Trust-Region Methods for the Derivative-Free Optimization of Nonsmooth Black-Box Functions[1]

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ICOTA 2019, Xiangtan University

Dedicated to the 60th Anniversary of Professor Ya-xiang Yuan

[1] joint work with G.Liuzzi, S.Lucidi, F.Rinaldi

Presentation outline

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Problem definition

Problem to be solved:

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

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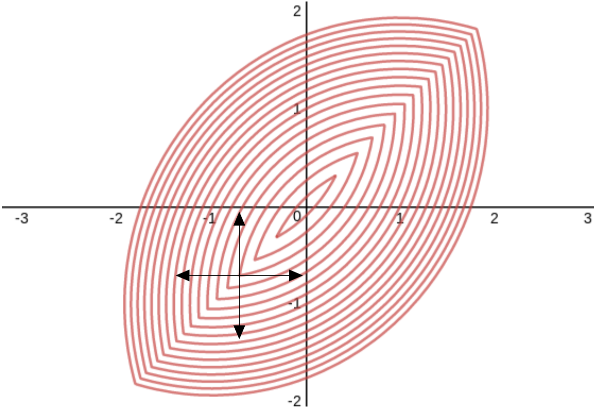
Assumptions:

- $f : \mathbb{R}^n \to \mathbb{R}$ is nonsmooth but Lipschitz continuous
- Mathematical representation of the objective function not available: **No knowledge about source of nonsmoothness**
- Function evaluations costly

Coordinate search failure



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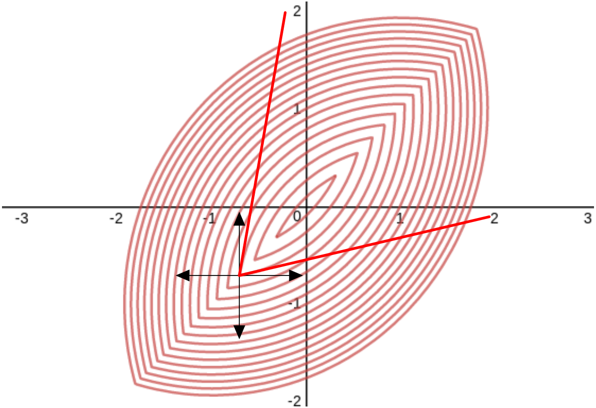
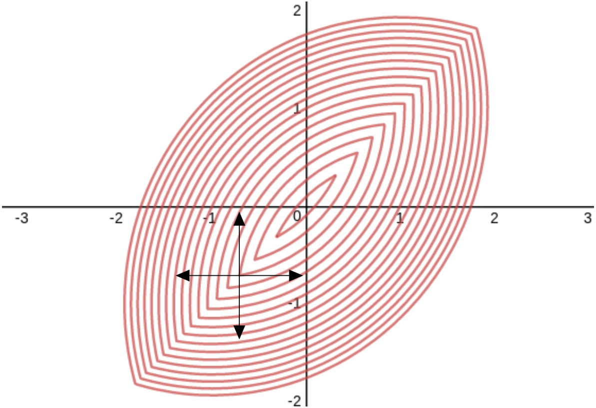


Drawback

Method gets stuck ... no search direction is in the cone of descent directions!

Convergence to non-stationary point

Asymptotically dense sets of search directions



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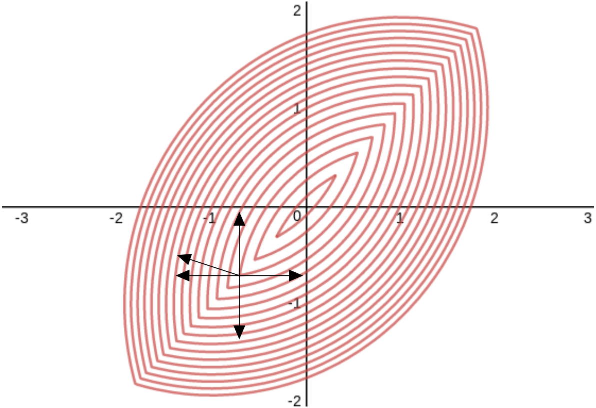
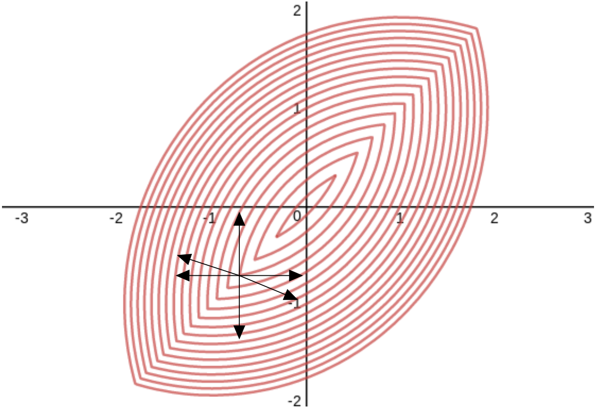


Trick

Enrich the set with new search directions

Asymptotically dense sets of search directions



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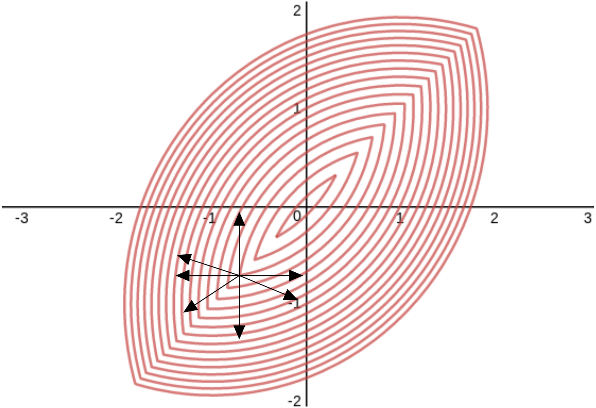

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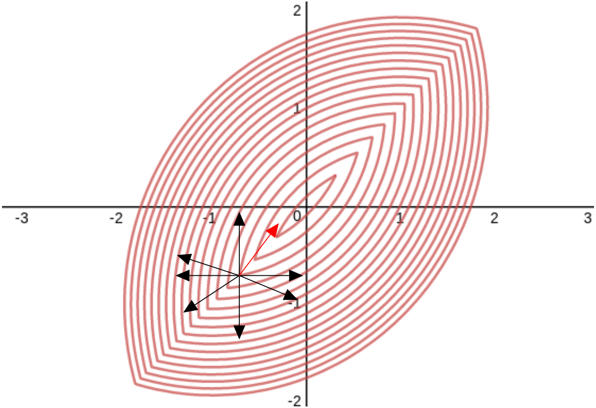

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Enrich the set with new search directions

How to handle black-box nonsmoothness?

- Directional approaches based on random directions asymptotically dense on the unit sphere:

  [Audet, Dennis, 2006]
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- Other convergent approaches require knowledge of nonsmoothness

Basic tools in non-smooth context

Clarke Directional Derivative

Given a point $x \in \mathbb{R}^n$ and a direction $d \in \mathbb{R}^n$, the Clarke directional derivative of f at x along d is defined as

$$f^\circ(x; d) = \limsup_{y \to x, t \downarrow 0} \frac{f(y + td) - f(y)}{t}$$

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Clarke Stationary Point

A point $x^* \in \mathbb{R}^n$ is Clarke stationary when $f^\circ(x^*, d) \geq 0$, for all $d \in \mathbb{R}^n$.

Algorithm Basic DFO-TRNS

Initialization. Select $x_0 \in \mathbb{R}^n$, $\eta > 0$, $0 < \gamma_1 < 1 \leq \gamma_2$, $\Delta_0 > 0$, and $p > 0$.

For $k = 0, 1 \ldots$

Generate randomly g_k in the unit sphere. Build a symmetric matrix B_k.

Let

$$\begin{aligned} s_k &\in \underset{\|s\|^2 \leq \Delta_k^2}{\operatorname{argmin}}\ m_k(s) = f(x_k) + {g_k}^\top s + \frac{1}{2} s^\top B_k s \\ \rho_k &= \frac{f(x_k) - f(x_k + s_k)}{\|s_k\|^{1+p}} \end{aligned}$$

If $\rho_k \geq \eta$, **Then** (**Success**), $x_{k+1} \leftarrow x_k + s_k$, $\Delta_{k+1} \leftarrow \gamma_2 \Delta_k$.

Else (**Failure**), $x_{k+1} \leftarrow x_k$, $\Delta_{k+1} \leftarrow \gamma_1 \Delta_k$.

End for

Why will Clarke be nonnegative along limiting TR steps

Mechanism

Predicted reduction

$$o(\|s_k\|) \;=\; \theta\|s\|^{1+p}$$

used in place of reduction in quadratic model $m_k(\mathbf{0}) - m_k(s_k)$.

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Reason

In unsuccessful iterations iterations, one has ($\rho_k < \eta$)

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Taking limits will when $\|s_k\| \longrightarrow 0$, will yield the **Clark derivative non-negative along limiting TR steps**

Asymptotic behavior of trust radius

Because in successful iterations we have

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Trust-region radius converges to zero

Assume that f is bounded from below. Any sequence $\{\Delta_k\}$ of trust-region radii produced by Algorithm **Basic DFO-TRNS** is such that

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The result is true even if B_k is unbounded as long as bounded by a power of Δ_k^{-q}, $q \in (0, 1)$.

Why will the TR steps also cover the unit sphere

Property

Any sequence $\{(x_k, s_k, \Delta_k)\}$ *generated by Algorithm* **Basic DFO-TRNS** *is such that*

$$s_k \;=\; -\Delta_k D_k g_k$$

with $D_k \in \mathbb{R}^{n\times n}$ *satisfying*

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Theorem

Property is satisfied when TR subproblems are solved up to optimality

Main result

$\{x_k\}$ sequence generated by Algorithm **Basic DFO-TRNS**. ASSUME:

- x^* limit point of $\{x_k\}_K$ with $K \subseteq \{k : \Delta_{k+1} < \Delta_k\}$
- $\{g_k\}_K$ dense in the unit sphere

Then x^* Clarke stationary

How to deal with nonsmoothness in practice?

IDEA: Embed **Basic DFO-TRNS** into an existing code

- Exploit the fact that f differentiable almost everywhere
- Combine **Basic DFO-TRNS** with approach for smooth problems (for quadratic term $\frac{1}{2}s^\top B_k s$):
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We weight the quadratic term of the model:

$$\omega \frac{1}{2} s^\top B_k s$$

with $\omega \in [0, 1]$

Test problems

- 51 nonsmooth problems
- Dimension $10 \leq n \leq 30$
- From 2 different collections [L. Lukšan, J. Vlček, 2000] [J.J. Moré, S. M. Wild, 2009]

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Analysis of numerical performance

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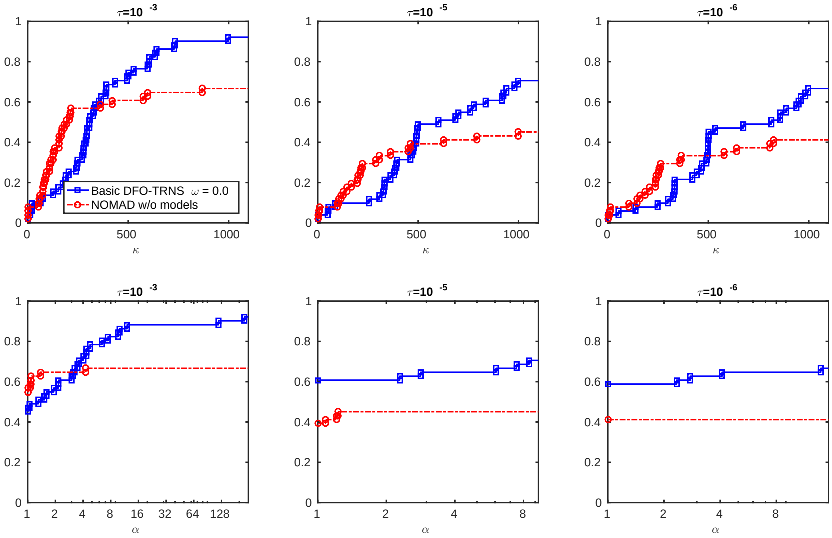
Software Used

- **Basic DFO-TRNS** (Combined with DFO-TR) $\omega = 0$
- **NOMAD** package [C. Audet et al.] without models

Basic DFO-TRNS vs NOMAD (w/o models)



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IDEA

Use a Bundle-like approach to handle nonsmoothness

Presentation outline

1. Introduction
2. A basic TR method for black-box functions
3. An advanced TR model

How to handle nosmoothness in TR methods

Smooth setting

Trust-region model is given by the sum of a linear term and a quadratic one

$$\bar{m}_k(s) + \frac{1}{2}s^\top B_k s \;=\; f(x_k) + \nabla f(x_k)^\top s + \frac{1}{2}s^\top B_k s$$

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Nonsmooth setting

Use a new linear term $m_k(s) \;=\; f(x_k) + f^\circ(x_k; s)$

$$\bar{m}_k(s) \;=\; \max_{\xi \in \partial f(x_k)} \left\{ f(x_k) + \xi^\top s \right\}$$

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Remark

Since the set $\partial f(x_k)$ is unknown, the above model cannot be used in practice!

Classic bundle approach (convex case)

How to replace $\partial f(x_k)$

Exploit the information obtained on a set of points $\{y^j : j \in J_k\}$ approaching x_k, where J_k is an index set.

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New model

Approximate model: $\bar{m}_k(s) \;=\; \max_{\xi \in \partial f(x_k)} \left\{ f(x_k) + \xi^\top s \right\}$

with the following model: $\bar{m}_k(s) \;=\; \max_{j \in J_k} \left\{ f(y^j) + (\xi^j)^\top (x_k + s - y^j) \right\}$

where $\xi^j \in \partial f(y^j), j \in J_k$.

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How to rewrite the model

Final model is

$$\bar{m}_k(s) \; = \; \max_{j \in J_k} \left\{ f(x_k) + (\xi^j)^\top s - \beta_k^j \right\}$$

with $\beta_k^j \; = \; f(x_k) + (\xi^j)^\top (y^j - x_k) - f(y^j)$ displacement related to point y^j.

The derivative-free context

Main Issue

- Element $\xi \in \partial f(y)$ cannot be computed.
- How to adapt the bundle approach to our derivative-free setting?

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Idea: Replace the information of ξ

Use a set of randomly generated normalized directions

$$G_k \;=\; \{g_i : \|g_i\| = 1, i \in I_k\}$$

where I_k is another index set.

A nonsmooth model

Displacements

Compute for each $(i, j) \in I_k \times J_k$, the displacements

$$\beta_k^{ij} \;=\; \max\left\{0, f(x_k) - f(y_k^j) + (g_i)^\top (y_k^j - x_k)\right\}$$

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New model

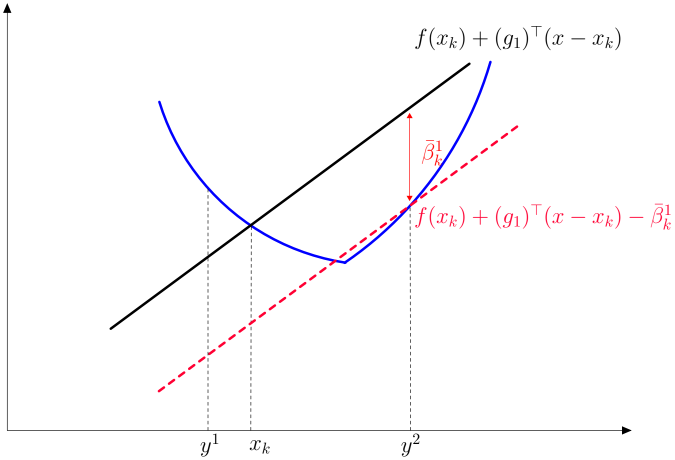
Introduce the following model

$$\bar{m}_k(s) \; = \; \max_{i \in I_k}\left\{ f(x_k) + (g_i)^\top s - \bar{\beta}_k^i \right\}$$

where

$$\bar{\beta}_k^i \; = \; \max_{j \in J_k}\{\beta_k^{ij}\}$$

Example of our nonsmooth model in convex case



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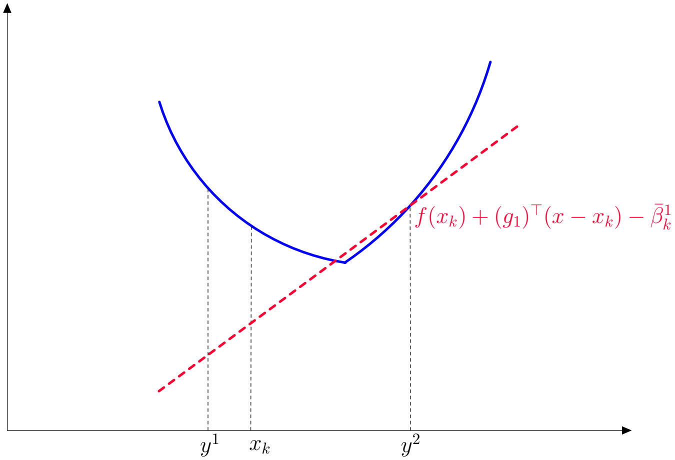

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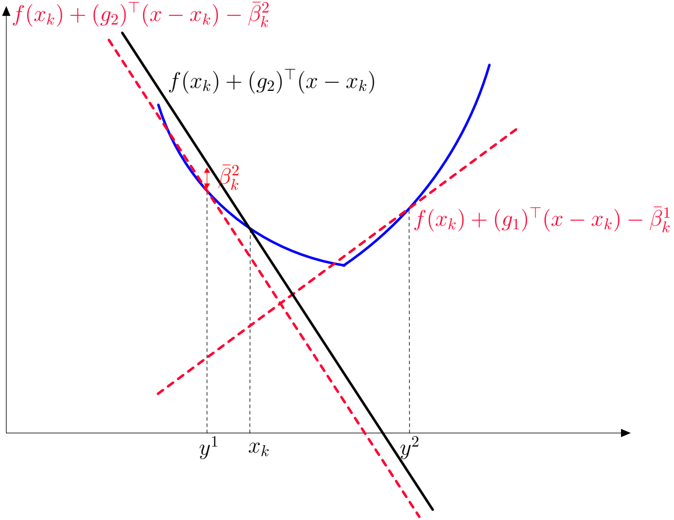

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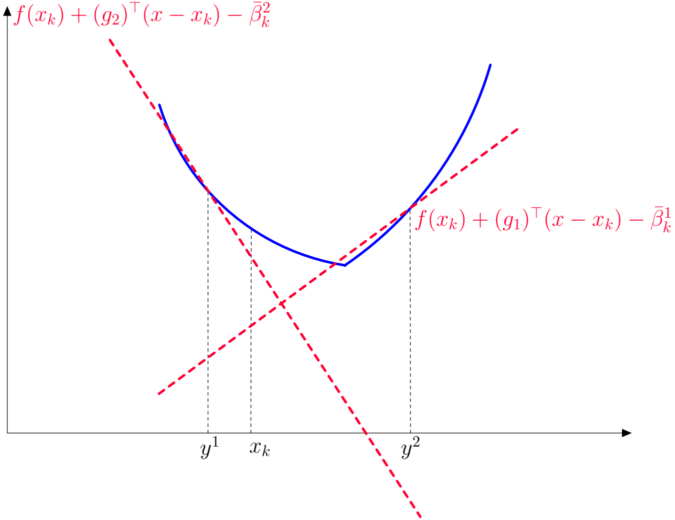

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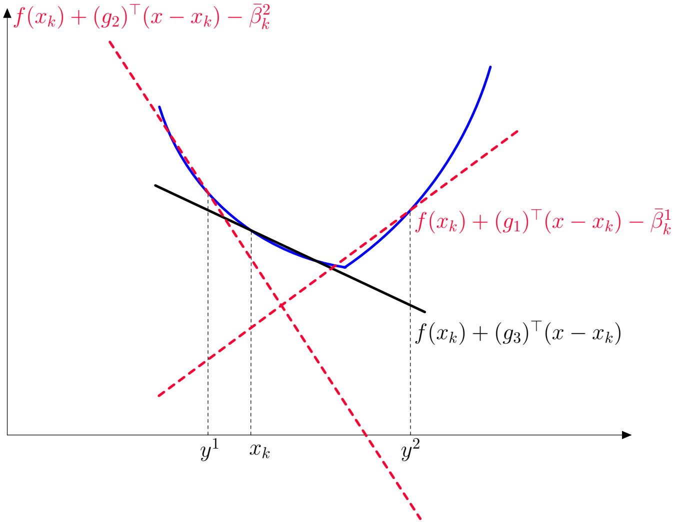

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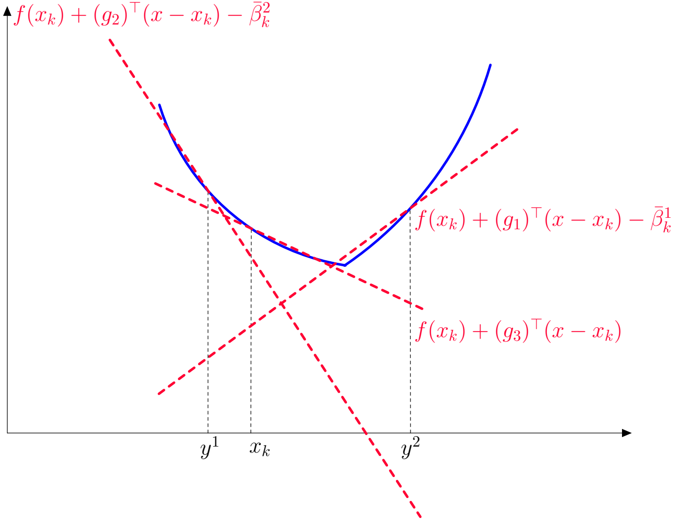

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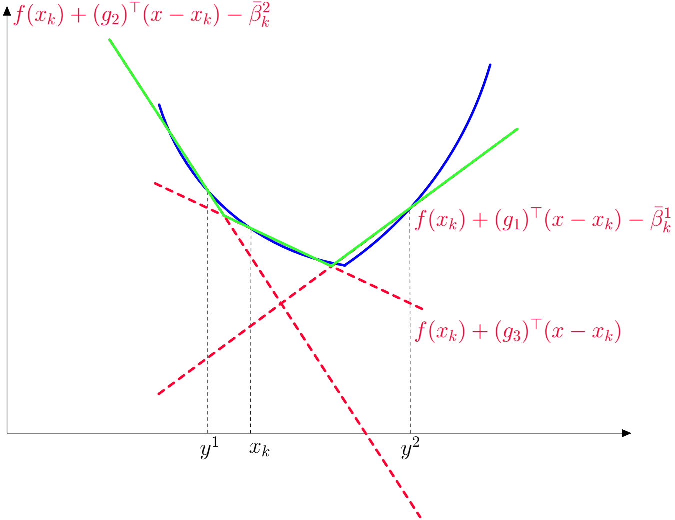

Dealing with nonconvexity

Bundle idea

- Hyperplanes might cut off solution.
- Lower all hyperplanes down.
- Amount will depend on the distance to the generating point.

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New displacements in the DFO case

Set

$$\beta_k^{ij} = \max\{0, f(x_k) - f(y_k^j) - (g_i)^\top (x_k - y_k^j) + \quad ? \quad \}$$

$$\bar{\beta}_k^i = \max_j \{\beta_k^{ij}\}$$

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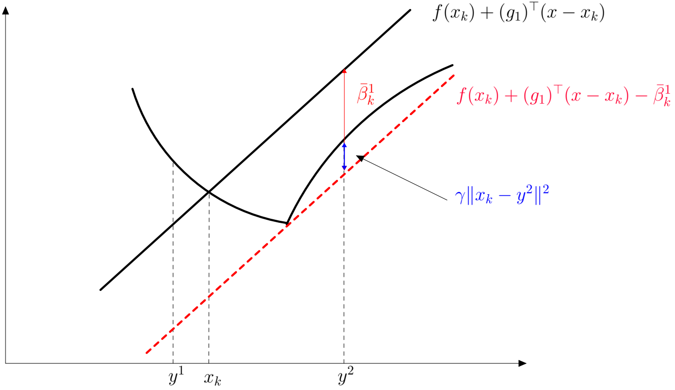

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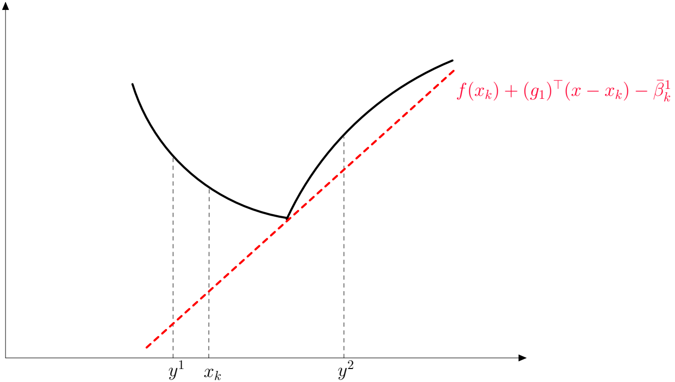

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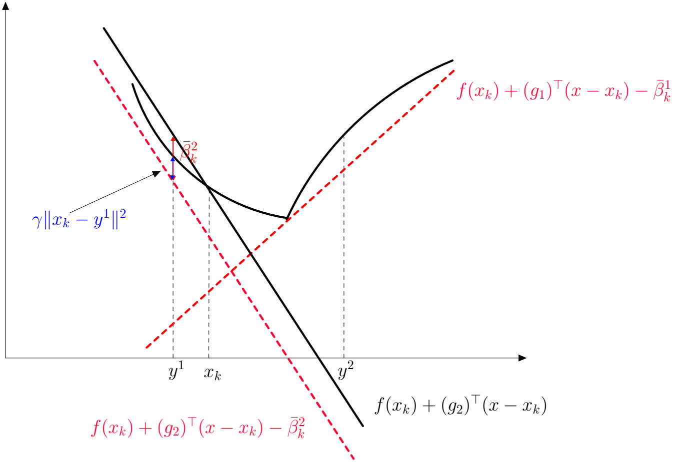

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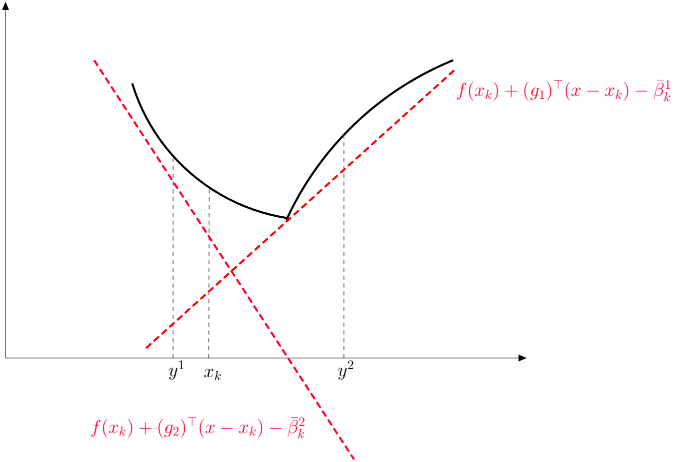

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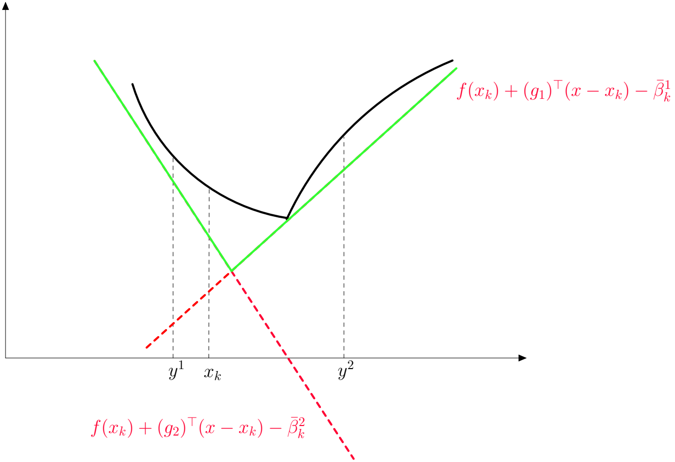


Our nonsmooth TR model

Nonsmooth approximating TR model

$$m_k(s) \;=\; \max_{i\in I_k}\left\{ f(x_k) + (g_i)^\top s - \tilde{\beta}_k^i \right\} + \frac{1}{2} s^\top B_k s$$

where

- I_k is an index set for generated directions g_i
- $\tilde{\beta}_k^i$ are as in the pictures...
- B_k is a symmetric matrix built out from interpolation or regression on a sample set of points

A revelation: the convex combination vector

The TR is equivalent to:

$$\begin{aligned} \min_{s,\alpha} \quad & \tfrac{1}{2} s^\top B_k s + \alpha \\ \text{s.t.} \quad & [f(x_k) - \tilde{\beta}_k^i] + (g_i)^\top s \;\le\; \alpha, \quad \forall\, i \in I_k \\ & \|s\|^2 \;\le\; \Delta_k^2 \end{aligned}$$

A revelation: the convex combination vector

The TR is equivalent to:

$$\begin{aligned} \min_{s,\alpha} \quad & \tfrac{1}{2} s^\top B_k s + \alpha \\ \text{s.t.} \quad & [f(x_k) - \tilde{\beta}_k^i] + (g_i)^\top s \;\le\; \alpha, \quad \forall\, i \in I_k \\ & \|s\|^2 \;\le\; \Delta_k^2 \end{aligned}$$

Such a step solves an auxiliary problem:

$$\begin{aligned} \min \quad & \tilde{m}_k(s) = f(x_k) + \tilde{g}_k{}^\top s + \frac{1}{2} s^\top B_k s \\ \text{s.t.} \quad & \|s\|^2 \le \Delta_k^2 \end{aligned}$$

where

$$\tilde{g}_k \;=\; \sum_{i \in I_k} \lambda_i g_i \quad \text{with} \quad \sum_{i \in I_k} \lambda_i = 1, \quad \text{and} \quad \lambda_i \ge 0,\ \forall i \in I_k$$

and λ are the multipliers associated with the α constraints

Algorithm Advanced DFO-TRNS

Initialization. Select $x_0 \in \mathbb{R}^n$, $\eta, \gamma > 0$, $0 < \gamma_1 < 1 \leq \gamma_2$, $\bar{\epsilon} > 0$, $\Delta_0 > 0$, and $p > 0$. Set $G_0 = \emptyset$.

For $k = 0, 1 \ldots$

Generate randomly g_k in the unit sphere. Build a symmetric matrix B_k.

Set $G_k = G_{k-1} \cup \{g_k\}$.

Let s be a solution of NTRS for this G_k, and λ the associate multipliers.

If $\|\tilde{g}_k\| < \bar{\epsilon}\Delta_k^{\frac{1}{2}}$ **Then** Reset $G_k = \{g_k\}$. Let s be a solution of NTRS for G_k.

Set $s_k = s$ and $\rho_k = \dfrac{f(x_k) - f(x_k + s_k)}{\|s_k\|^{p+1}}$.

If $\rho_k \geq \eta$

Then set $\texttt{SUCCESS} \leftarrow \texttt{true}$, $x_{k+1} \leftarrow x_k + s_k$, $\Delta_{k+1} \leftarrow \gamma_2 \Delta_k$,

Else set $\texttt{SUCCESS} \leftarrow \texttt{false}$, $x_{k+1} \leftarrow x_k$, $\Delta_{k+1} \leftarrow \gamma_1 \Delta_k$.

End If

End For

Convergence analysis

Assumption on the sample set

Points in the sample set $\{y_k^j : \ j \in J_k\}$ verify

$$\|x_k - y_k^j\| \ \leq \ \gamma \Delta_k, \quad \forall j \in J_k$$

Comments

- Assumptions and results are the **SAME** as for the basic version
- Convergence analysis follows **REMARKABLY** the lines of the basic version
- Main difference: use of the convex combination vector $\tilde{g}_k$ instead of g_k

Preliminary Numerical Results

Problems & Analysis

- Same problems as before
- Performance and data profiles used
- Budget = **10000** function evaluations

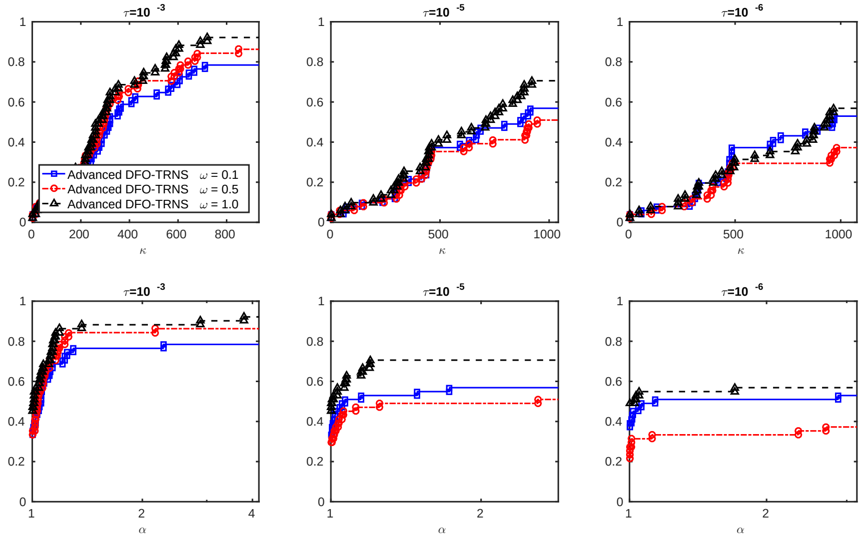
Software Used

- **Basic DFO-TRNS** (Combined with DFO-TR)
- **Advanced DFO-TRNS** (Combined with DFO-TR)
- **NOMAD** package [C. Audet et al.]

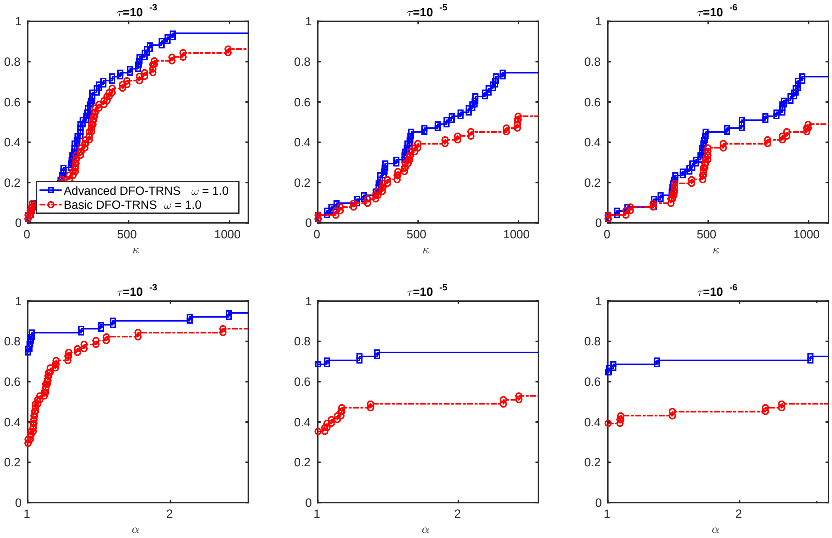
Details

- Different ω for the quadratic term in the models
- **NOMAD** used was WITH models

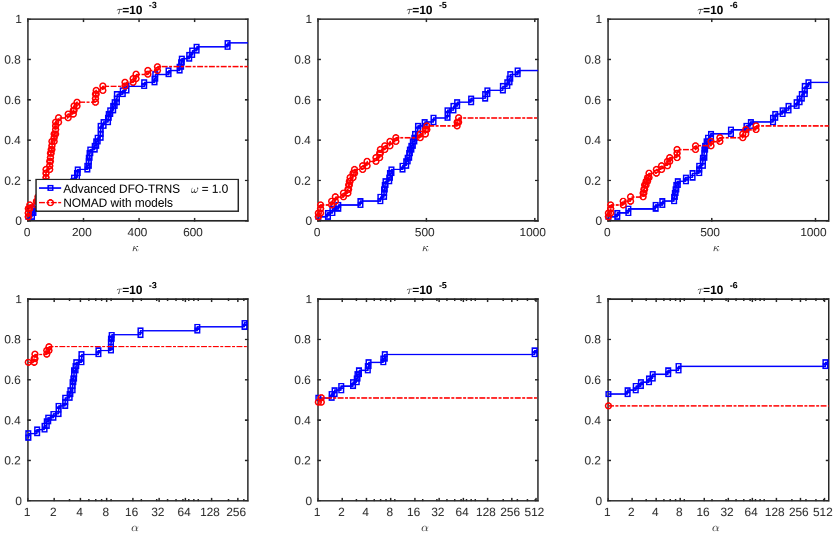
Comparison of **Adv. DFO-TRNS** varying ω's in $\frac{\omega}{2}s^\top B_k s$



Basic vs Adv. DFO-TRNS with $\omega = 1$



Adv. DFO-TRNS $(\omega = 1)$ vs NOMAD with models



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For further details: G. Liuzzi, S. Lucidi, F. Rinaldi and L.N. Vicente, *Trust-region methods for the derivative-free optimization of nonsmooth black-box functions*, SIAM Journal on Optimization, 29 (2019) 3012-3035