ISMP 2012

The mesh adaptive direct search algorithm with reduced number of directions

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Presentation outline

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Reducing the size of the poll set

Numerical results

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We consider the optimization problem:

\[ \min_{x \in \Omega} f(x) \]

where evaluations of \( f \) and the functions defining \( \Omega \) are usually the result of a computer code (a blackbox).
Blackboxes as illustrated by J. Simonis [ISMP 2009]

- Long runtime
- Large memory requirement
- Software might fail
- No derivatives available
- Local optima
- Non-smooth, noisy

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The MADS acronyms

- **MADS** *(Mesh Adaptive Direct Search)*
  → The algorithmic framework without the definition of the polling directions.

- **LT-MADS**: Original MADS implementation.

- **Ortho-MADS**: Second MADS implementation.

- **NOMAD** *(Nonlinear Optimization with the MADS algorithm)*:
  → The software package. Includes LT-MADS and Ortho-MADS.
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- NOMADS does not exist.
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 $k$:

- $M_k = \bigcup_{x \in V_k} \{ x + \Delta_k Dz : z \in \mathbb{N}^{nD} \}$.
- $V_k$ 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.
  - etc.
[0] **Initializations** \( (x_0, \Delta_0) \)

[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 \( P_k = \{x_k + \Delta_k d : d \in D_k\} \)
- \( \text{sort}(P_k) \)
- evaluate candidates opportunistically

[2] **Updates**
- if success
  - \( x_{k+1} \leftarrow \text{success point} \)
  - increase \( \Delta_k \)
- else
  - \( x_{k+1} \leftarrow x_k \)
  - decrease \( \Delta_k \)
  - \( k \leftarrow k + 1 \), 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:

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$n + 1$</td>
<td>✓</td>
<td>X</td>
</tr>
<tr>
<td>$2n$</td>
<td>✓</td>
<td>✓</td>
</tr>
</tbody>
</table>

▶ 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.
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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.

<table>
<thead>
<tr>
<th>Poll at iteration $k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P^o_k = {x_k + \Delta_k d : d \in D^o_k}$ (original poll set)</td>
</tr>
<tr>
<td>extract $D'_k \subset D^o_k$</td>
</tr>
<tr>
<td>compute new direction $d_k$</td>
</tr>
<tr>
<td>$D_k = D'_k \cup {d_k}$</td>
</tr>
<tr>
<td>construct $P_k = {x_k + \Delta_k d : d \in D_k}$ (reduced poll set)</td>
</tr>
<tr>
<td>sort($P_k$)</td>
</tr>
<tr>
<td>evaluate($P_k$) (opportunistically)</td>
</tr>
</tbody>
</table>

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

- $D^o_k = [H_k - H_k]$ 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 $D^o_k$ 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 $D_k^0$ \hspace{2cm} $n + 1$ 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 than $2n$ points.

- The first framework is decomposed allowing to evaluate $n$ trial points in a first step and possibly one 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

\begin{itemize}
  \item interrupt iteration
\end{itemize}

Failure

\begin{itemize}
  \item compute new direction $d_k$
  \item evaluate $(x_k + \Delta_k d_k)$
\end{itemize}
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 $2n \text{ vs } n + 1$

![Graph showing data profile and number of problems for Ortho-MADS $2n$ and $n + 1$.]
3. LT-MADS vs Ortho-MADS

![Graph comparing LT-MADS and Ortho-MADS]

ISMP 2012: $n + 1$ directions
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- 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.