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Reducing the number of function evaluations in MADS algorithms

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Presentation outline

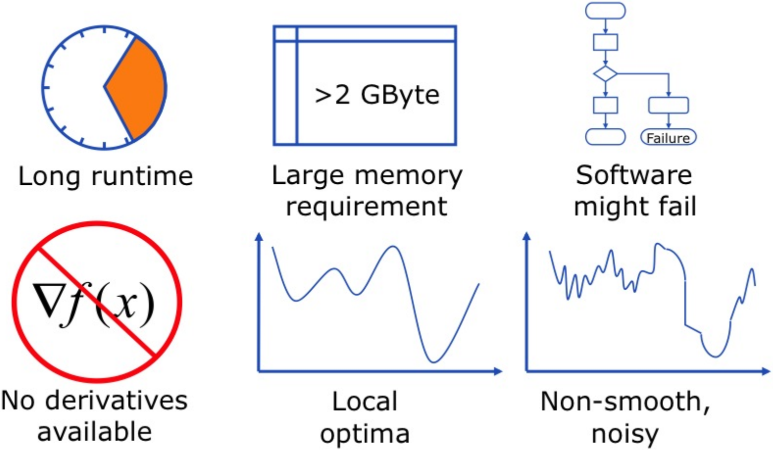
Blackbox optimization problems

We consider the optimization problem:

$$\min_{x \in \Omega} \quad f(x)$$

where evaluations of f and the functions defining Ω are usually the result of a computer code (a blackbox).

Blackboxes as illustrated by J. Simonis [ISMP 2009]



Blackbox optimization problems

The MADS algorithm

Reducing the size of the poll set

Numerical results

Discussion

Mesh Adaptive Direct Search (MADS)

- Audet and Dennis [SIOPT, 2006]
- Iterative algorithm that evaluates the blackbox at some trial points on a spatial discretization called the mesh.
- One iteration = search and poll.
- The search allows trial points generated anywhere on the mesh.
- The poll consists in generating a list of trial points constructed from poll directions. These directions grow dense.
- At the end of the iteration, the mesh size is reduced if no new iterate is found.
- Algorithm is backed by a convergence analysis based on the Clarke Calculus for nonsmooth functions.

The poll (1/2)

- Mesh at iteration k:
  - $M_k = \bigcup_{x \in V_k} \{x + \Delta_k D z : z \in \mathbb{N}^{n_D}\}$.
  - V_k is the "cache".
  - $\Delta_k > 0$ is the mesh size parameter.
  - D is a fixed set of directions typically set to $[I \ \ -I]$.

- Poll directions: A positive spanning set $D_k \subset \mathbb{R}^n$ where each direction $d \in D_k$ can be written as a nonnegative integer combination of directions of D.

- The directions correspond typically to a minimal positive basis ($n+1$ directions) or a maximal positive basis ($2n$ directions).

The poll (2/2)

- Poll set: $P_k = \{x_k + \Delta_k d : d \in D_k\}$ where x_k is the current incumbent, or the poll center.
- The trial points in P_k are evaluated following the opportunistic strategy: evaluations are interrupted as soon as a new better solution is found.
- Trial points ordering is then crucial in practice. It can be based on:
  - Model or surrogate values.
  - Angle with the gradient of a model.
  - Angle with the last direction of success.

[0] Initializations (x_0, Δ_0)

[1] Iteration k

- **[1.1] Search**
  - select a finite number of mesh points
  - evaluate candidates opportunistically
- **[1.2] Poll** (if the Search failed)
  - construct poll set $P_k = \{x_k + \Delta_k d : d \in D_k\}$
  - sort(P_k)
  - evaluate candidates opportunistically

[2] Updates

- if success
  - $x_{k+1} \leftarrow$ success point
  - increase Δ_k
- else
  - $x_{k+1} \leftarrow x_k$
  - decrease Δ_k
- $k \leftarrow k + 1$, stop or go to **[1]**

Motivation

- MADS is a generic algorithmic framework with two practical implementations: LT-MADS and Ortho-MADS.
- For various reasons, Ortho-MADS is preferred to LT-MADS. LT-MADS defines $n+1$ and $2n$ types of directions, and Ortho-MADS has only the $2n$ variant:

	LT-MADS(2006)	Ortho-MADS (2009)
$n+1$	✓	X
$2n$	✓	✓

- Some tests suggest that the LT-MADS implementation is more efficient with $n+1$ directions. We want to define an Ortho-MADS variant using $n+1$ directions.

General framework (1)

Idea: Given a poll set of $2n$ trial points, prune it to n points and add a direction to obtain $n+1$ points.

Poll at iteration k

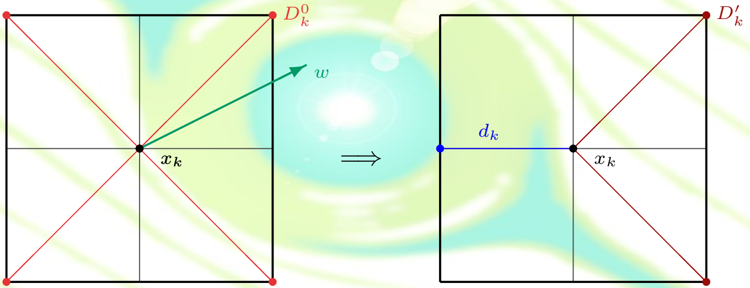
$P_k^o = \{x_k + \Delta_k d : d \in D_k^o\}$ (original poll set)
extract $D'_k \subset D_k^o$
compute new direction d_k
$D_k = D'_k \cup \{d_k\}$
construct $P_k = \{x_k + \Delta_k d : d \in D_k\}$ (reduced poll set)
sort(P_k)
evaluate(P_k) (opportunistically)

Ortho-MADS $n+1$ is a simple first implementation of this general framework.

Ortho-Mads $n+1$

- $D_k^o = [H_k \ \ -H_k]$ is the original Ortho-MADS spanning set with $2n$ directions and $H_k \in \mathbb{Z}^{n\times n}$ an orthogonal basis with integer coefficients.
- The selection of n columns of D_k^o to obtain D'_k is based on a target direction $w \in \mathbb{R}^n$.
- The target direction is taken as the last direction of success.
- The $(n+1)$th direction is $d_k = -\sum_{d \in D'_k} d$.

Ortho-MADS $n+1$: Idea



$2n$ directions D_k^0 $\qquad$ $n+1$ directions $D_k = D'_k \cup \{d_k\}$

Completion using function values

- We now present a second and more general framework.
- This version is not limited to Ortho-MADS and may be applied to any poll sets. For example hybrid versions with more that $2n$ points.
- The first framework is decomposed allowing to evaluate n trial points in a first step and possibly a last $(n+1)$th point $y_k = x_k + d_k\Delta_k$.
- y_k is constructed by exploiting the function values at the first n points.
- y_k must lie on the mesh and d_k must be inside the cone of the negative directions of D'_k so that the poll directions remain a positive spanning set.

General framework (2)

Poll at iteration k

- $P_k^o = \{x_k + \Delta_k d : d \in D_k^o\}$ (original poll set)
- extract $D'_k \subset D_k^o$ and construct P'_k
- sort (P'_k)
- evaluate (P'_k) (opportunistically)
- Success
  - interrupt iteration
- Failure
  - compute new direction d_k
  - evaluate $(x_k + \Delta_k d_k)$

Use of quadratic models

Quadratic models may be used at two different levels:

1. In Ortho-MADS $n+1$: The simplex gradient is taken as the target direction w.
2. In Framework (2): Optimize a model to determine the last trial point $y_k = x_k + \Delta_k d_k$.

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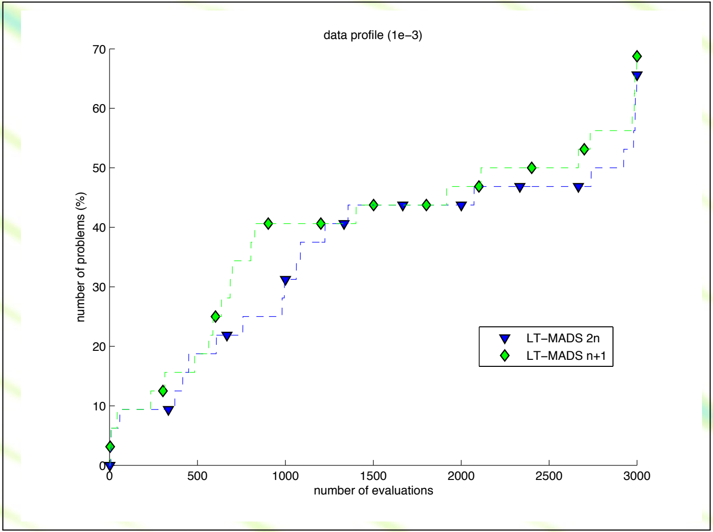
Set of problems and conditions

- These are preliminary tests.
- 32 analytic problems from the DFO literature.
- Number of variables: n ranges from 2 to 12.
- Constraints: 7 problems have from 1 to 15 constraints.
- A budget of 3000 evaluations is considered.
- Results are illustrated by data profiles with a precision of 10^{-3}.

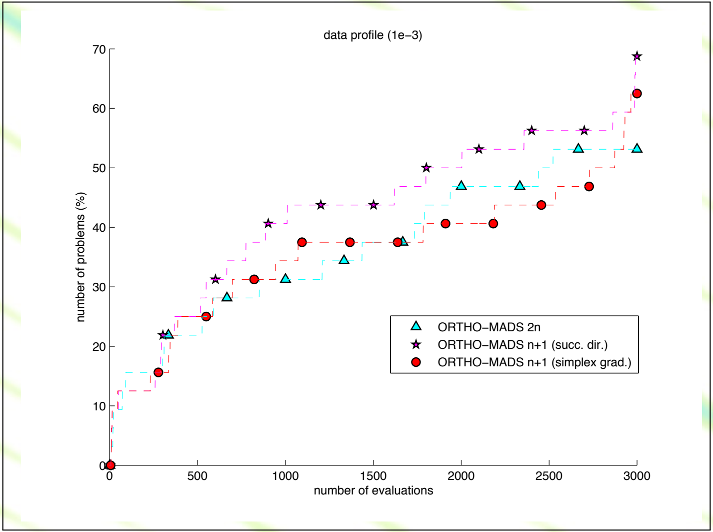
Summary of the tests

1. LT-MADS $2n$ vs $n+1$.
2. Ortho-MADS $2n$ vs Ortho-MADS $n+1$ with two variants: w success direction or simplex gradient.
3. LT-MADS vs Ortho-MADS.

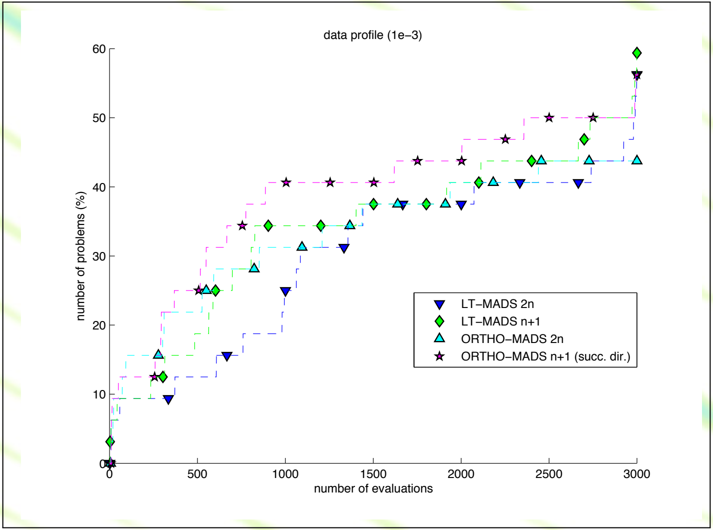
1. LT-MADS $2n$ vs $n+1$



2. Ortho-MADS $2n$ vs $n+1$



3. LT-MADS vs Ortho-MADS



Discussion

- This work is based on the remark that using minimal positive bases instead of maximal positive bases seems preferable.
- It defines several methods in order to achieve the reduction of poll directions from $2n$ to $n+1$ points.
- Preliminary tests demonstrate significative improvements.
- Future work includes more testing on true applications and development of smarter ways to use quadratic models and to treat the constraints.
- Our blackbox optimization solver: www.gerad.ca/nomad.