

Sparse and Smoothing Methods for Nonlinear Optimization Without Derivatives

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joint work with A. Bandeira (Princeton) and K. Scheinberg (Lehigh) (sparse)
R. Garmanjani (smoothing)

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<http://www.mat.uc.pt/~lnv>

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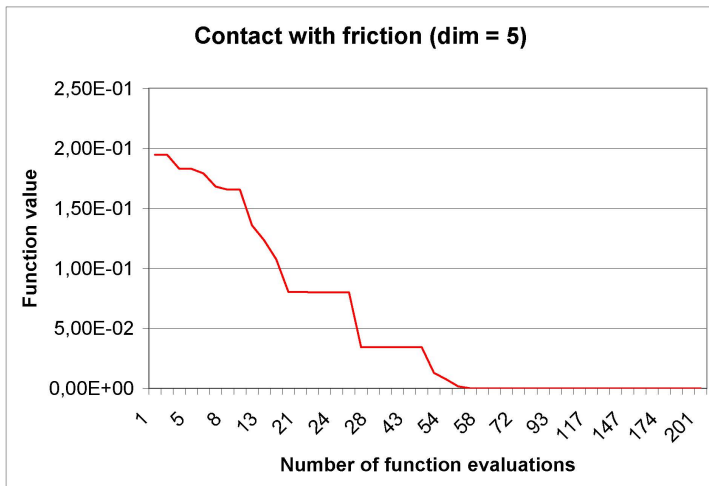
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- **Binary codes** (source code not available) and **random simulations** — making automatic differentiation impossible to apply.
- **Legacy codes** (written in the past and not maintained by the original authors).
- **Lack of sophistication** of the user (users need improvement but want to use something **simple**).

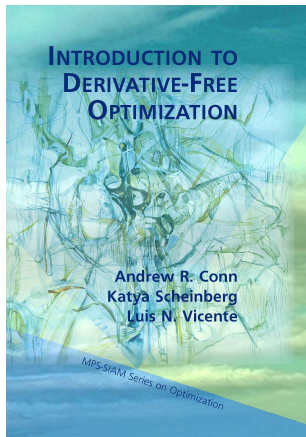
Limitations of Derivative-Free Optimization

In DFO **convergence/stopping** is typically **slow** (per function evaluation):



The book!

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



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- **Model-based methods**, of local nature.

Examples of models are **polynomials** or radial basis functions (**RBFs**).

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1st order Taylor:

$$m(y) = f(x) + \nabla f(x)^\top (y - x)$$

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Fully linear models can be quadratic (or even nonlinear).

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For a **class of fully quadratic models**, the (unknown) constants $\kappa_{ef}, \kappa_{eg}, \kappa_{eh} > 0$ must be **independent of x and Δ** .

Fully quadratic models are only necessary for global convergence to 2nd order stationary points.

Polynomial interpolation models

Given a **sample set** $Y = \{y^0, y^1, \dots, y^p\}$, a **polynomial basis** ϕ , and a **polynomial model** $m(y) = \alpha^\top \phi(y)$, the interpolating conditions form the linear system:

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where

$$M(\phi, Y) = \begin{bmatrix} \phi_0(y^0) & \phi_1(y^0) & \cdots & \phi_p(y^0) \\ \phi_0(y^1) & \phi_1(y^1) & \cdots & \phi_p(y^1) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_0(y^p) & \phi_1(y^p) & \cdots & \phi_p(y^p) \end{bmatrix} \quad f(Y) = \begin{bmatrix} f(y^0) \\ f(y^1) \\ \vdots \\ f(y^p) \end{bmatrix}.$$

Natural/canonical basis

The **natural/canonical basis** appears in a **Taylor expansion** and is given by:

$$\bar{\phi} = \left\{ \frac{1}{2}y_1^2, \dots, \frac{1}{2}y_n^2, y_1y_2, \dots, y_{n-1}y_n, y_1, \dots, y_n, 1 \right\}.$$

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Under appropriate smoothness, the second order Taylor model, centered at 0, is:

$$\begin{aligned} f(0) [1] &+ \frac{\partial f}{\partial x_1}(0)[y_1] + \frac{\partial f}{\partial x_2}(0)[y_2] \\ &+ \frac{\partial^2 f}{\partial x_1^2}(0)[y_1^2/2] + \frac{\partial^2 f}{\partial x_1 x_2}(0)[y_1 y_2] + \frac{\partial^2 f}{\partial x_2^2}(0)[y_2^2/2]. \end{aligned}$$

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An equivalent definition of Λ -poisedness is ($|Y| = |\alpha|$)

$$\|M(\bar{\phi}, Y_{scaled})^{-1}\| \leq \Lambda,$$

with Y_{scaled} obtained from Y such that $Y_{scaled} \subset B(0; 1)$.

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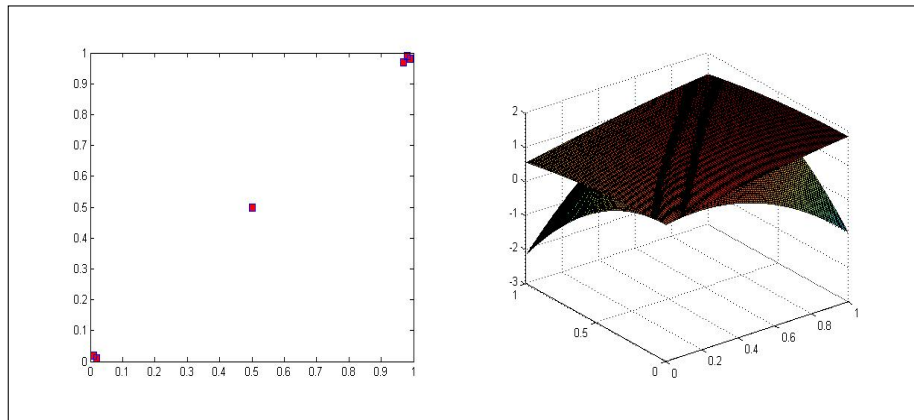
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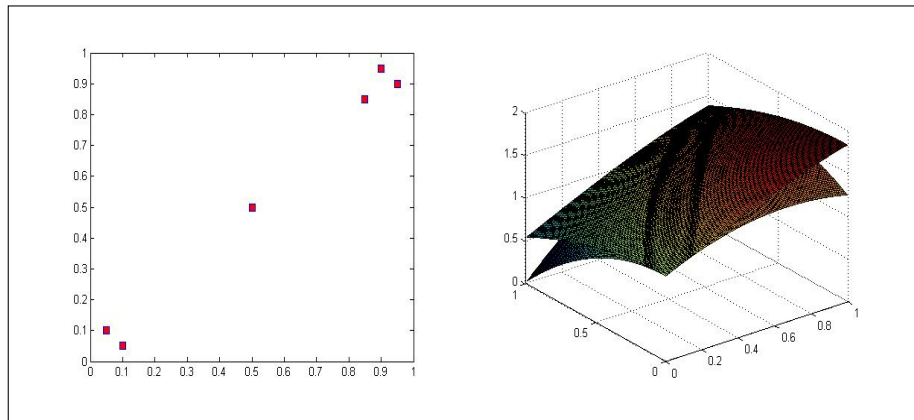
Non-squared cases are defined analogously (IDFO).

A badly poised set



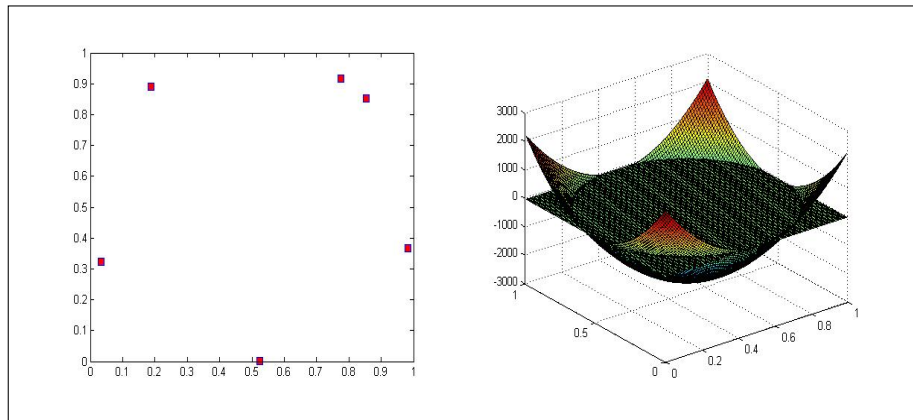
$$\Lambda = 5324.$$

A not so badly poised set



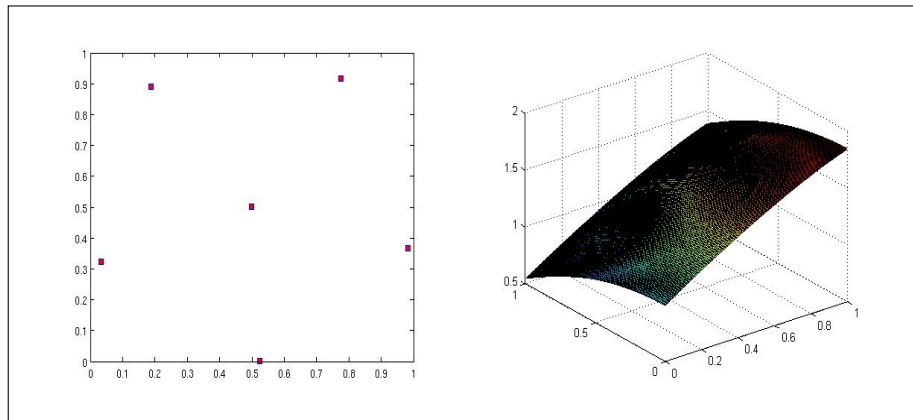
$$\Lambda = 295.$$

Another badly poised set



$$\Lambda = 492625.$$

An ideal set



$$\Lambda = 1.$$

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 - **Other approaches?...**

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Theorem (IDFO book)

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$$\|\nabla f(y) - \nabla m(y)\| \leq \Lambda_L [C_f + \|H\|] \Delta \quad \forall y \in B(x; \Delta).$$

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→ One should build models by **minimizing** the norm of H .

Minimum Frobenius norm models

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$$m(y) = \alpha_Q^T \bar{\phi}_Q(y) + \alpha_L^T \bar{\phi}_L(y).$$

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Then, build models by minimizing the entries of the Hessian ('Frobenius norm'):

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The solution of this convex QP problem requires a linear solve with:

$$\begin{bmatrix} M_Q M_Q^\top & M_L \\ M_L^\top & 0 \end{bmatrix} \quad \text{where} \quad M(\bar{\phi}, Y) = [M_Q \quad M_L].$$

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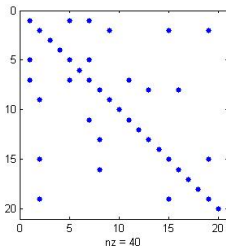
→ MFN models are fully linear.

Sparsity on the Hessian

- In many problems, pairs of variables have no 'correlation', leading to **zero** second order partial derivatives in f :

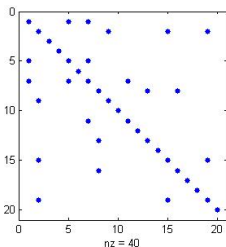
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- Thus, the Hessian $\nabla^2 m(x=0)$ of the model (i.e., the vector α_Q in the basis $\bar{\phi}$) should be **sparse**.

Our main question

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An answer will be given by building the models using instead the ℓ_1 -norm and relaxing the interpolating conditions for noisy recovery

$$\begin{aligned} \min \quad & \|\alpha_Q\|_1 \\ \text{s.t.} \quad & \|M(\bar{\phi}, Y)\alpha - f(Y)\|_2 \leq \eta. \end{aligned}$$

Compressed sensing — sparse recovery

- Objective: Find **sparse** α subject to a **highly underdetermined** linear system $M\alpha = f$.

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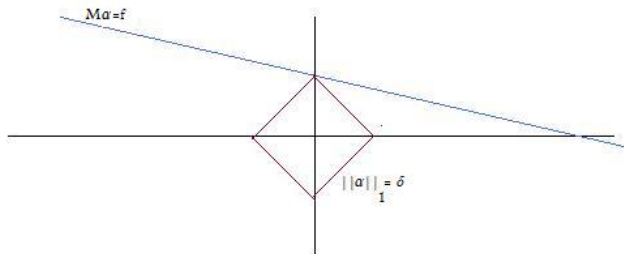
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The *RIP Constant* of order s of M ($p \times N$) is the smallest δ_s such that

$$(1 - \delta_s)\|\alpha\|_2^2 \leq \|M\alpha\|_2^2 \leq (1 + \delta_s)\|\alpha\|_2^2$$

for all s -sparse α ($\|\alpha\|_0 \leq s$).

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Theorem (Candès, Tao, 2005, 2006)

If $\bar{\alpha}$ is s -sparse and M satisfies RIP of order $2s$ with $\delta_{2s} < \frac{1}{3}$, then $\bar{\alpha}$ can be recovered by ℓ_1 -minimization:

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i.e., the optimal solution α^* of this problem is unique and given by $\alpha^* = \bar{\alpha}$.

Theorem (Candès 2009)

Let $M \in \mathbb{R}^{p \times N}$ satisfy RIP of order $2s$ with

$$\delta_{2s} < \sqrt{2} - 1.$$

For every s -sparse vector $\bar{\alpha} \in \mathbb{R}^N$, let noisy measurements $f = M\bar{\alpha} + \epsilon$ be given satisfying $\|\epsilon\|_2 \leq \eta$.

Let α^* be a solution of

$$\min_{\alpha \in \mathbb{R}^N} \|\alpha\|_1 \quad \text{s. t.} \quad \|M\alpha - f\|_2 \leq \eta.$$

Then

$$\|\alpha^* - \bar{\alpha}\|_2 \leq c_{total} \eta,$$

for a constant c_{total} only depending on the RIP constant.

Theorem (Jacques 2010, Bandeira, Scheinberg, and Vicente 2011)

Let $M = (M_1, M_2) \in \mathbb{R}^{p \times (N-r)} \times \mathbb{R}^{p \times r}$ satisfy RIP of order $2(s-r)$ with

$$\delta_{2(s-r)} < \sqrt{2} - 1.$$

For every $(s-r)$ -sparse vector $\bar{\alpha}_1$, with $\bar{\alpha} = (\bar{\alpha}_1, \bar{\alpha}_2)$, let noisy measurements $f = M\bar{\alpha} + \epsilon$ be given satisfying $\|\epsilon\|_2 \leq \eta$.

Let $\alpha^* = (\alpha_1^*, \alpha_2^*)$ be a solution of

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- It is **hard** to find **deterministic** matrices that satisfy the RIP for large s .

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- Using **Random Matrix Theory** it is possible to prove RIP for

$$p = \mathcal{O}(s \log N).$$

- Matrices with Gaussian entries.
- Matrices with Bernoulli entries.
- Uniformly chosen subsets of discrete Fourier transform.
- ...

Bounded orthonormal expansions (Rauhut)

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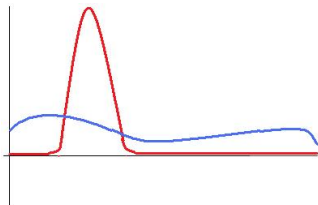
- Choose orthonormal bases (leads to uncorrelated matrix entries).

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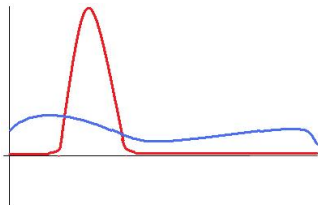


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- Select Y **randomly**.

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Then,

$$\|\alpha^* - \bar{\alpha}\|_2 \leq c_{total} \eta.$$

What basis do we need for sparse Hessian recovery?

Remember the second order Taylor model

$$\begin{aligned} & f(0) [1] + \frac{\partial f}{\partial x_1}(0)[y_1] + \frac{\partial f}{\partial x_2}(0)[y_2] \\ & + \frac{\partial^2 f}{\partial x_1^2}(0)[y_1^2/2] + \frac{\partial^2 f}{\partial x_1 x_2}(0)[y_1 y_2] + \frac{\partial^2 f}{\partial x_2^2}(0)[y_2^2/2]. \end{aligned}$$

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So, we want something like the **natural/canonical basis**:

$$\bar{\phi} = \left\{ \frac{1}{2}y_1^2, \dots, \frac{1}{2}y_n^2, y_1 y_2, \dots, y_{n-1} y_n, y_1, \dots, y_n, 1 \right\}.$$

An orthonormal basis for quadratics (appropriate for sparse Hessian recovery)

Proposition (Bandeira, Scheinberg, and Vicente, 2011)

The following basis ψ for quadratics is orthonormal (w.r.t. the uniform measure on $B_\infty(0; \Delta)$) and satisfies $\|\psi_\iota\|_{L^\infty} \leq 3$.

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→ ψ is **very similar** to the canonical basis, and preserves the **sparsity** of the Hessian (at 0).

Let us look again at

$$\min \|\alpha_Q\|_1 \quad \text{s. t.} \quad \|M(\phi, Y)\alpha - f\|_2 \leq \eta,$$

where

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Thus, in $\|\epsilon\| \leq \eta$, one has $\eta = \mathcal{O}(\Delta^3)$.

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$$q^* = \sum \alpha_i^* \psi_i$$

obtained by solving the *noisy and partial ℓ_1 -minimization problem* is a *fully quadratic model* for f (with error constants not depending on Δ).

An answer to our main question

- For instance, when the number of non-zeros of the Hessian is $h = \mathcal{O}(n)$, we are able to construct **fully quadratic models** with

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- Also, we **recover both** the function and its sparsity structure.

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- Deal with **small n** (from the DFO setting) and the bound we obtain is asymptotical.
- Use **deterministic** sampling.

A practical interpolation-based trust-region solver

We have tested the effect of minimum ℓ_1 -norm Hessian models in a practical trust-region DFO algorithm:

- New sample points are only defined by the trust-region step $x + \Delta x$ (no model management iterations).

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- Points too far from the current iterate are thrown away (sort of a criticality step).
- Trust-region radius is not reduced when the sample set has less than $n + 1$ points.

Performance profiles (accuracy of 10^{-4} in function values)

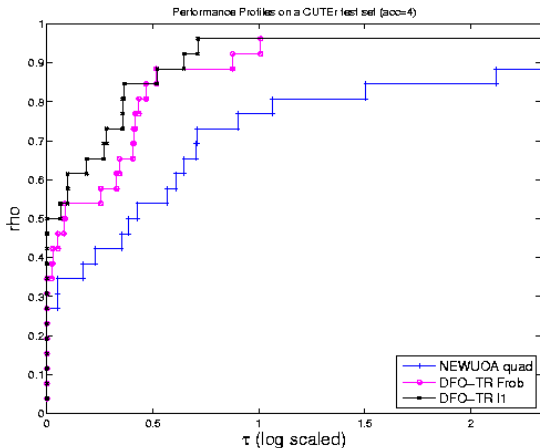


Figure: Performance profiles comparing DFO-TR (ℓ_1 and Frobenius) and NEWUOA (Powell) in a test set from CUTEr (Fasano et al.).

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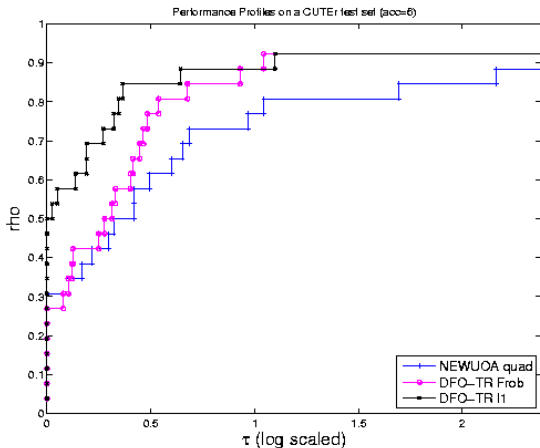


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Concluding remarks

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Concluding remarks

- Optimization is a fundamental tool in Compressed Sensing. However, this work shows that CS can also be 'applied to' Optimization.
- In a sparse scenario, we were able to construct fully quadratic models with samples of size $\mathcal{O}(n \log^4 n)$ instead of the classical $\mathcal{O}(n^2)$.
- We proposed a practical DFO method (using ℓ_1 -minimization) that was able to outperform state-of-the-art methods in several numerical tests (in the already 'tough' DFO scenario where n is small).

- Improve the efficiency of the model ℓ_1 -minimization, by properly [warmstarting](#) it (currently we solve it as an LP using `lipsol` by Y. Zhang).

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- Study the convergence properties of possibly **stochastic** interpolation-based trust-region methods.

- A. Bandeira, K. Scheinberg, and L. N. Vicente, [Computation of sparse low degree interpolating polynomials and their application to derivative-free optimization](#), 2011.
- A. Bandeira, K. Scheinberg, and L. N. Vicente, [On partially sparse recovery](#), 2011.
- A. R. Conn, K. Scheinberg, and L. N. Vicente, [Global convergence of general derivative-free trust-region algorithms to first and second order critical points](#), SIAM J. Optim., 20 (2009) 387–415.
- S. Gratton and L. N. Vicente, [A surrogate management framework using rigorous trust-regions steps](#), 2011.

Definition

- *Sample* the objective function at a *finite number* of points at each iteration.
- *Base actions* on those function values.

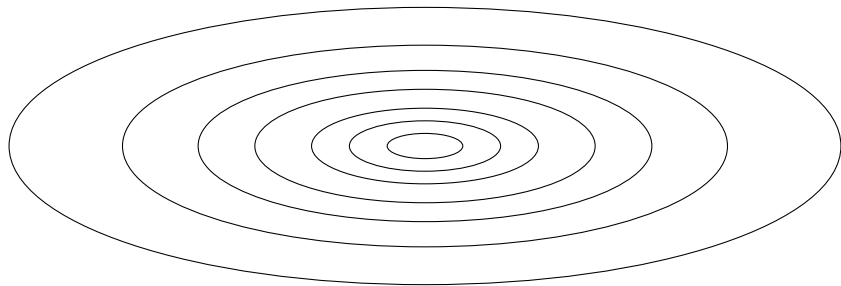
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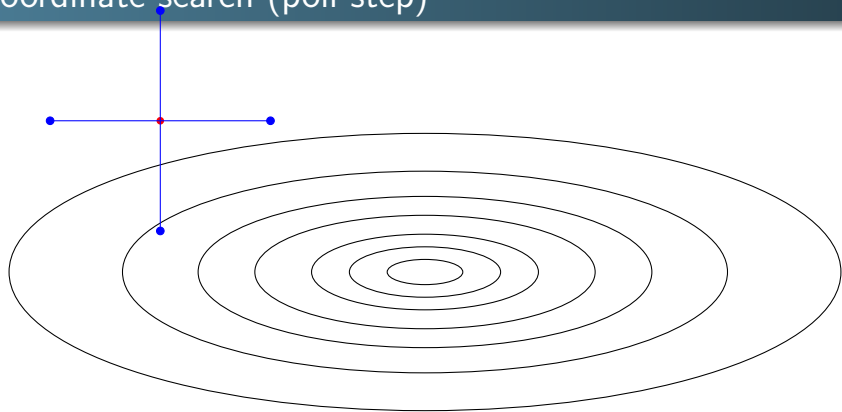
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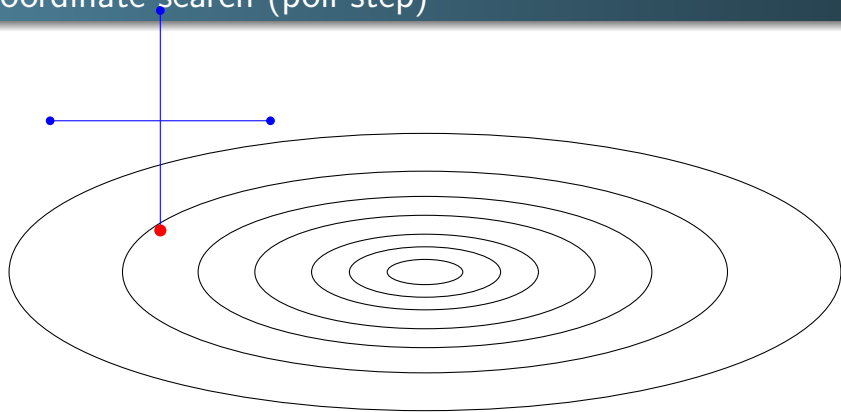
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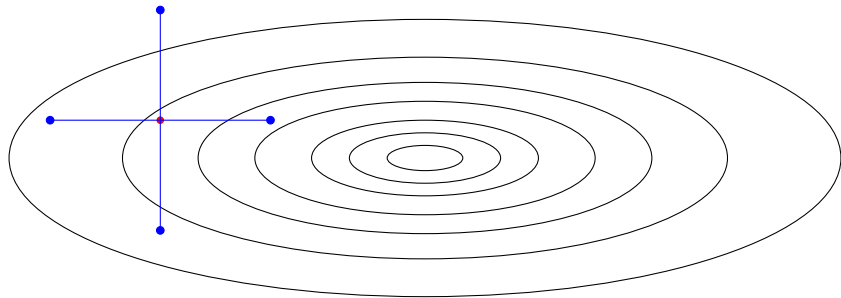
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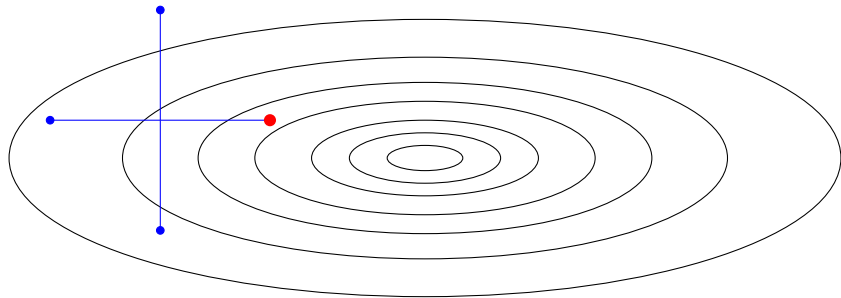
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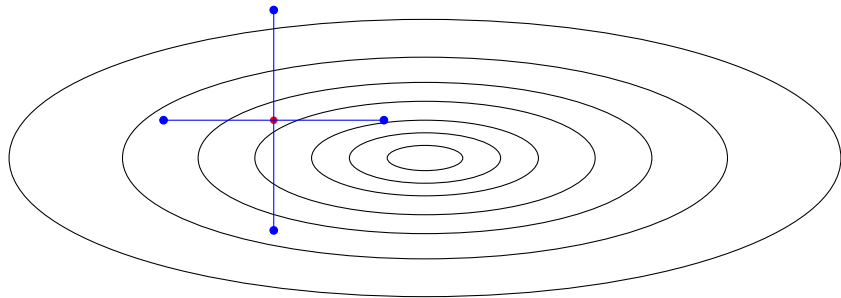
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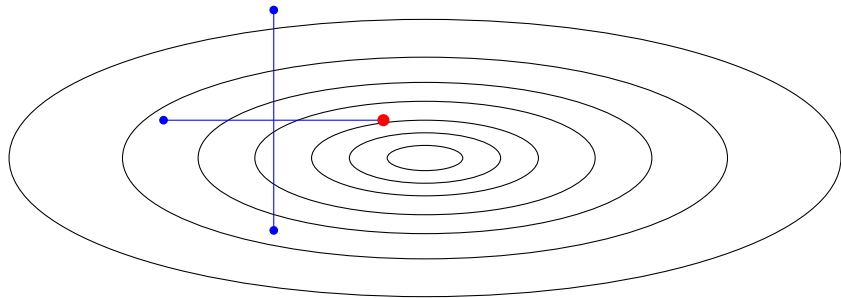
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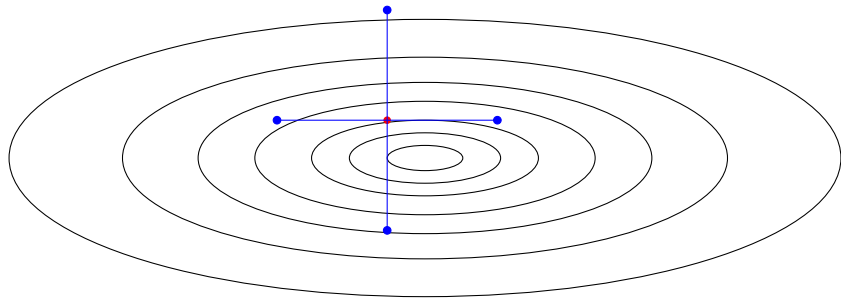
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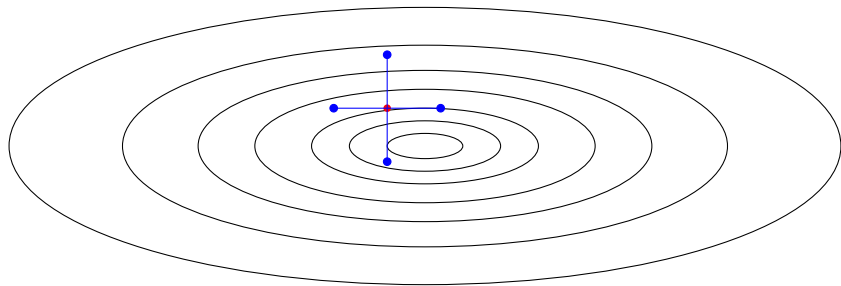
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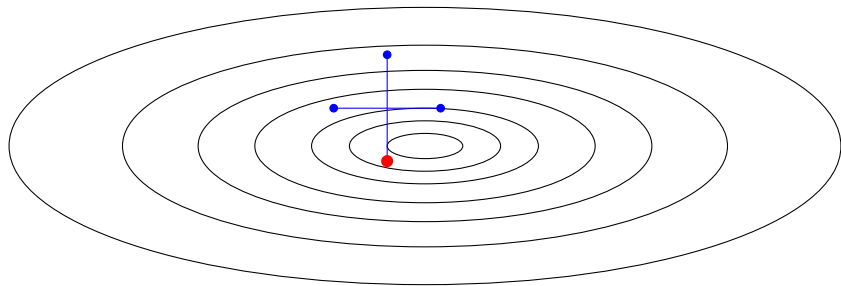
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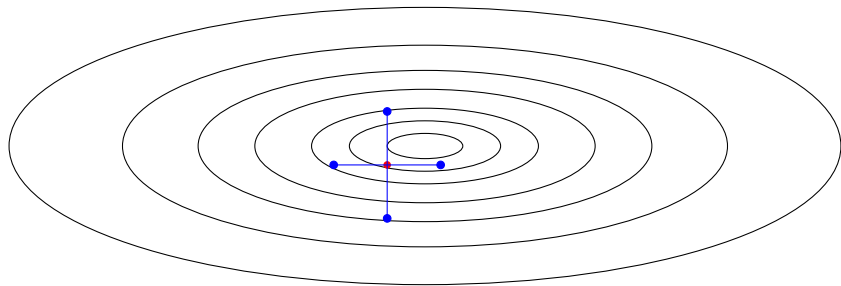
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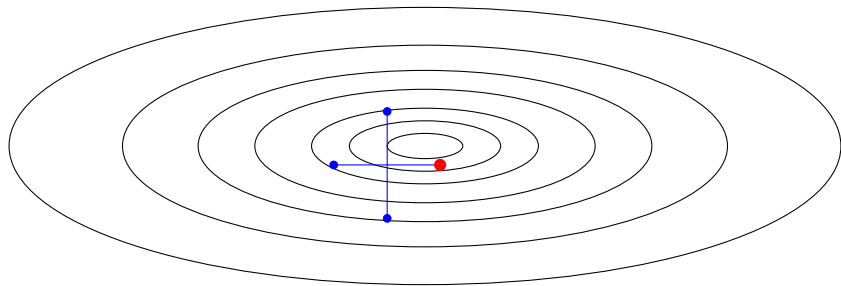
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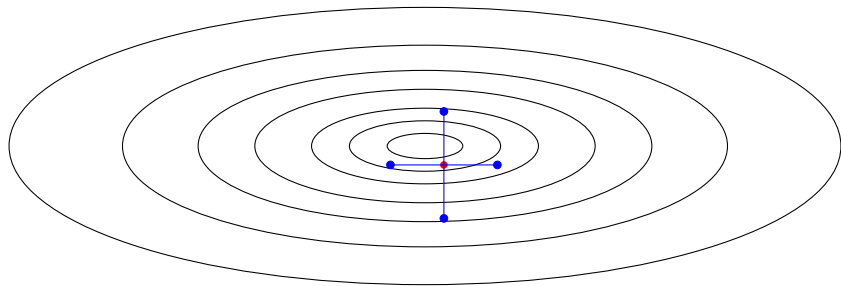
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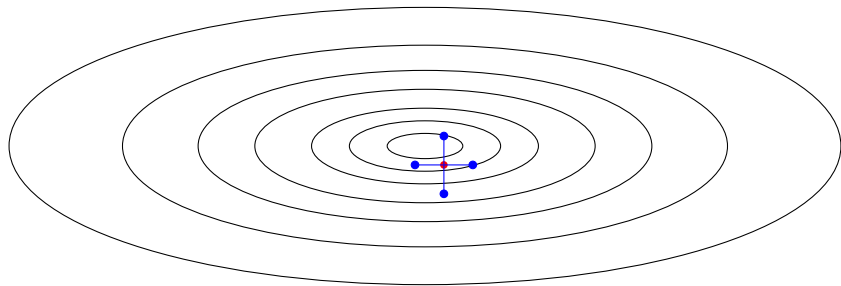
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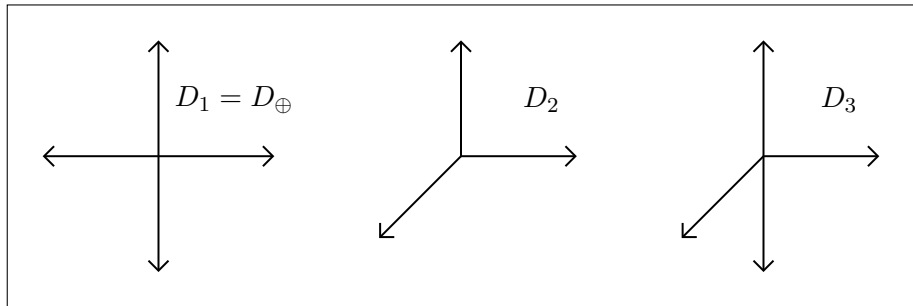
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Positive spanning sets / positive bases



All of them are positive spanning sets (since they span \mathbb{R}^n ($n = 2$) with nonnegative coefficients).

D_1 and D_2 are positive bases.

Unconstrained optimization

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

$$f : \mathbb{R}^n \rightarrow \mathbb{R}$$

f is at least locally Lipschitz continuous

Forcing function

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A simple example of a forcing function is when $p = 2$: $\rho(\alpha) = \alpha^2$.

A class of direct-search methods

Initialization: Choose x_0 and $\alpha_0 > 0$.

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

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

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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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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 $x_{k+1} = x_k$.

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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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From such a result, one can then prove global convergence results (some form of stationarity independently of the starting point).

The question that interest us (smooth case)

Question

Given $\epsilon \in (0, 1)$, how many iterations k are needed to reach

$$\|\nabla f(x_{k+1})\| \leq \epsilon.$$

Worst case complexity of direct search (smooth case)

Assumption

The norm of the vectors of any positive spanning set D_k are bounded above and away from zero.

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Theorem (Lewis, Tolda, and Torczon 2003)

Let D_k be a positive spanning set.

Assume that ∇f is Lipschitz continuous (with constant $L_f > 0$).

If $f(x_k + \alpha_k d) \geq f(x_k) - \rho(\alpha_k)$, for all $d \in D_k$, then

$$\|\nabla f(x_k)\| \leq C(L_f, \text{bounds}) \times \alpha_k \quad \dots \text{ in the case } \rho(\alpha) = \alpha^2.$$

Note that global convergence is deduced from here: $\|\nabla f(x_k)\| \xrightarrow{K} 0$.

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Theorem (LNV 2010)

Any direct-search method (based on sufficient decrease) takes at most

$$\mathcal{O}\left(\epsilon^{-\frac{p}{\min(p-1,1)}}\right)$$

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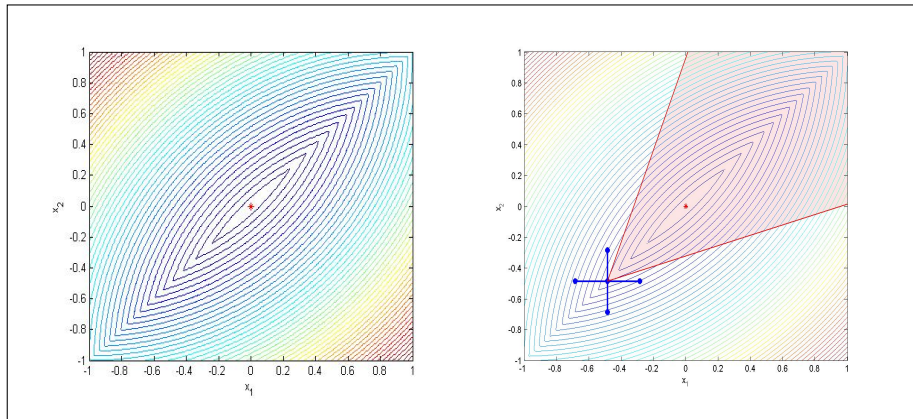
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Reference:

- L. N. Vicente, [Worst case complexity of direct search](#), preprint 10-17, Dept. of Mathematics, Univ. Coimbra, 2010.

Difficulties in the nonsmooth case



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

Difficulties in the nonsmooth case

Thus, one needs to use an **infinite number of polling directions**.

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... and thus to relate some form of stationarity (Clarke) to the step size.

One possible fix: Smoothing functions

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We call $\tilde{f} : \mathbb{R}^n \times \mathbb{R}^+ \rightarrow \mathbb{R}$ a smoothing function of f if

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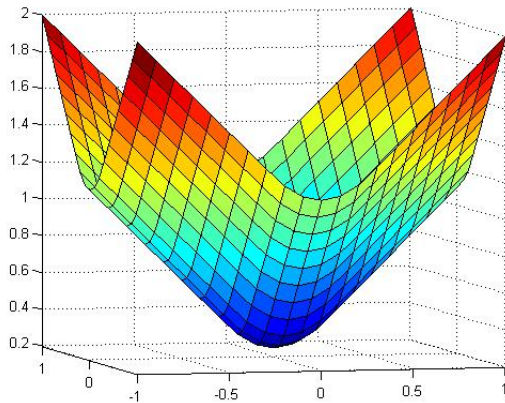
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- 2 and, for any $x \in \mathbb{R}^n$,

$$\lim_{z \rightarrow x, \mu \downarrow 0} \tilde{f}(z, \mu) = f(x).$$

Example of a smoothing function



A smoothing function of $|x_1| + |x_2|$ for $\mu = 0.5$.

A class of smoothing DS methods

Initialization: Choose a function $r(\cdot)$ such that $\lim_{\mu \downarrow 0} r(\mu) = 0$.

Choose $\mu_0 > 0$ and $\sigma \in (0, 1)$.

Choose $x_0 \in \mathbb{R}^n$.

For $k = 0, 1, \dots$

- Apply DS to $\tilde{f}(\cdot, \mu_k)$ (starting from $y_{0,k} = x_k$) generating points $y_{0,k}, \dots, y_{j,k}$ until $\alpha_{j+1,k} < r(\mu_k)$.
- Set $x_{k+1} = y_{j,k}$ and decrease the smoothing parameter: $\mu_{k+1} \in (0, \sigma \mu_k]$.

Assumption (for all k)

*The level sets $L(y_{0,k}) = \{y \in \mathbb{R}^n : \tilde{f}(y, \mu_k) \leq \tilde{f}(y_{0,k}, \mu_k)\}$ are bounded.
The functions $\tilde{f}(\cdot, \mu_k)$ are bounded below in $L(y_{0,k})$.*

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Theorem

The smoothing parameter goes to zero:

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

Global convergence of smoothing DS

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After having proved that μ_k goes to zero, one then obtains:

Theorem

- 1 $\lim_{k \rightarrow +\infty} \alpha_{j_k,k} = 0$.
- 2 *There exists a point x^* and a subsequence $K \subseteq \{j_1, j_2, \dots\}$ of unsucc. DS iterates such that $x_k = y_{j_k,k} \xrightarrow{K} x_*$.*

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Definition

We say that x^* is a *stationary point associated with the smoothing function \tilde{f}* if $0 \in G_{\tilde{f}}(x_*)$, where

$$G_{\tilde{f}}(x_*) = \{v : \exists N : x \xrightarrow[N]{} x_*, \mu \downarrow 0 \text{ with } \nabla_x \tilde{f}(x, \mu) \xrightarrow[N]{} v\}.$$

Does $0 \in G_{\bar{f}}(x_*)$ mean any form of true stationarity?

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Theorem

Let f be Lipschitz continuous near x_ .*

Let D_f be the subset of \mathbb{R}^n where f is differentiable.

Clarke subdifferential (alternative characterization)

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Then the Clarke subdifferential can be given by

$$\partial f(x_*) = \text{co}\{\lim \nabla f(x) : x \rightarrow x_*, x \in D_f\},$$

where co represents the convex hull.

Definition

We say that the sequence $\{\psi^\mu : \mathbb{R}^n \rightarrow \mathbb{R}^+, \mu \in \mathbb{R}^{++}\}$ is a *mollifier* if:

- $B^\mu = \{z : \psi^\mu(z) > 0\}$ converges to $\{0\}$, as $\mu \downarrow 0$,
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If the mollifiers $\{\psi^\mu\}$ are bounded and continuous on \mathbb{R}^n , then \tilde{f} is a smoothing function of f and one has the *gradient consistency property*

$$\partial f(x_*) = \text{co } G_{\tilde{f}}(x_*).$$

How to construct smoothing functions

In particular, mollifiers can be built from density functions.

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Let B be a bounded set and $\psi : B \rightarrow \mathbb{R}^+$ be a density function with $\int_B \psi(z) dz = 1$. The following is a mollifier:

$$\psi^\mu(z) = \begin{cases} \frac{\psi(x/\mu)}{\mu^n} & \text{if } z \in \mu B, \\ 0 & \text{otherwise.} \end{cases}$$

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There are other forms of building smoothing functions such that

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Worst case complexity of smoothing DS

Theorem

Any smoothing DS (based on sufficient decrease) takes at most (when $r(\mu) = \mu^q$)

$$\mathcal{O}((-\log \xi)\xi^{-pq})$$

iterations to reduce μ below $\xi \in (0, 1)$.

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Optimal choices consist of $q = 2$ and $p = 3/2$, leading to a worst case cost of

$$\mathcal{O}((-\log(\xi))\xi^{-3}).$$

A smoothing function for $\|F(\cdot)\|_1$

Chen and Zhou have introduced the following smoothing function of $|t|$:

$$\tilde{s}(t, \mu) = \int_{-\infty}^{\infty} |t - \mu\tau| \rho(\tau) d\tau,$$

where $\rho : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ is a piecewise continuous density function with a finite number of pieces satisfying

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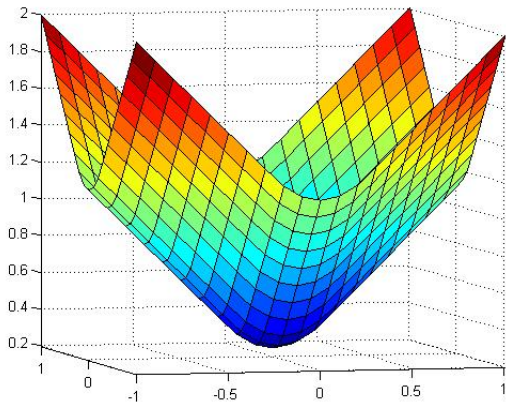
Using the density corresponding to the so-called Steklov mollifier,

$$\rho(\tau) = \begin{cases} 1 & \text{if } \tau \in [-\frac{1}{2}, \frac{1}{2}], \\ 0 & \text{otherwise,} \end{cases}$$

one obtains

$$\tilde{s}(t, \mu) = \begin{cases} \frac{t^2}{\mu} + \frac{\mu}{4} & \text{if } t \in [-\frac{\mu}{2}, \frac{\mu}{2}], \\ |t| & \text{otherwise.} \end{cases}$$

Example of this smoothing function



The smoothing function $\tilde{s}(x_1, \mu) + \tilde{s}(x_2, \mu)$ of $|x_1| + |x_2|$ for $\mu = 0.5$.

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$$\left\{ \lim_{t \rightarrow 0, \mu \downarrow 0} \tilde{s}'(t, \mu) \right\} = [-1, 1] = \partial|\cdot|(0).$$

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Now, let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be C^1 . Then $\tilde{s}(f)$ is a smoothing function of $|f|$.

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(i) $\tilde{F} = \sum_{i=1}^m \tilde{s}(F_i)$ is a smoothing function of $\|F\|_1 = \sum_{i=1}^m |F_i|$.

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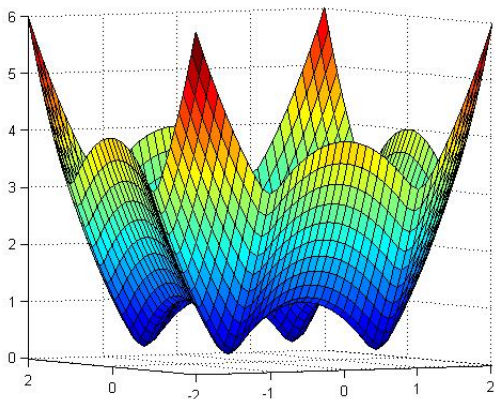
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Example of this smoothing function



The smoothing function $\tilde{F}(x_1, x_2, \mu)$
for $\|F(x_1, x_2)\|_1 = \|(x_1^2 - 1, x_2^2 - 1)\|_1$ and $\mu = 0.5$.

Some numerical experiments

We have tested the smoothing direct-search approach on the MATLAB direct-search `sid-psm` code:

- A. L. Custódio and L. N. Vicente, *Using sampling and simplex derivatives in pattern search methods*, SIAM Journal on Optimization, 18 (2007), 537-555.
- A. L. Custódio, H. Rocha, and L. N. Vicente, *Incorporating minimum Frobenius norm models in direct search*, Computational Optimization and Applications, 46 (2010) 265–278.

Some numerical experiments

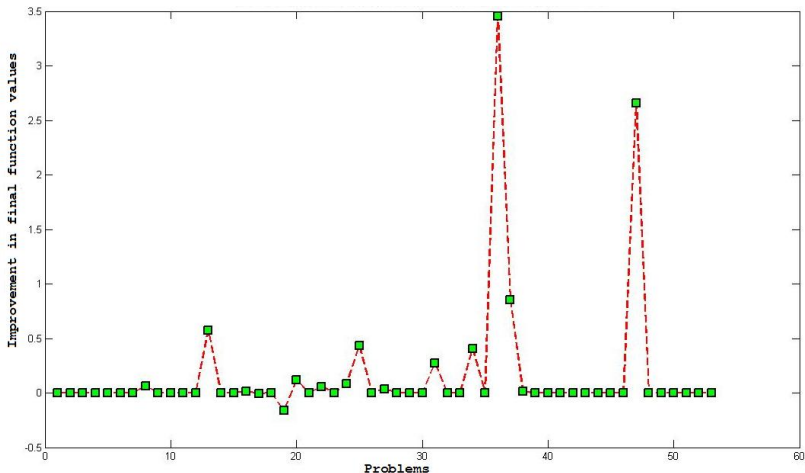
We have tested the smoothing direct-search approach on the MATLAB direct-search `sid-psm` code:

- A. L. Custódio and L. N. Vicente, *Using sampling and simplex derivatives in pattern search methods*, SIAM Journal on Optimization, 18 (2007), 537-555.
- A. L. Custódio, H. Rocha, and L. N. Vicente, *Incorporating minimum Frobenius norm models in direct search*, Computational Optimization and Applications, 46 (2010) 265–278.

We tested the `piecewise-linear problems` ($\min \|F(\cdot)\|_1$) from:

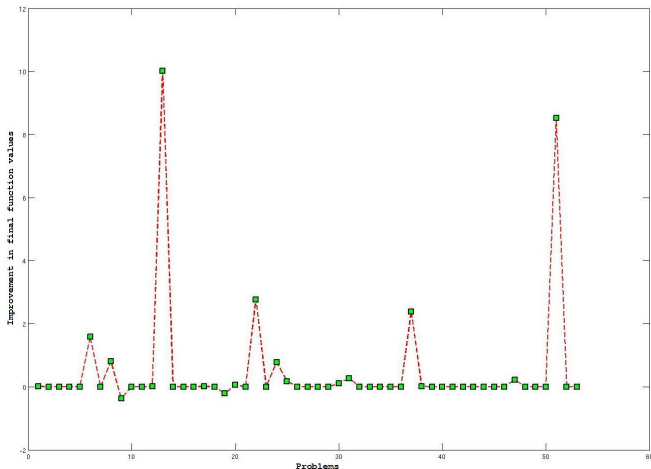
- J. J. Moré and S. M. Wild, *Benchmarking derivative-free optimization algorithms*, SIAM Journal on Optimization, 20 (2009), 172–191.

Some numerical experiments



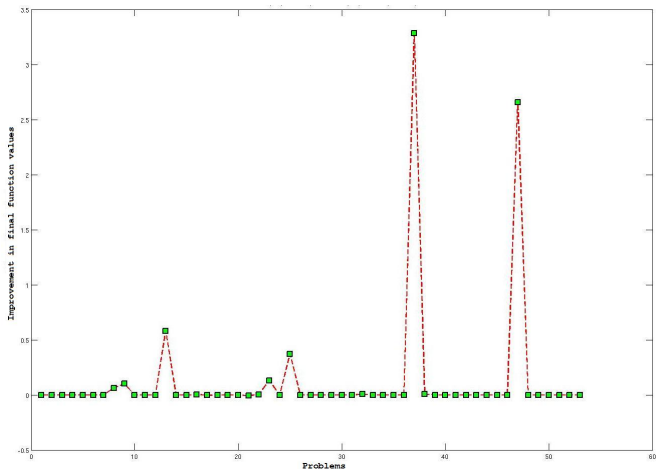
Smoothing DS with $\mu_0 = 10^{-2}$ vs DS
(no search step, cycling polling).

Some numerical experiments



Smoothing DS with $\mu_0 = 10^{-2}$ vs DS
(search step using smoothing function with $\mu = 10^{-4}$, cycling polling).

Some numerical experiments



Smoothing DS with $\mu_0 = 10^{-2}$ vs DS

(no search step, polling using simplex gradient of smoothing function with $\mu = 10^{-4}$).

We have developed a [smoothing direct-search approach](#) using smoothing functions.

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We have proved that the smoothing DS method is [globally convergent](#).

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Conclusions

We have developed a **smoothing direct-search approach** using smoothing functions.

We have proved that the smoothing DS method is **globally convergent**.

Smoothing DS is **costly** but seems able to find **better solutions**.

We have derived a **complexity** worst case bound for direct-search methods in the **non-smooth case**.