The Mesh Adaptive Direct Search Algorithm for Discrete Blackbox Optimization

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ICCOPT, Tokyo

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

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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 \( x \).

- \( f(x_0) \approx 3h45 \) 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 $f(\hat{x}) \approx 2h50$. 

$$x \in \mathbb{R}^4_+$$

Blackbox
Run TR on collection
Return CPU time

MADS Algorithm

$f(x)$

$$f(\hat{x}) \approx 2h50.$$
Motivating example: Parameters tuning (2/2)

- This optimization produced $\hat{x}$ with $f(\hat{x}) \simeq 2h50$. Victory?
Motivating example: Parameters tuning (2/2)

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

\[ x \in \mathbb{R}^4_+ \]
**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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- 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
  
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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.
Blackbox optimization

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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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- 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.
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.

- 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.
<table>
<thead>
<tr>
<th></th>
<th>Initialization ( (x_0, \Delta_0: \text{initial poll size}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Iteration ( k )</td>
</tr>
<tr>
<td></td>
<td>let ( \delta^k \leq \Delta^k ) be the mesh size parameter</td>
</tr>
<tr>
<td></td>
<td><strong>Search</strong></td>
</tr>
<tr>
<td></td>
<td>test a finite number of mesh points</td>
</tr>
<tr>
<td></td>
<td><strong>Poll</strong> (if the Search failed)</td>
</tr>
<tr>
<td></td>
<td>construct set of directions ( D^k )</td>
</tr>
<tr>
<td></td>
<td>test poll set ( P^k = {x_k + \delta^k d : d \in D^k} )</td>
</tr>
<tr>
<td></td>
<td>with ( |\delta^k d| \approx \Delta^k )</td>
</tr>
<tr>
<td>2</td>
<td><strong>Updates</strong></td>
</tr>
<tr>
<td></td>
<td>if success</td>
</tr>
<tr>
<td></td>
<td>( x_{k+1} \leftarrow \text{success point} )</td>
</tr>
<tr>
<td></td>
<td>increase ( \Delta^k )</td>
</tr>
<tr>
<td></td>
<td>else</td>
</tr>
<tr>
<td></td>
<td>( x_{k+1} \leftarrow x_k )</td>
</tr>
<tr>
<td></td>
<td>decrease ( \Delta^k )</td>
</tr>
<tr>
<td></td>
<td>( k \leftarrow k + 1 ), stop if ( \Delta^k \leq \Delta_{\text{min}} ) or go to [1]</td>
</tr>
</tbody>
</table>
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)

\[
\begin{align*}
\delta^k &= 1 \\
\Delta^k &= 1 \\
\delta^{k+1} &= 1/4 \\
\Delta^{k+1} &= 1/2
\end{align*}
\]

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

\[
\begin{align*}
\delta^k &= 1 \\
\Delta^k &= 1 \\
\delta^{k+1} &= 1/4 \\
\Delta^{k+1} &= 1/2 \\
\delta^{k+2} &= 1/16 \\
\Delta^{k+2} &= 1/4
\end{align*}
\]

trial points \(= \{p_1, p_2, p_3\} \quad = \{p_4, p_5, p_6\} \quad = \{p_7, p_8, p_9\} \)
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 work, 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>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>0.125</td>
<td>0.375</td>
</tr>
<tr>
<td>0.0625</td>
<td>0.3125</td>
</tr>
<tr>
<td>0.03125</td>
<td>0.34375</td>
</tr>
<tr>
<td>0.015625</td>
<td>0.328125</td>
</tr>
<tr>
<td>0.0078125</td>
<td>0.3359375</td>
</tr>
<tr>
<td>0.00390625</td>
<td>0.33203125</td>
</tr>
<tr>
<td>0.001953125</td>
<td>0.333984375</td>
</tr>
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<tbody>
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<td>1</td>
<td>0</td>
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<td>0</td>
</tr>
<tr>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>0.25</td>
<td>0.25</td>
<td>0.2</td>
<td>0.4</td>
</tr>
<tr>
<td>0.125</td>
<td>0.375</td>
<td>0.125</td>
<td>0.35</td>
</tr>
<tr>
<td>0.0625</td>
<td>0.3125</td>
<td>0.05</td>
<td>0.35</td>
</tr>
<tr>
<td>0.03125</td>
<td>0.34375</td>
<td>0.02</td>
<td>0.34</td>
</tr>
<tr>
<td>0.015625</td>
<td>0.328125</td>
<td>0.01</td>
<td>0.33</td>
</tr>
<tr>
<td>0.0078125</td>
<td>0.3359375</td>
<td>0.005</td>
<td>0.335</td>
</tr>
<tr>
<td>0.00390625</td>
<td>0.33203125</td>
<td>0.002</td>
<td>0.332</td>
</tr>
<tr>
<td>0.001953125</td>
<td>0.333984375</td>
<td>0.001</td>
<td>0.333</td>
</tr>
</tbody>
</table>

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 $2 \times 10^b$
- $2 \times 10^b$ refines to $1 \times 10^b$
Mesh refinement on $\min(x - 1/3)^2$

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<td>1</td>
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<td>0</td>
</tr>
<tr>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>0.2</td>
<td>0.4</td>
</tr>
<tr>
<td>0.1</td>
<td>0.3</td>
</tr>
<tr>
<td>0.05</td>
<td>0.35</td>
</tr>
<tr>
<td>0.02</td>
<td>0.34</td>
</tr>
<tr>
<td>0.01</td>
<td>0.33</td>
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- $2 \times 10^b$ 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 $\mathcal{G} = 1$. 
Poll and mesh size parameter update

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

- 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>
<tr>
<th>$\delta^k$</th>
<th>$\Delta^k$</th>
</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>
</tr>
<tr>
<td>0.01</td>
<td>0.1</td>
</tr>
<tr>
<td>0.005</td>
<td>0.05</td>
</tr>
<tr>
<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 \leftarrow \text{stop}</td>
</tr>
<tr>
<td>Initialization</td>
<td>Iteration</td>
</tr>
<tr>
<td>---------------</td>
<td>-----------</td>
</tr>
<tr>
<td>( x_0, \Delta_0 \in {1, 2, 5} \times 10^b, G ) granularity</td>
<td>[1] let ( \delta^k \leq \Delta^k ) be the mesh size parameter</td>
</tr>
<tr>
<td></td>
<td>[2] Updates</td>
</tr>
<tr>
<td></td>
<td>Search</td>
</tr>
<tr>
<td></td>
<td>Poll (if the Search failed)</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
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<tr>
<td></td>
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</tr>
</tbody>
</table>
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.

- A surrogate function \( s \) is defined as the time to solve a collection of small-sized problems.
- In 2005, \( f(x) \approx 3\text{h}-4\text{h} \) and \( s(x) \approx 1\text{m} \). The surrogate was 200 times faster (now \( \approx 140 \) times).
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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 ( \times 2 \div 2 )</th>
<th>New ( {1, 2, 5} \times 10^b )</th>
<th>Granularity</th>
<th>0.01</th>
<th>0.05</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU:</td>
<td>228 s</td>
<td>207 s</td>
<td>205 s</td>
<td>220 s</td>
<td></td>
</tr>
<tr>
<td>( \eta_1 )</td>
<td>0.2508936274</td>
<td>0.5325498121</td>
<td>0.35</td>
<td>0.35</td>
<td></td>
</tr>
<tr>
<td>( \eta_2 )</td>
<td>0.9008242693</td>
<td>0.9938378210</td>
<td>0.99</td>
<td>0.95</td>
<td></td>
</tr>
<tr>
<td>( \alpha_1 )</td>
<td>0.5464425868</td>
<td>0.4817164472</td>
<td>0.50</td>
<td>0.45</td>
<td></td>
</tr>
<tr>
<td>( \alpha_2 )</td>
<td>1.5505441560</td>
<td>3.5206901980</td>
<td>2.82</td>
<td>3.20</td>
<td></td>
</tr>
</tbody>
</table>

Observations:

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

\[
(\eta_1, \eta_2, \alpha_1, \alpha_2) = (0.35, 0.99, 0.5, 2.82).
\]
Results on a collection of mixed-integer problems

- 43 problems taken from 3 papers by J. Müller et al.:
  - SO-MI [Müller et al., 2013]: 19 problems, mixed, constrained.
  - SO-I [Müller et al., 2014]: 16 problems, discrete, constrained.
  - MISO [Müller, 2016]: 8 problems, mixed, unconstrained.

- 10 LHS starting points are considered for each problem, for a total of 430 instances.

- NOMAD 3.7.3 (current release, classic mesh) vs NOMAD 3.8.Dev (prototype, new mesh).

- Performance and data profiles [Moré and Wild, 2009].
Performance profiles for the 430 instances

Performance profiles (43x10 instances)

BBO: Algorithm and Applications 24/32
Data profiles for the 430 instances (precision $10^{-1}$)
Data profiles for the 430 instances (precision $10^{-3}$)
Data profiles for the 430 instances (precision $10^{-7}$)
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Discussion
Discussion (1/2)

▶ 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 $G = 1$. 
Discussion (1/2)

- 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 \( G = 1 \).

- Computational 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 (1/2)

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  - A native way to handle granularity of variables \(G\).
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  - Experiments on other test problems in progress.

- Computational experiments on analytical problems:
  \(\simeq 3\%\) performance improvement over the previous NOMAD version.
Discussion (2/2)

▶ 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


References II


