Blackbox optimization with the MADS algorithm and the NOMAD software

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Presentation outline

Introduction

The MADS algorithm

The NOMAD software package

Example 1: Aircraft takeoff trajectories

Example 2: Characterization of objects from radiographs

Example 3: Hyperparameters Optimization

References
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References
Blackbox / Derivative-Free Optimization

We consider

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

where the evaluations of $f$ and the functions defining $\Omega$ are the result of a computer simulation (a blackbox)

- Each call to the simulation may be expensive
- The simulation can fail
- Sometimes $f(x) \neq f(x)$
- Derivatives are not available and cannot be approximated
Blackboxes as illustrated by a Boeing engineer

- Long runtime
- Large memory requirement
- No derivatives available
- Local optima
- Non-smooth, noisy
Terms

▶ “Derivative-Free Optimization (DFO) is the mathematical study of optimization algorithms that do not use derivatives” [Audet and Hare, 2017]
  ▶ Optimization without using derivatives
  ▶ Derivatives may exist but are not available
  ▶ Obj./constraints may be analytical or given by a blackbox

▶ “Blackbox Optimization (BBO) is the study of design and analysis of algorithms that assume the objective and/or constraints functions are given by blackboxes” [Audet and Hare, 2017]
  ▶ A simulation, or a blackbox, is involved
  ▶ Obj./constraints may be analytical functions of the outputs
  ▶ Derivatives may be available (ex.: PDEs)
  ▶ Sometimes referred as Simulation-Based Optimization (SBO)
Optimization: Global view
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Typical setting

Unconstrained case, with one initial starting solution

Algorithm

\[ x_0 \xrightarrow{\text{Algorithm}} x^* \]

\[ x_1, x_2, \ldots \xrightarrow{f(x_1), f(x_2), \ldots} f \]

\( f \) (blackbox)
# Algorithms for blackbox optimization

A method for blackbox optimization should ideally:

- Be efficient given a **limited budget of evaluations**
- Be **robust** to noise and blackbox failures
- Natively handle **general constraints**
- Have **convergence properties** ensuring first-order local optimality in the smooth case – otherwise why using it on more complicated problems?
- Easily exploit **parallelism**
- Deal with **multiobjective optimization**
- Deal with **integer and categorical variables**
- Have a publicly available **implementation**
Families of methods

- **“Computer science”** methods:
  - Heuristics such as genetic algorithms
  - No convergence properties
  - Cost a lot of evaluations
  - Should be used only in last resort for desperate cases

- **Statistical methods:**
  - Design of experiments – out of date compared to modern DFO methods
  - Bayesian optimization: EGO algorithm based on surrogates and expected improvement
  - Still limited in terms of dimension
  - Does not natively handle constraints
  - Better to use these tools in conjunction with DFO methods

- **Derivative-Free Optimization methods (DFO)**
DFO methods

- Model-based methods:
  - Derivative-Free Trust-Region (DFTR) methods.
  - Based on quadratic models or radial-basis functions.
  - Use of a trust-region.
  - Better for \{ DFO \setminus BBO \}.
  - Not resilient to noise and hidden constraints.
  - Not easy to parallelize.

- Direct-search methods:
  - Classical methods: Coordinate search, Nelder-Mead – the other simplex method.
  - Modern methods: Generalized Pattern Search (GPS), Generating Set Search (GSS), Mesh Adaptive Direct Search (MADS).

So far, the size of the instances (variables and constraints) is typically limited to $\simeq 50$, and we target local optimization.
The MADS algorithm [Audet and Dennis, Jr., 2006]
MADS illustration with $n = 2$: Poll step

$$\Delta^m_k = \Delta^p_k = 1$$

poll trial points $= \{t_1, t_2, t_3\}$
MADS illustration with $n = 2$: Poll step

\[ \Delta^m_k = \Delta^p_k = 1 \]
\[ \Delta^m_{k+1} = \frac{1}{4} \]
\[ \Delta^p_{k+1} = \frac{1}{2} \]

poll trial points = \{t_1, t_2, t_3\} = \{t_4, t_5, t_6\}
MADS illustration with $n = 2$: Poll step

$$\Delta^m_k = \Delta^p_k = 1$$

$$\Delta^m_{k+1} = \frac{1}{4}$$
$$\Delta^p_{k+1} = \frac{1}{2}$$

$$\Delta^m_{k+2} = \frac{1}{16}$$
$$\Delta^p_{k+2} = \frac{1}{4}$$

Poll trial points:
- $\{t_1, t_2, t_3\}$
- $\{t_4, t_5, t_6\}$
- $\{t_7, t_8, t_9\}$
Special features of MADS

- Constraints handling with the Progressive Barrier technique [Audet and Dennis, Jr., 2009]
- Surrogates [Talgorn et al., 2015]
- Categorical variables [Abramson, 2004]
- Granular and discrete variables [Audet et al., 2019b]
- Global optimization [Audet et al., 2008a]
- Parallelism [Le Digabel et al., 2010, Audet et al., 2008b]
- Multiobjective optimization [Audet et al., 2008c]
- Sensitivity analysis [Audet et al., 2012]
- Handling of stochastic blackboxes [Alarie et al., 2019, Audet et al., 2019a]
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NOMAD (Nonlinear Optimization with MADS)

- C++ implementation of the MADS algorithm [Audet and Dennis, Jr., 2006]
- Standard C++. Runs on Linux, Mac OS X and Windows
- Parallel versions with MPI
- MATLAB versions; Multiple interfaces (Python, Excel, etc.)
- Open and free – LGPL license
- Download at https://www.gerad.ca/nomad
- Support at nomad@gerad.ca

- Related article in TOMS [Le Digabel, 2011] (WoS Highly Cited Paper)
NOMAD: History and team

- Developed since 2000
- Current version: 3.9 (June 2018)
- Algorithm designers, developers:
  - M. Abramson, C. Audet, G. Couture, J. Dennis, S. Le Digabel, V. Rochon-Montplaisir, C. Tribes

- Developers:
  - Versions 1 and 2: G. Couture
  - **Version 3 (2008)**: S. Le Digabel, C. Tribes
  - **Version 4 (2020)**: V. Rochon-Montplaisir, C. Tribes
≈12,000 certified downloads since 2008
Main functionalities (1/2)

- Single or biobjective optimization

- Variables:
  - Continuous, integer, binary, categorical, granular
  - Periodic
  - Fixed
  - Groups of variables

- Searches:
  - Latin-Hypercube
  - Variable Neighborhood Search
  - Nelder-Mead Search
  - Quadratic models
  - Statistical surrogates
  - User search
Main functionalities (2/2)

- Constraints treated with 4 different methods:
  - Progressive Barrier (default)
  - Extreme Barrier
  - Progressive-to-Extreme Barrier
  - Filter method

- Several direction types:
  - Coordinate directions
  - LT-MADS
  - OrthoMADS
  - Hybrid combinations

- Sensitivity analysis

(all items correspond to published or submitted papers)
Blackbox conception (batch mode)

- Command-line program that takes in argument a file containing \( x \), and displays the values of \( f(x) \) and the \( c_j(x) \)’s

- Can be coded in any language

- Typically: `> bb.exe x.txt` displays `f c1 c2` (objective and two constraints)
Run NOMAD

> nomad parameters.txt

[...]

NOMAD - version 3.8.1 has been created by
Charles Audet - Ecole Polytechnique de Montreal
Sebastien Le Digabel - Ecole Polytechnique de Montreal
Christophe Tribes - Ecole Polytechnique de Montreal

The copyright of NOMAD - version 3.8.1 is owned by
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Christophe Tribes - Ecole Polytechnique de Montreal

NOMAD v3 has been funded by AFOER, Exxon Mobil, Hydro Quebec, Rio Tinto and TVADO.

NOMAD v3 is a new version of NOMAD v1 and v2. NOMAD v1 and v2 were created and developed by Mark Abramson, Charles Audet, Gilles Couture, and John E. Dennis Jr., and were funded by AFOER and Exxon Mobil.

License : '$NOMAD_HOME/src/lgpl.txt'
User guide: '$NOMAD_HOME/doc/user_guide.pdf'
Examples : '$NOMAD_HOME/examples'
Tools : '$NOMAD_HOME/tools'

Please report bugs to nomad@gerad.ca

Seed: 0

MADS run {

<table>
<thead>
<tr>
<th>BHN</th>
<th>OBJ</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>0.0000000000</td>
</tr>
<tr>
<td>21</td>
<td>-1.0000000000</td>
</tr>
<tr>
<td>23</td>
<td>-3.0000000000</td>
</tr>
<tr>
<td>51</td>
<td>-4.0000000000</td>
</tr>
<tr>
<td>563</td>
<td>-4.0000000000</td>
</tr>
</tbody>
</table>

} end of run (mesh size reached NOMAD precision)

blackbox evaluations: 563
best infeasible solution (min. violation): ( 1.0000000013 1.0000000048 0.9999999797 0.99999992 -4 ) h=1.10134e-13 f=-4
best feasible solution: ( 1 1 1 1 -4 ) h=0 f=-4
### Introduction

The **MADS** algorithm

The **NOMAD** software package

**Example 1: Aircraft trajectories**

**Example 2: Radiographs**

**Example 3: HPO**

### References
Aircraft takeoff trajectories

- [Torres et al., 2011]


- Biobjective optimization

- Must execute on different platforms including some old Solaris distributions
Definition of the optimization problem

- Concept: Optimization of vertical flight path based on procedures designed to reduce noise emission at departure to protect airport vicinity.

- Minimization of environmental and economical impact: Noise and fuel consumption.

- NADP (Noise Abatement Departure Procedure), variables: During departure phase, the aircraft will target its climb configuration:
  - Increase the speed up to climb speed (acceleration phase)
  - Reduce the engine rate to climb thrust (reduction phase)
  - Gain altitude
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References
Characterization of objects from radiographs - LANL

We want to identify an unknown object inside a box, using a x-ray source that gives an image on a detector.

In this work, the unknown object is supposed to be spherical.
Radiograph

A radiograph is the observed image on the detector. For example:
Description of the problem

- The problem consist to **identify the unknown object** with sufficient precision so that the object can be classified as dangerous or not
- Must work **rapidly**
- Must work for radiographs **not created on a well-controlled experimental environment**
- Must **not crash** for unreasonable user inputs
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HPO with HyperNOMAD

- PhD project of Dounia Lakhmiri

- Technical report [Lakhmiri et al., 2019]

- We focus on the HPO of deep neural networks

- Our advantages:
  - Blackbox optimization problem:
    \[ \text{One blackbox call} = \text{Training} + \text{validation} + \text{test, for a fixed set of hyperparameters} \]
  - Presence of categorical variables (ex.: number of layers)
  - Existing methods are mostly heuristics (grid search, random search, GAs, etc.)

- Based on the NOMAD implementation of MADS
Principle

Blackbox

- Construct the network
- Network training, validation, testing

Accuracy

HyperNOMAD optimizer

- Hyperparameters
- Block structure
- Neighbors
- NOMAD

Initialization:
- dataset,
- starting point,
- evaluation budget
HyperNOMAD

- HyperNOMAD is the interface between NOMAD and a deep learning platform
- Based on the PyTorch library
- Works with preexisting datasets such as MNIST or CIFAR-10, or on custom data
- Available at https://github.com/bbopt/HyperNOMAD
- We consider three types of hyperparameters:
  - Architecture of the neural network
  - Optimizer
  - Plus one for the size of mini-batches
Hyperparameters for the architecture \((5n_1 + n_2 + 4)\)

<table>
<thead>
<tr>
<th>Hyperparameter</th>
<th>Type</th>
<th>Scope</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of convolutional layers ((n_1))</td>
<td>Categorical</td>
<td>[0;20]</td>
</tr>
<tr>
<td>Number of output channels</td>
<td>Integer</td>
<td>[0;50]</td>
</tr>
<tr>
<td>Kernel size</td>
<td>Integer</td>
<td>[0;10]</td>
</tr>
<tr>
<td>Stride</td>
<td>Integer</td>
<td>[1;3]</td>
</tr>
<tr>
<td>Padding</td>
<td>Integer</td>
<td>[0;2]</td>
</tr>
<tr>
<td>Do a pooling</td>
<td>Boolean</td>
<td>0 or 1</td>
</tr>
<tr>
<td>Number of full layers ((n_2))</td>
<td>Categorical</td>
<td>[0;30]</td>
</tr>
<tr>
<td>Size of the full layer</td>
<td>Integer</td>
<td>[0;500]</td>
</tr>
<tr>
<td>Dropout rate</td>
<td>Real</td>
<td>[0;1]</td>
</tr>
<tr>
<td>Activation function</td>
<td>Categorical</td>
<td>ReLU, Sigmoid, Tanh</td>
</tr>
</tbody>
</table>
### Hyperparameters for the optimizer (5)

<table>
<thead>
<tr>
<th>Optimizer</th>
<th>Hyperparameter</th>
<th>Type</th>
<th>Scope</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stochastic Gradient Descent (SGD)</td>
<td>Learning rate</td>
<td>Real</td>
<td>[0;1]</td>
</tr>
<tr>
<td></td>
<td>Momentum</td>
<td>Real</td>
<td>[0;1]</td>
</tr>
<tr>
<td></td>
<td>Dampening</td>
<td>Real</td>
<td>[0;1]</td>
</tr>
<tr>
<td></td>
<td>Weight decay</td>
<td>Real</td>
<td>[0;1]</td>
</tr>
<tr>
<td>Adam</td>
<td>Learning rate</td>
<td>Real</td>
<td>[0;1]</td>
</tr>
<tr>
<td></td>
<td>$\beta_1$</td>
<td>Real</td>
<td>[0;1]</td>
</tr>
<tr>
<td></td>
<td>$\beta_2$</td>
<td>Real</td>
<td>[0;1]</td>
</tr>
<tr>
<td></td>
<td>Weight decay</td>
<td>Real</td>
<td>[0;1]</td>
</tr>
<tr>
<td>Adagrad</td>
<td>Learning rate</td>
<td>Real</td>
<td>[0;1]</td>
</tr>
<tr>
<td></td>
<td>Learning rate decay</td>
<td>Real</td>
<td>[0;1]</td>
</tr>
<tr>
<td></td>
<td>Initial accumulator</td>
<td>Real</td>
<td>[0;1]</td>
</tr>
<tr>
<td></td>
<td>Weight decay</td>
<td>Real</td>
<td>[0;1]</td>
</tr>
<tr>
<td>RMSProp</td>
<td>Learning rate</td>
<td>Real</td>
<td>[0;1]</td>
</tr>
<tr>
<td></td>
<td>Momentum</td>
<td>Real</td>
<td>[0;1]</td>
</tr>
<tr>
<td></td>
<td>$\alpha$</td>
<td>Real</td>
<td>[0;1]</td>
</tr>
<tr>
<td></td>
<td>Weight decay</td>
<td>Real</td>
<td>[0;1]</td>
</tr>
</tbody>
</table>
Blocks of hyperparameters

- **Convolution block:** 2 convolutional layers with
  (number of output channels, kernel size, stride, padding, pooling) = (16, 5, 1, 1, 0) and (7, 3, 1, 1, 1):

  ![Convolution Block Table]

- **Fully connected block:** 3 fully connected layers with sizes of output = 1200, 512, 20:

  ![Fully Connected Block Table]

- **Optimizer block:** SGD with learning rate = 0.1, momentum = 0.9, dampening = $1e^{-4}$, and weight decay = 0:

  ![Optimizer Block Table]
Average results on MNIST

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Avg accuracy on validation set</th>
<th>Avg accuracy on test set</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rand. search [Bergstra and Bengio, 2012]</td>
<td>94.02</td>
<td>89.07</td>
</tr>
<tr>
<td>SMAC [Hutter et al., 2011]</td>
<td>95.48</td>
<td>97.54</td>
</tr>
<tr>
<td>RBFOpt [Diaz et al., 2017]</td>
<td>95.66</td>
<td>97.93</td>
</tr>
<tr>
<td>NOMAD</td>
<td><strong>96.81</strong></td>
<td><strong>97.98</strong></td>
</tr>
</tbody>
</table>
MNIST results with HyperNOMAD

Comparison between HyperNOMAD, TPE and RS when launched from the default starting point of HyperNOMAD, on the MNIST data set. Best solution with HyperNOMAD: 99.61%
Results on CIFAR-10 (vs Hyperopt)

- Training with 40,000 images, validation/test on 10,000 images
- One evaluation (training+test) $\sim$ 2 hours
  (i7-6700@3.4 GHz, GeForce GTX 1070)

![Graphs showing test accuracy vs number of blackbox evaluations for different optimization methods.](image)

(a) Default starting point

(b) From a VGG architecture
Summary

- Blackbox optimization motivated by industrial applications
- Algorithmic features backed by mathematical convergence analyses and published in optimization journals
- NOMAD: Software package implementing MADS
- Open source; LGPL license
- Features: Constraints, biobjective, global optimization, surrogates, several types of variables, parallelism
- HyperNOMAD: Library for the HPO problem.
- Fast support at nomad@gerad.ca
- NOMAD has become the baseline for benchmarking DFO algorithms
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