $k \in L$).

Focus first on the unconstrained case

For the analysis, let us consider first the case $\Omega = \mathbb{R}^n$.

Clarke generalized directional derivative

Definition

For f Lipschitz continuous near x_*, the Clarke generalized directional derivative is:

$$f_C^\circ(x_*; v) = \limsup_{x' \to x_* \; t \downarrow 0} \frac{f(x' + tv) - f(x')}{t}.$$

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Definition

x_* is a Clarke stationary point if

$$f_C^\circ(x_*;v) \ \geq \ 0, \quad \forall v \in \mathbb{R}^n.$$

Analysis of MADS or of the suff. decrease variant

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Theorem

If v *is a refining direction for* x_*:

$$f_C^\circ(x_*;v) \ \geq \ 0.$$

For the case of MADS, the proof is due to Audet and Dennis, 2006.

Non-Lipschitzian case

What happens in the case where f is not Lipschitz continuous near x_*?

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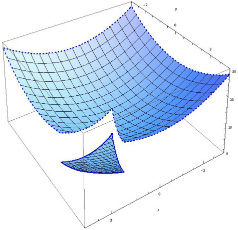
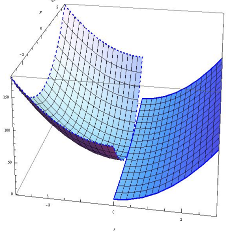
- However, f could still have directional derivatives...
- and they could be nonnegative!





Rockafellar generalized directional derivative

Definition

For f lower semicontinuous at x_*, the Rockafellar generalized directional derivative is:

$$f_R^\circ(x_*; v) = \limsup_{x' \to_f x_*, t \downarrow 0} \frac{f(x' + tv) - f(x')}{t}.$$

The notation $x' \to_f x_*$ represents $x' \to x_*$ and $f(x') \to f(x_*)$.

The next question is...

When do these derivatives exist?

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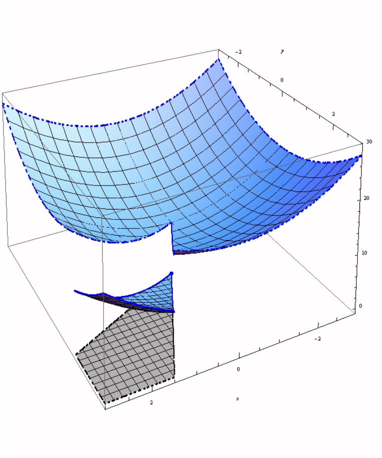


Directionally Lipschitzian function w.r.t. a direction

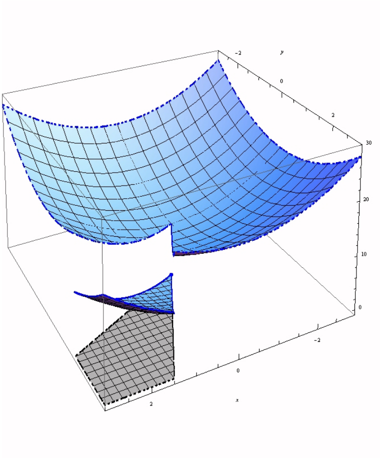
They exist when the following property holds:

Definition

f *directionally Lipschitzian at* x_* *with respect to* v *when*

$$\limsup_{x' \to_f x_*, t \downarrow 0} \sup_{v' \to v} \frac{f(x' + tv') - f(x')}{t} < +\infty.$$

Directionally Lipschitzian function w.r.t. a direction



This function is directionally Lipschitzian w.r.t. the directions in the interior of the shaded region.

Back to our direct-search results...

Assumption

- $\{x_k\}_{k \in K}$ *refining subsequence converging to* $x_* \in \Omega$.
- f *lower semicontinuous at* x_*.
- $\lim_{k \in K} f(x_k) = f(x_*)$.

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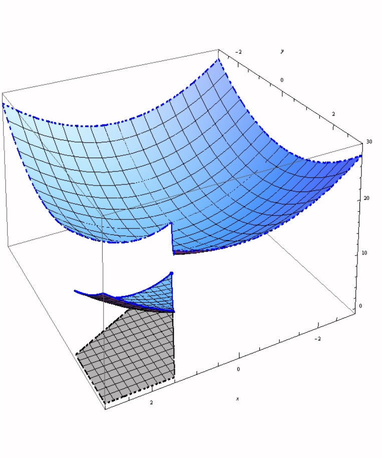
Theorem

If v *is a refining direction for* x_* *w.r.t. which* f *directionally Lipschitzian at* x_**:*

$$f_R^\circ(x_*; v) \ \geq \ 0.$$

Directionally Lipschitzian function w.r.t. a direction



This theorem allow us to state results in the interior of the shaded region.

One also has

Definition

The Rockafellar upper subderivative is defined by

$$f^{\uparrow}(x_*;v) \;=\; \limsup_{x' \to_f x_*,\, t \downarrow 0} \; \inf_{v' \to v} \frac{f(x'+tv') - f(x')}{t}.$$

Rockafellar upper subderivative

Due to...

Theorem (Rockafellar)

$$f^{\uparrow}(x_*; v) \;=\; \liminf_{v' \to v} f_R^{\circ}(x_*; v').$$

... we would also get, in this example, $f^{\uparrow}(x_*; v) \geq 0$ along the border of the shaded region.

The constrained case

As in the continuous case (Audet and Dennis, 2006):

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(3) For directions in the tangent cone (not in the hypertangent cone) use continuity of $f_R^\circ(x_*; v)$ and l.s.c. of $f^\uparrow(x_*; v)$.

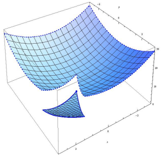
Finite number of step discontinuities

Let us look, now, at functions locally defined by a finite number of steps or branches:

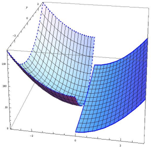
Assumption

There exists a neighborhood $B = \bigcup_{i=1}^{n_B} B_i$ *of* x_* *such that:*

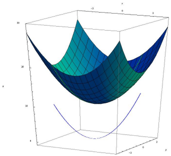
- $int(B_i) \neq \emptyset$
- $cl(B_i)$ *has the exterior cone property*
- f *is Lipschitz continuous in* $int(B_i)$ *and can be cont. extended to* ∂B_i



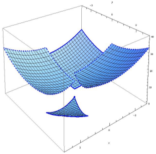
f_1



f_2



f_4 fails!



f_5

Finite number of step discontinuities

Theorem

If x_* belongs to the interior of a partition set, then $f_C^\circ(x_*; v) \geq 0$ for all refining directions $v \in T_\Omega(x_*)$.

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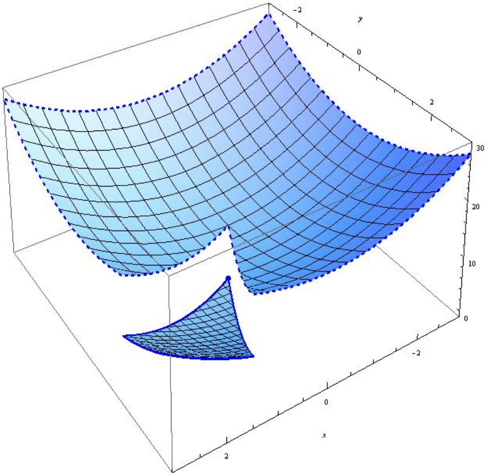
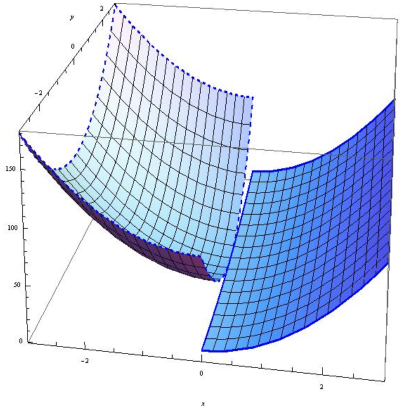
Corollary

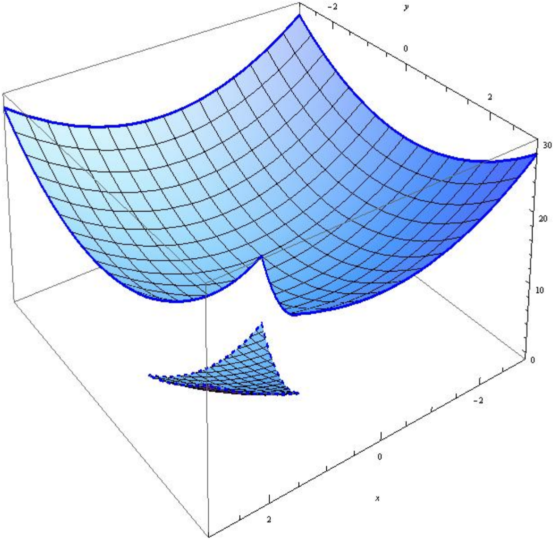
Additionally, if $n_B = 2$, then f attains its lowest values around x_* in B' and $\lim_{k \in K_*} f(x_k) = f(x_*)$ for $K_* \subset K'$.



-2
y
0
2
30
20
10
0
-2
0
x
2

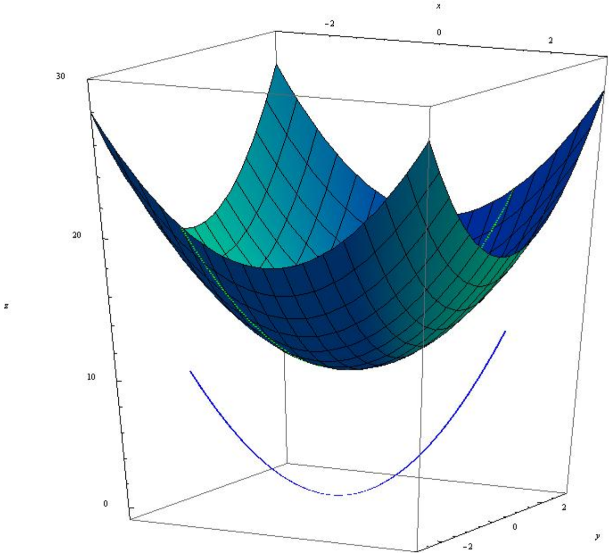
Function f_2



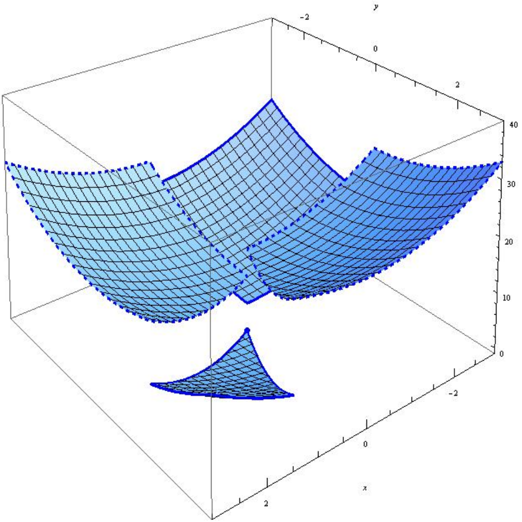


-2
y
0
2
30
20
10
0
-2
0
x
2

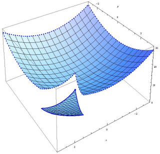
Function f_4



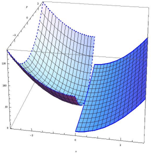
Function f_5



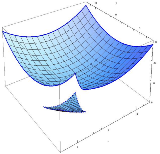
Numerical illustration



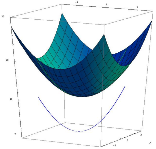
f_1



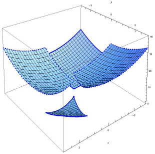
f_2



f_3

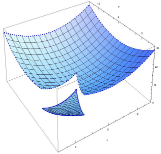


f_4

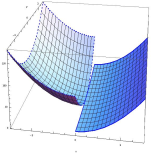


f_5

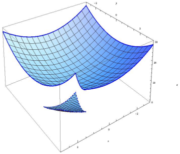
function	10 runs for the same initial point			
	MADS		Suff. Decrease	
	#failures	#fevals	#failures	#fevals
f_1	0	233	0	175.6
f_2	0	193.9	0	494.6
f_3	0	228.8	0	175.6
f_4	10	173.7	10	144.4
f_5	2	220.6	1	177.7



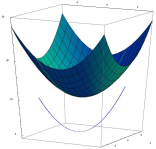
f_1



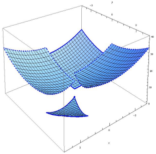
f_2



f_3



f_4



f_5

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Suff. Decrease	
function	#failures
f_1	2
f_2	0
f_3	2
f_4	1000
f_5	61

10 runs for
100 initial points

References

- L. N. Vicente and A. L. Custódio, Analysis of direct searches for non-Lipschitzian functions, 2009.

(2) Poll step: Choose a positive spanning set D_k from the set $\mathcal{D}$.

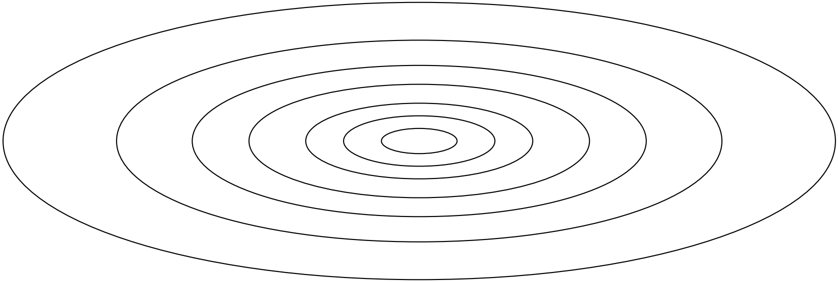
Order $P_k = \{x_k + \alpha_k d : \, d \in D_k\}$ and start evaluating f_Ω following the chosen order.

If a point $x_k + \alpha_k d_k$ is found such that

$$f_\Omega(x_k + \alpha_k d_k) < f(x_k) - \bar{\rho}(\alpha_k)$$

then stop polling, set $x_{k+1} = x_k + \alpha_k d_k$, and declare the iteration and the poll step successful.

Coordinate search (poll ordering — opportunistic)



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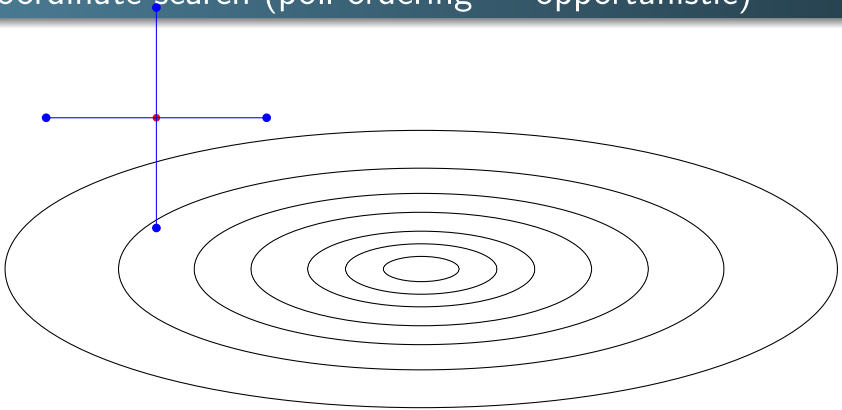

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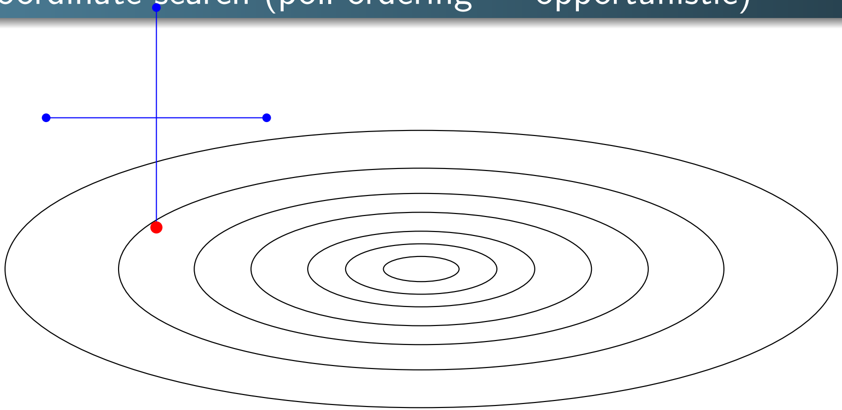

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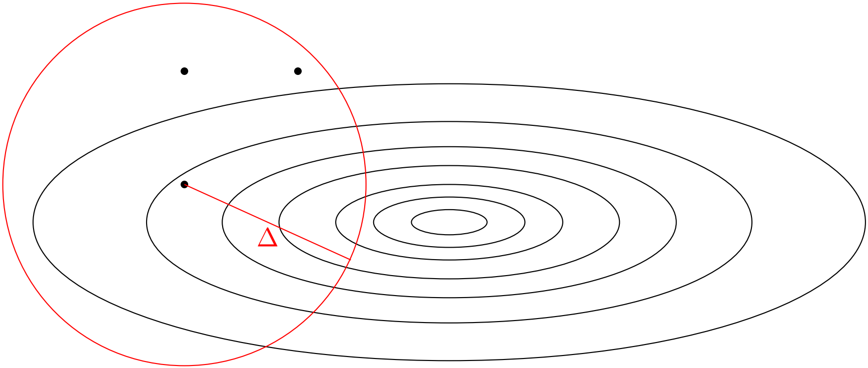

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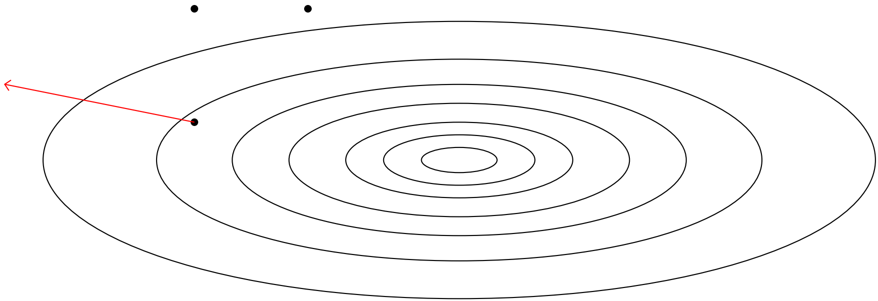

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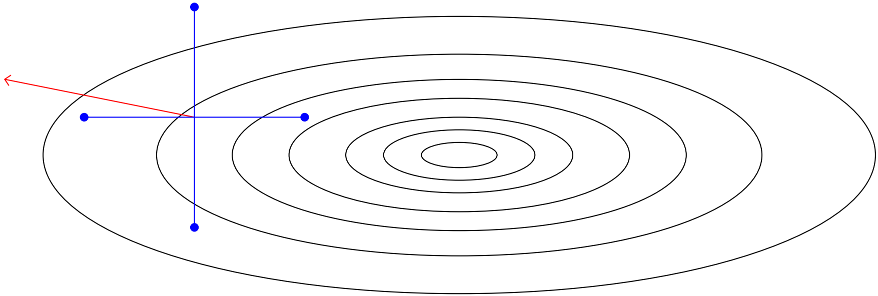

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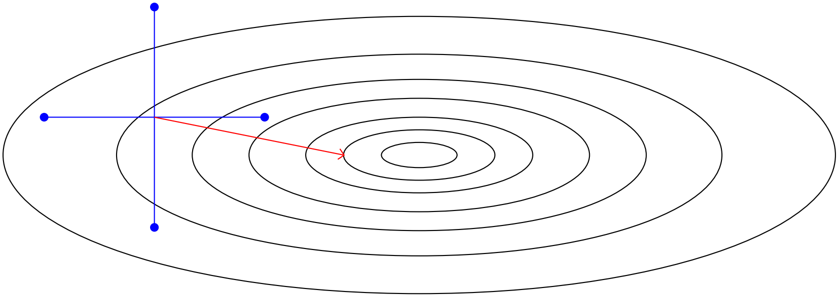

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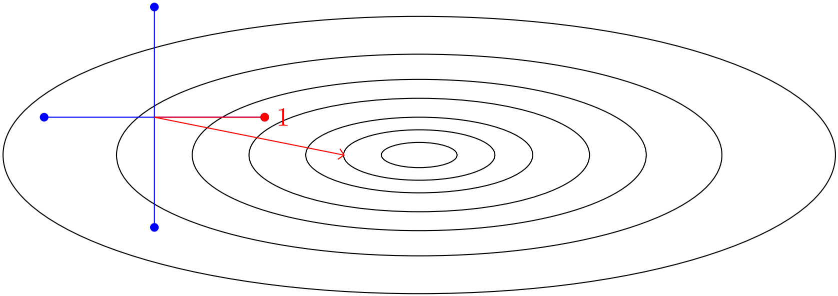

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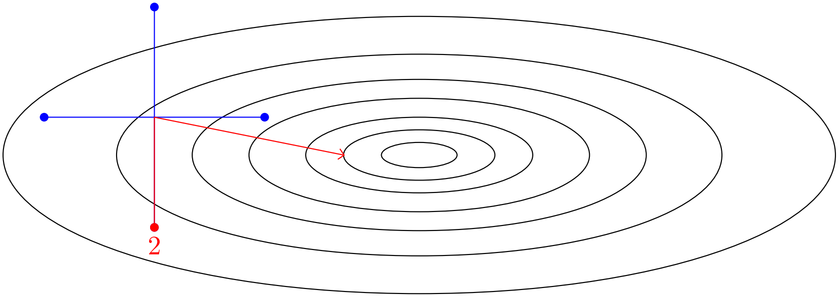

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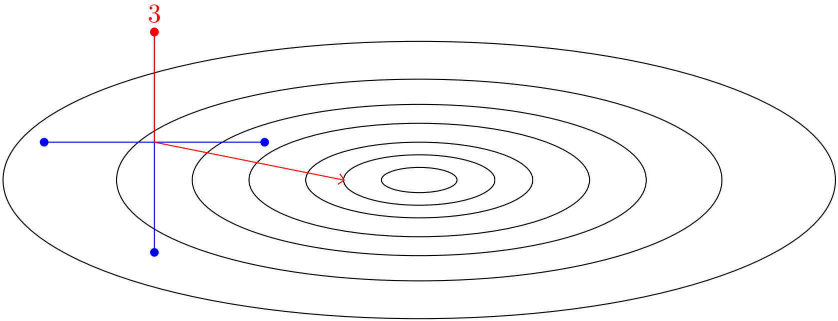
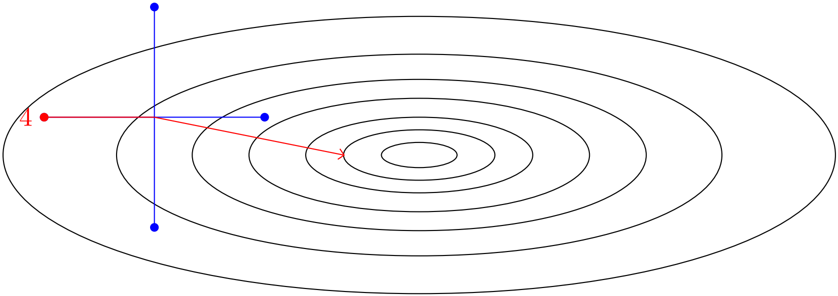


Coordinate search (poll ordering — opportunistic)



Poll ordering strategies

1. consecutive order of storage
2. random order

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   $\longrightarrow$ uses the negative simplex gradient

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7. model values order

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4. cycling order (start by the vector right after the last tested in the previous iteration)
5. (simplex descent) indicator order
   $\longrightarrow$ uses the negative simplex gradient
6. (model descent) indicator order
7. model values order
8. combinations of previous strategies:

Best strategy (for us):

negative simplex gradient + cycling order

Poll ordering by simplex gradients

$\longrightarrow$ Provided reductions of over 50% for smooth problems and over 25% for nonsmooth problems.

Poll ordering by simplex gradients

⟶ Provided reductions of over 50% for smooth problems and over 25% for nonsmooth problems.

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⟶ Analysis (in particular in the nonsmooth case) indicates favorable directional properties of the negative simplex gradient.

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1. A. L. Custódio and L. N. Vicente, Using sampling and simplex derivatives in pattern search methods, SIAM Journal on Optimization, 18 (2007), 537-555
2. A. L. Custódio, J. E. Dennis Jr., and L. N. Vicente, Using simplex gradients of nonsmooth functions in direct search methods, IMA Journal of Numerical Analysis, 28 (2008), 770-784

Recall... the class of directional direct-search methods

(1) Search step (optional): Try to compute a point x with

$$f_\Omega(x) < f(x_k) - \bar{\rho}(\alpha_k)$$

by evaluating the function f at a finite number of points.

If such a point is found then set $x_{k+1} = x$, declare the iteration and the search step successful, and skip the poll step.

Search step

The search step consists of evaluating the objective function at a finite number of points.

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The search step can take advantage of the existence of surrogate models for f to improve the efficiency of the direct-search method.

Search step requirements (when using simple decrease)

The search step must return a lattice point when $\bar{\rho}(\cdot) = 0$.

Minimum Frobenius Norm quadratic models

Given a sample set, MFN quadratic models are formed by:

$$\begin{aligned} \min \quad & \|\text{model Hessian}\|_F \\ \text{s.t} \quad & \text{interpolation conditions.} \end{aligned}$$

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$\longrightarrow$ MFN models can be shown 'fully linear' (see IDFO book).

$\longrightarrow$ MFN models provide very good numerical results when used in trust-region interpolation-based methods (within the codes `DFO` and `NEWUOA`).

Our search step

We collect previously evaluated poll points into a sample set.

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Then, our search step consists of:

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Then, our search step consists of:

- Computing a MFN quadratic model when interpolation is underdetermined.
- Computing an ℓ_2–regression quadratic model when interpolation is overdetermined.
- Minimizing the model in a trust region in $B(x_k; \Delta_k)$ with

$$\Delta_k \;=\; \mathcal{O}(\alpha_k),$$

where α_k is the step size parameter in direct search.

Our code sid-psm does essentially:

- Search step as described above.

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Software freely available at: `http://www.mat.uc.pt/sid-psm`

Numerical tests

Comparisons are made against the codes:

- APPSPACK — generalized pattern search (poll by random order), by T. G. Kolda's group.
- NEWUOA — interpolation-based trust-region method (least updating MFN models), by M. J. D. Powell.
- NMSMAX — Nelder-Mead method, by N. J. Higham.

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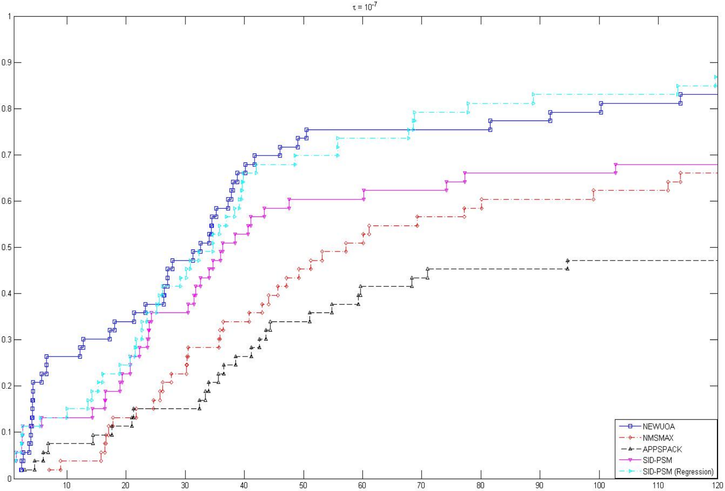
Using an unconstrained test set (Moré and Wild) formed by:

- Smooth (53 nonlinear least squares problems obtained from CUTEr functions, with $n \in [2, 12]$).
- Non-stochastic noisy (adding oscillatory noise to the smooth ones).
- Non-differentiable (as in the smooth case but by taking ℓ_1 norms).
- Stochastic noisy (adding random noise to the smooth ones).

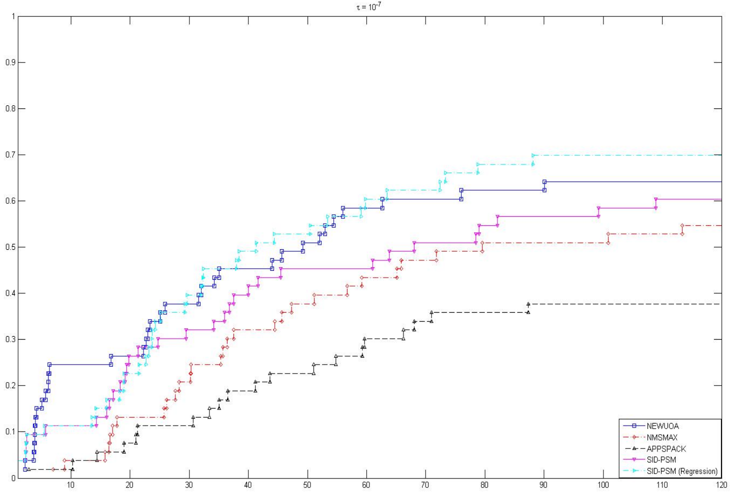
Data profiles — smooth

$\tau = 10^{-7}$



Data profiles — non-stochastic noisy

$\tau = 10^{-7}$



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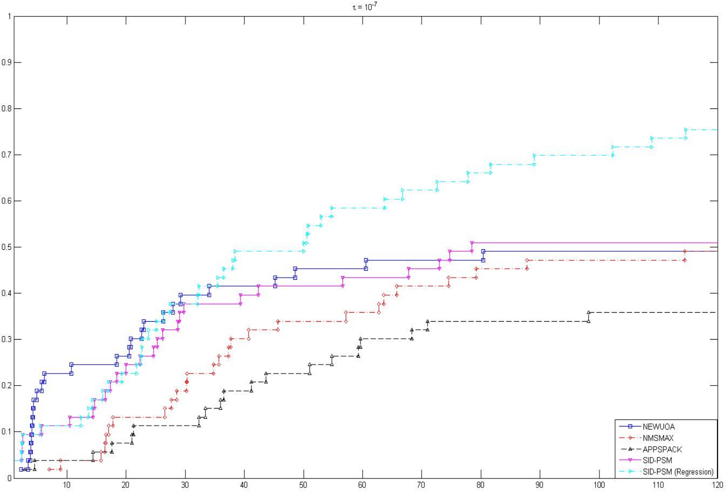
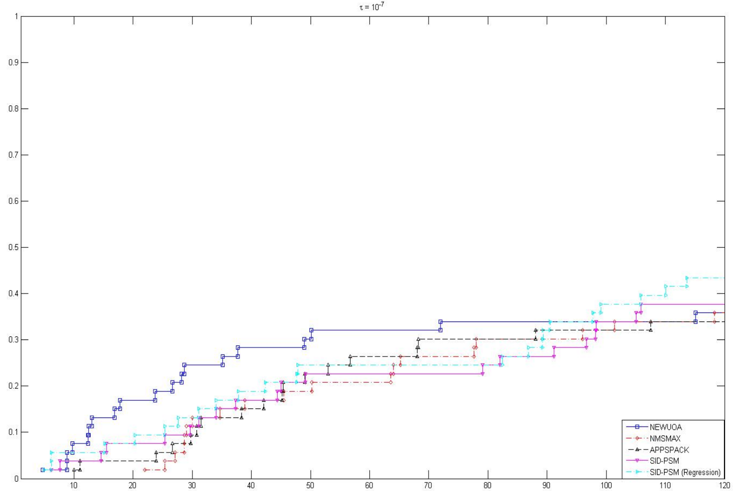

τ = 10^-7
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
10
20
30
40
50
60
70
80
90
100
110
120
NEWUOA
NMSMAX
APPSPACK
SID-PSM
SID-PSM (Regression)

$\tau = 10^{-7}$


τ = 10^-7
1
0.9
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20
30
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60
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The study by Sahinihis and Rios

23 DFO codes have recently been tested and compared by:

- L. M. Rios and N. Sahinidis, Derivative-free optimization: A review of algorithms and comparison of software implementations, 2010.

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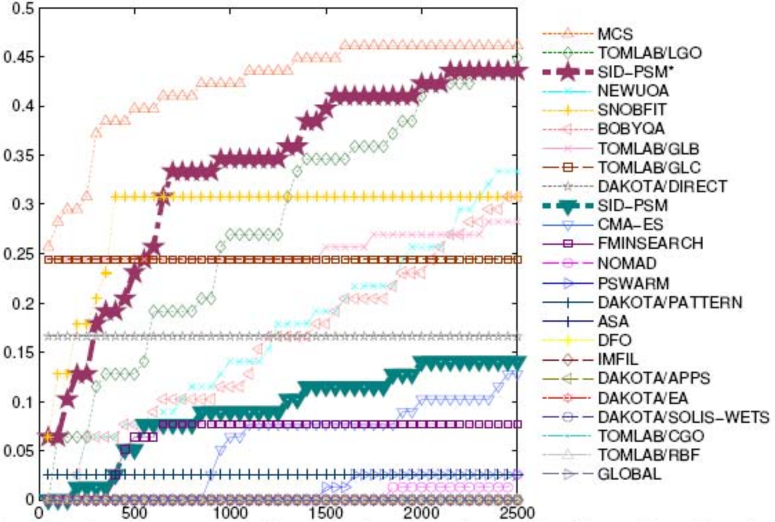
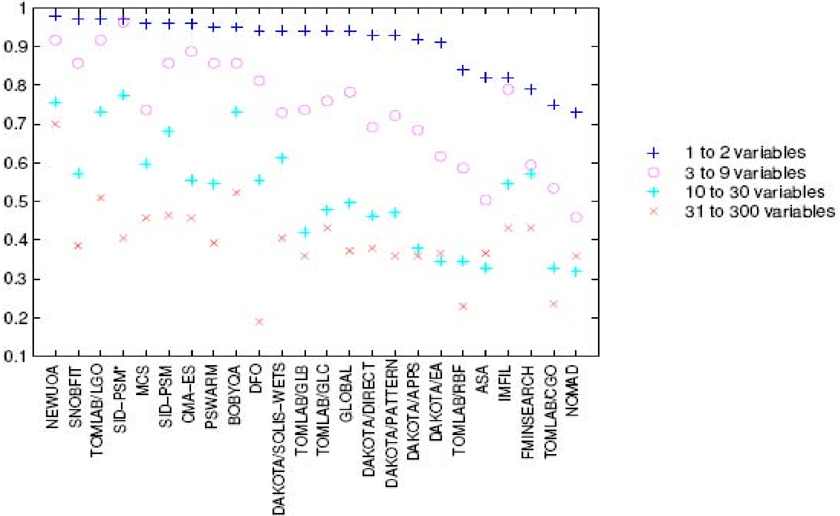
$\longrightarrow$ Test set of 505 problems (convex & nonconvex).



Fraction of convex smooth problems solved as a function of allowable number of function evaluations.



Fraction of problems solved from a near-optimal solution.

References

- A. L. Custódio, H. Rocha, and L. N. Vicente, Incorporating minimum Frobenius norm models in direct search, published online in Computational Optimization and Applications.

Upcoming papers

Model based:

- Bilevel Derivative-Free Optimization and its Application to Robust Optimization

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Direct search:

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- Complexity of Direct Search can be $\mathcal{O}(\epsilon^{-2})$

The book!

- A. R. Conn, K. Scheinberg, and L. N. Vicente, Introduction to Derivative-Free Optimization, MPS-SIAM Series on Optimization, SIAM, Philadelphia, 2009.