The Mesh Adaptive Direct Search Algorithm for Discrete Blackbox Optimization

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Presentation outline

Blackbox optimization

Motivating example

The MADS algorithm

Computational experiments

Discussion
Blackbox optimization

Motivating example

The MADS algorithm

Computational experiments

Discussion
Blackbox optimization (BBO) problems

- Optimization problem:
  \[
  \min_{x \in \Omega} f(x)
  \]

- Evaluations of \(f\) (the objective function) and of the functions defining \(\Omega\) are usually the result of a computer code (a blackbox).

- Variables are typically continuous, but in this work, some of them are discrete – integers or granular variables.
Blackboxes as illustrated by J. Simonis [ISMP 2009]

- Long runtime
- No derivatives available
- Large memory requirement
- Local optima
- Non-smooth, noisy
- Software might fail
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Discussion
Motivating example: Parameters tuning (1/2)

- [Audet and Orban, 2006].
- The classical Trust-Region algorithm depends on four parameters $x = (\eta_1, \eta_2, \alpha_1, \alpha_2) \in \mathbb{R}^4_+$. 
- Consider a collection of 55 test problems from CUTEr.
- Let $f(x)$ be the CPU time required to solve the collection of problems by a Trust-Region algorithm with parameters $x$.
- $f(x_0) \simeq 3h45$ with the textbook values $x_0 = (1/4, 3/4, 1/2, 2)$. 
Motivating example: Parameters tuning (2/2)

This optimization produced \( \hat{x} \) with \( f(\hat{x}) \approx 2h50 \).
Motivating example: Parameters tuning (2/2)

This optimization produced $\hat{x}$ with $f(\hat{x}) \simeq 2h50$. Victory?

\[ x \in \mathbb{R}^4_{+} \]
Motivating example: Parameters tuning (2/2)

This optimization produced $\hat{x}$ with $f(\hat{x}) \simeq 2h50$. Victory? No because
$\hat{x} = (0.22125, 0.94457031, 0.37933594, 2.3042969)$. 
Granular variables

The initial point \( x_0 = (0.25, 0.75, 0.50, 2.00) \) is frequently used because each entry is a multiple of 0.25.

Its granularity is \( G = 0.25 \)
Granular variables

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Its granularity is $G = 0.25$

- How can we devise a direct search algorithm so that it stops on a prescribed granularity?
  With a granularity of $G = 0.05$, the code might produce
  $$\hat{x} = (0.20, 0.95, 0.40, 2.30).$$
  Which is much nicer (for a human) than
  $$\hat{x} = (0.22125, 0.94457031, 0.37933594, 2.3042969).$$
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Which is much nicer (for a human) than
$$\hat{x} = (0.22125, 0.94457031, 0.37933594, 2.3042969).$$
This may be achieved using integer variables, together with a relative scaling, but there is a simpler way for mesh-based methods.
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Discussion
Mesh Adaptive Direct Search (MADS) in $\mathbb{R}^n$

- [Audet and Dennis, Jr., 2006].
Mesh Adaptive Direct Search (MADS) in $\mathbb{R}^n$

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- Iterative algorithm that evaluates the blackbox at some trial points on a spatial discretization called the mesh.
- One iteration = search and poll.
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- 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.
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- 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 success point is found.
[0] **Initializations** \((x_0, \Delta_0: \text{initial poll size})\)

[1] **Iteration** \(k\)

- let \(\delta^k \leq \Delta^k\) be the mesh size parameter
- **Search**
  - test a finite number of mesh points
- **Poll** (if the Search failed)
  - construct set of directions \(D_k\)
  - test poll set \(P_k = \{x_k + \delta^k d : d \in D_k\}\)
  - with \(\|\delta^k d\| \simeq \Delta_k\)

[2] **Updates**

- if success
  - \(x_{k+1} \leftarrow \text{success point}\)
  - increase \(\Delta^k\)
- else
  - \(x_{k+1} \leftarrow x_k\)
  - decrease \(\Delta^k\)
  - \(k \leftarrow k + 1, \text{stop if } \Delta^k \leq \Delta_{\text{min}} \text{ or go to [1]}\)
Poll illustration (successive fails and mesh shrinks)

\[
\delta^k = 1 \\
\Delta^k = 1
\]

trial points = \{p_1, p_2, p_3\}
Poll illustration (successive fails and mesh shrinks)

\[ \delta^k = 1 \]
\[ \Delta^k = 1 \]

\[ \delta^{k+1} = \frac{1}{4} \]
\[ \Delta^{k+1} = \frac{1}{2} \]

trial points = \{p_1, p_2, p_3\} = \{p_4, p_5, p_6\}
Poll illustration (successive fails and mesh shrinks)

\[ \delta^k = 1 \quad \Delta^k = 1 \]
\[ \delta^{k+1} = \frac{1}{4} \quad \Delta^{k+1} = \frac{1}{2} \]
\[ \delta^{k+2} = \frac{1}{16} \quad \Delta^{k+2} = \frac{1}{4} \]

trial points = \{p_1, p_2, p_3\} = \{p_4, p_5, p_6\} = \{p_7, p_8, p_9\}
Discrete variables in MADS – so far

- MADS has been designed for continuous variables.
- Some theory exists for categorical variables [Abramson, 2004].
- So far: Only a patch allows to handle integer variables: Rounding + minimal mesh size of one.

In this talk, we start from scratch and present direct search methods with a natural way of handling discrete variables.
Mesh refinement on \( \min(x - 1/3)^2 \)

<table>
<thead>
<tr>
<th>( \Delta^k )</th>
<th>( x^k )</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
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Mesh refinement on $\min(x - 1/3)^2$

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Idea: Instead of dividing $\Delta^k$ by 2, change it so that
- $10 \times 10^b$ refines to $5 \times 10^b$
- $5 \times 10^b$ refines to $2 \times 10^b$
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- $5 \times 10^b$ refines to $2 \times 10^b$
- $2 \times 10^b$ refines to $1 \times 10^b$

To get three decimals, one simply sets the granularity to $0.001$. Integer variables are treated by setting the granularity to $G = 1$. 
Poll and mesh size parameter update

- The poll size parameter $\Delta^k$ is updated as
  $10 \times 10^b \leftrightarrow 5 \times 10^b \leftrightarrow 2 \times 10^b \leftrightarrow 1 \times 10^b$

- The fine underlying mesh is defined with the mesh size parameter
  $\delta^k = \begin{cases} 
  1 & \text{if } \Delta^k \geq 1, \\
  \max\{10^{2b}, G\} & \text{otherwise, i.e. } \Delta^k \in \{1, 2, 5\} \times 10^b.
  \end{cases}$

- Example: Granularity of $G = 0.005$ :

<table>
<thead>
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</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>0.01</td>
<td>0.5</td>
</tr>
<tr>
<td>0.01</td>
<td>0.2</td>
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<tr>
<td>0.01</td>
<td>0.1</td>
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<tr>
<td>0.005</td>
<td>0.05</td>
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<td>0.005</td>
<td>0.02</td>
</tr>
<tr>
<td>0.005</td>
<td>0.01</td>
</tr>
<tr>
<td>0.005</td>
<td>0.005 ← stop</td>
</tr>
</tbody>
</table>
[0] **Initializations** \((x_0, \Delta_0 \in \{1, 2, 5\} \times 10^b, G \text{ granularity})\)

[1] **Iteration** \(k\)

- let \(\delta^k \leq \Delta^k\) be the mesh size parameter

**Search**
- test a finite number of mesh points

**Poll** (if the Search failed)
- construct set of directions \(D_k\)
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Theory

- MADS analysis relies on “the sequence of trial points are located on some discretization of the space of variables called the mesh”.

- By multiplying or dividing $\Delta^k$ by a rational number $\tau$, [Torczon, 1997] showed that all trial points from iteration 0 to $\ell$ were located on a fine underlying mesh. The proof is not trivial and uses the fact that $\tau \in \mathbb{Q}$, and does not work for $\tau \in \mathbb{R}$ (paper won SIAM Outstanding Paper Prize).
Theory

- MADS analysis relies on “the sequence of trial points are located on some discretization of the space of variables called the mesh”.
- By multiplying or dividing $\Delta^k$ by a rational number $\tau$, [Torczon, 1997] showed that all trial points from iteration 0 to $\ell$ were located on a fine underlying mesh.
- With the new mesh, that technical part of the proof becomes:

Consider any trial point $t$ considered from iteration $k = 0$ to $\ell$. If a granularity of $G_i$ is requested on variable $i$, $t_i$ lies on the mesh of granularity $G_i$ if no granularity is requested on variable $i$, $t_i$ lies on the mesh of granularity $10^{b_i}$ with $b_i = \min\{b_i^k : k = 0, 1, \ldots, \ell\}$. 
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Discussion
Trust-Region parameters tuning

Find the values of the four parameters $x = (\eta_1, \eta_2, \alpha_1, \alpha_2) \in \mathbb{R}_+^4$ that minimize the overall CPU time to solve 55 CUTEr problems.

- The surrogate function $s$ is defined as the time to solve a collection of small-sized problems.
- In 2005, $f(x) \simeq 3h - 4h$ and $s(x) \simeq 1m$. The surrogate is 200 times faster.
Trust-Region parameters tuning

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**Theorem (Moore’s Law is valid)**

<table>
<thead>
<tr>
<th>Year</th>
<th>CPU ( f(x) )</th>
<th>CPU ( s(x) )</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>2005</td>
<td>13800 s</td>
<td>69 s</td>
<td>42</td>
</tr>
<tr>
<td>2016</td>
<td>330 s</td>
<td>2.3 s</td>
<td>30</td>
</tr>
</tbody>
</table>

Moore’s Law: Speed doubles every 2 years:
2016-2005 = 11 \( \Rightarrow \) 5.5 cycles,
speedup of \( 2^{5.5} \simeq 45 \).
Standard $\times 2 \div 2$ versus New $\{1, 2, 5\} \times 10^b$
## Trust-Region parameter tuning: Results

<table>
<thead>
<tr>
<th></th>
<th>Standard</th>
<th>New</th>
<th>Granularity</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \times 2 \div 2 )</td>
<td>{1, 2, 5} ( \times 10^6 )</td>
<td>0.01</td>
</tr>
<tr>
<td>CPU:</td>
<td>228 s</td>
<td>207 s</td>
<td>0.05</td>
</tr>
<tr>
<td>( \eta_1 )</td>
<td>0.2508936274</td>
<td>0.5325498121</td>
<td>0.35</td>
</tr>
<tr>
<td>( \eta_2 )</td>
<td>0.9008242693</td>
<td>0.9938378210</td>
<td>0.99</td>
</tr>
<tr>
<td>( \alpha_1 )</td>
<td>0.5464425868</td>
<td>0.4817164472</td>
<td>0.50</td>
</tr>
<tr>
<td>( \alpha_2 )</td>
<td>1.5505441560</td>
<td>3.5206901980</td>
<td>2.82</td>
</tr>
</tbody>
</table>

Observations:

- On this example, the new strategies are preferable.
- Trust-region recommendation for humans:

\[
(\eta_1, \eta_2, \alpha_1, \alpha_2) = (0.35, 0.99, 0.5, 2.82).
\]
Preliminary results on mixed-integer problems

- Data profiles [Moré and Wild, 2009].
- 11 analytical problems from the literature.
- Continuous + integer variables.
- No constraints.
- 10 random starting points for each problem (110 executions).
- “classic” VS new mesh.
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- New mesh parameter update rules to control the number of decimals \( \{1, 2, 5\} \times 10^b \)
  - A native way to handle granularity of variables \( G \).
  - Integer variables are handled by setting \( G = 1 \).
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  - A native way to handle granularity of variables \( G \).
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- Numerical experiments on trust region parameters
  - New parameters reduce CPU time by 35% (versus textbook).
  - New parameters have granularity 0.01 (readable by humans).
  - Experiments on other test problems in progress.
Discussion

- New mesh parameter update rules to control the number of decimals $\{1, 2, 5\} \times 10^b$
  - A native way to handle granularity of variables $G$.
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- Numerical experiments on trust region parameters
  - New parameters reduce CPU time by 35% (versus textbook).
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  - Experiments on other test problems in progress.

- This will be part of our NOMAD 3.8 software
  - the only additional input from the user is $G$.
  - ... and it is optional.
  - www.gerad.ca/nomad.
References I

Mixed variable optimization of a Load-Bearing thermal insulation system using a filter pattern search algorithm.

Audet, C. and Dennis, Jr., J. (2006).
Mesh adaptive direct search algorithms for constrained optimization.

Finding optimal algorithmic parameters using derivative-free optimization.

Algorithm 909: NOMAD: Nonlinear Optimization with the MADS algorithm.

Benchmarking derivative-free optimization algorithms.

On the convergence of pattern search algorithms.