Blackbox optimization with the NOMAD software

Sébastien Le Digabel
Charles Audet
Viviane Rochon-Montplaisir
Christophe Tribes

GERAD and École Polytechnique de Montréal (MAGI)

UQAC, 2018–03–21

Presentation outline

Blackbox optimization

The MADS algorithm

The NOMAD software package

References

Blackbox optimization problems

- Optimization problem:

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

- Evaluations of f (the objective function) and of the functions defining Ω are usually the result of a computer code (a blackbox).
- n variables, m general constraints.
- $\Omega = \left\{x \in \mathcal{X} : c_j(x) \leq 0, j \in \{1, 2, \ldots, m\}\right\} \subseteq \mathbb{R}^n$.
- $\mathcal{X}$: Bounds and/or nonquantifiable constraints.

[0] Initializations (x_0, Δ_0^m)

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

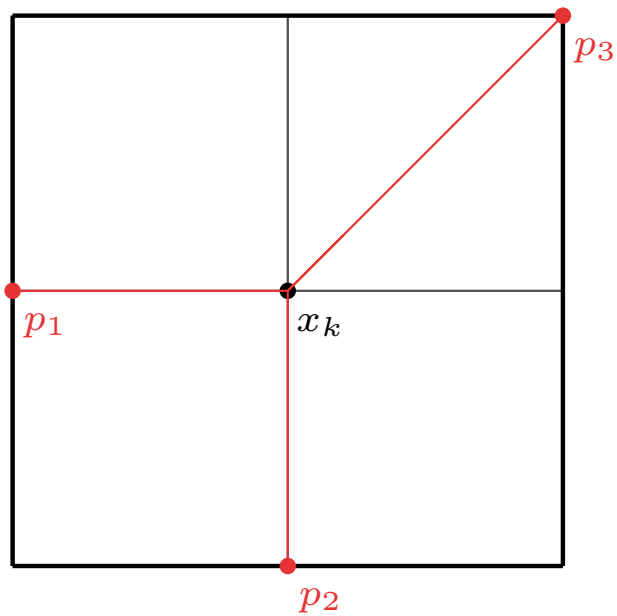
[2] Updates

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

From the MADS original paper [Audet and Dennis, Jr., 2006].

Poll illustration (successive fails and mesh shrink)

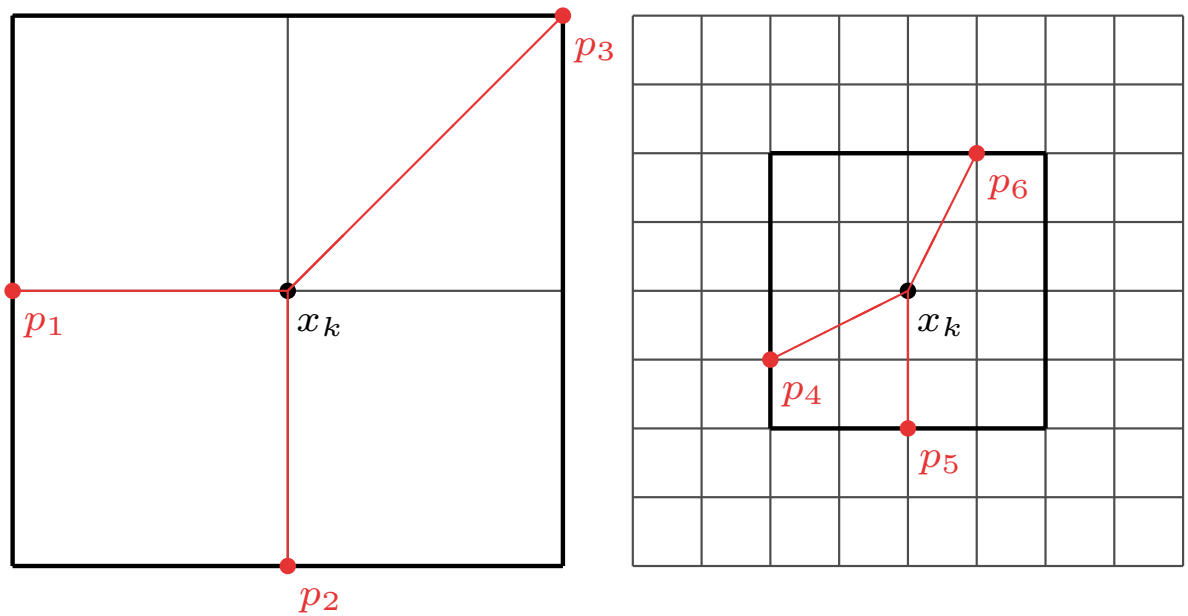
$$\Delta_k = 1$$



trial points=$\{p_1, p_2, p_3\}$

Poll illustration (successive fails and mesh shrink)

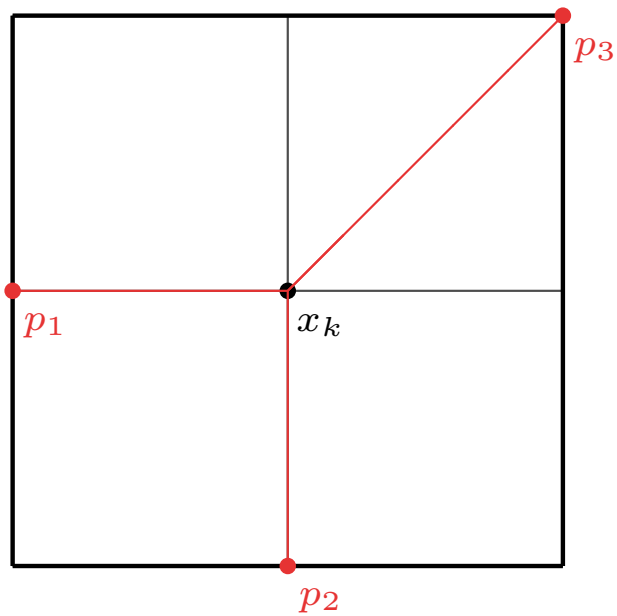
$\Delta_k = 1$ $\Delta_{k+1} = 1/4$

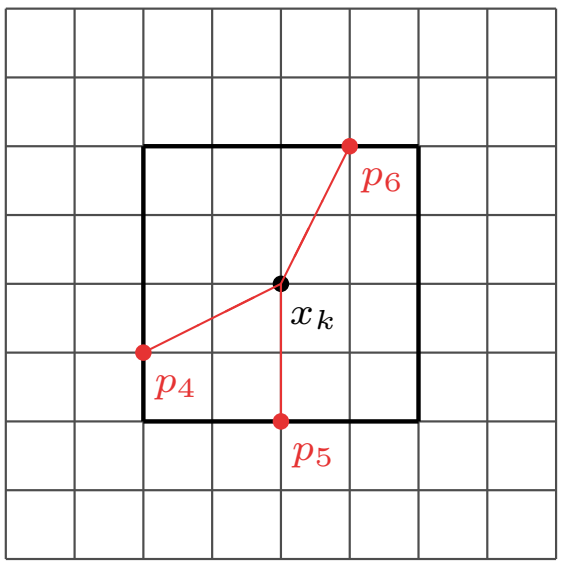


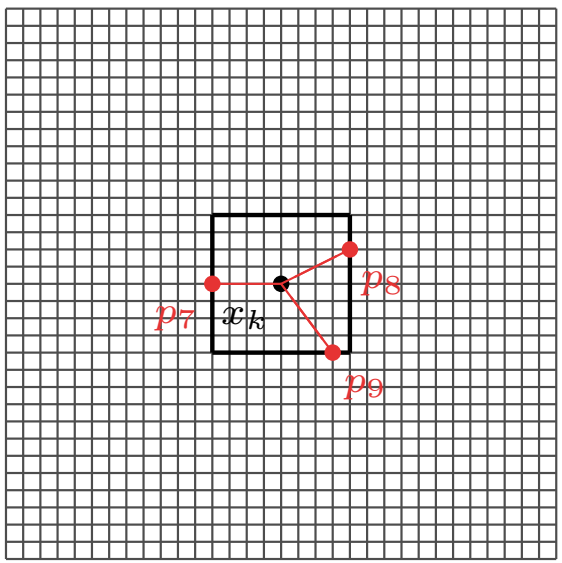
trial points$=\{p_1, p_2, p_3\}$ $= \{p_4, p_5, p_6\}$

Poll illustration (successive fails and mesh shrink)

$\Delta_k = 1$ $\Delta_{k+1} = 1/4$ $\Delta_{k+2} = 1/16$







trial points$=\{p_1, p_2, p_3\}$ $= \{p_4, p_5, p_6\}$ $= \{p_7, p_8, p_9\}$

MADS extensions

- 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., 2018].
- 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].

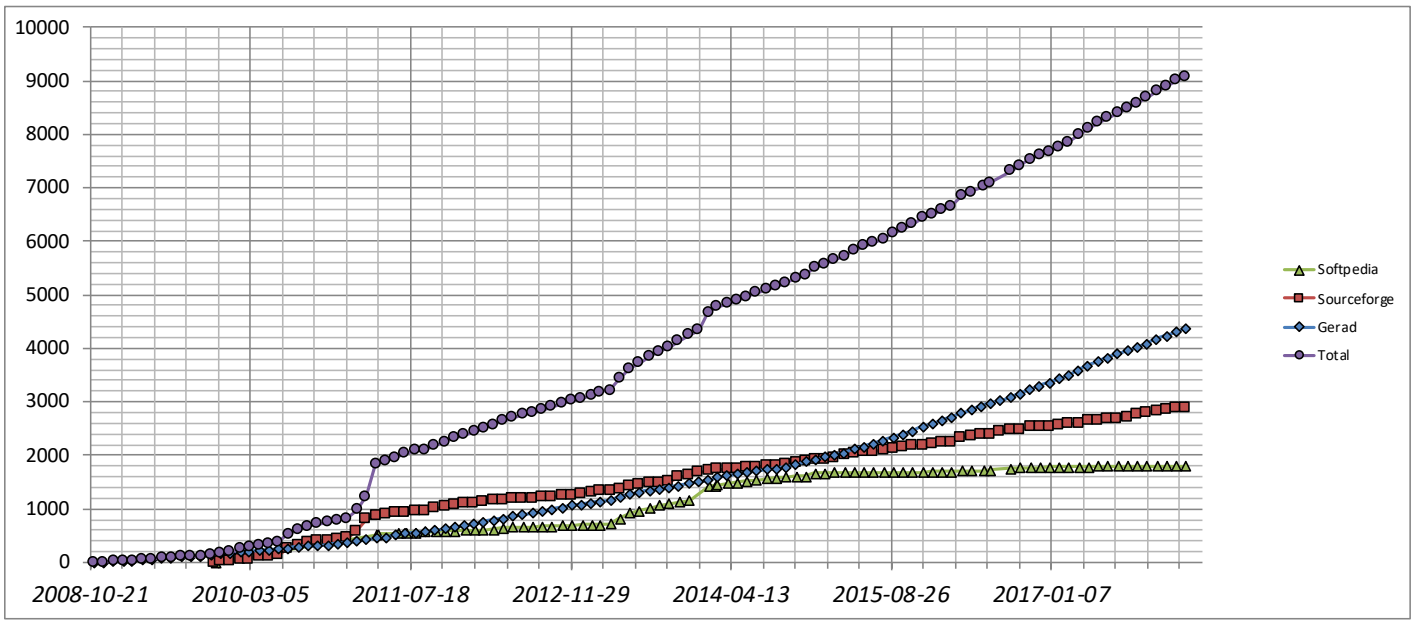
NOMAD (Nonlinear Optimization with MADS)

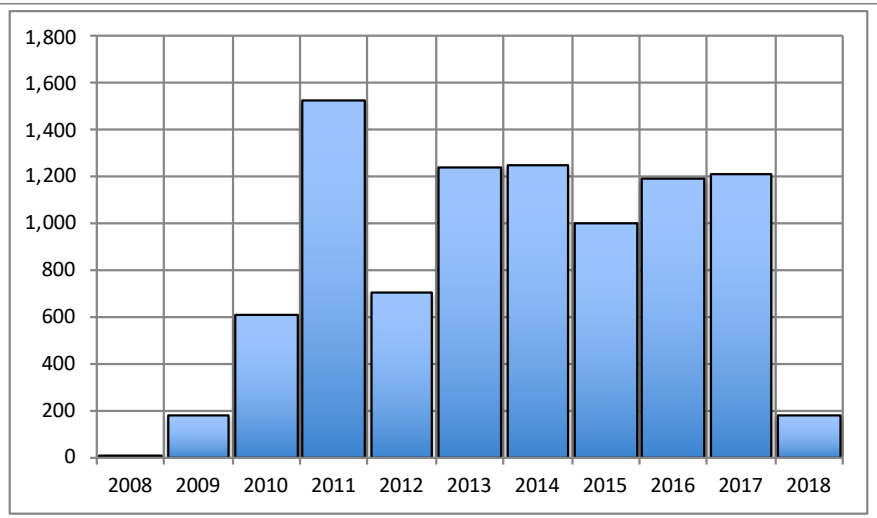
- C++ implementation of MADS.
- Standard C++, no other package needed.
- Parallel versions with MPI.
- Runs on Linux, Mac OS X and Windows.
- MATLAB versions; Multiple interfaces (Python, Excel, etc.)
- Command-line and library interfaces.
- Distributed under the LGPL license.
- Complete user guide available in the package.
- Doxygen documentation available online.
- Download at https://www.gerad.ca/nomad.

NOMAD: History and team

- Developed since 2000.
- Current version: 3.8.
- Algorithm designers:
  - M. Abramson, C. Audet, J. Dennis, S. Le Digabel, C. Tribes, V. Rochon-Montplaisir.
- Developers:
  - Versions 1 and 2: G. Couture.
  - **Version 3 (2008)**: S. Le Digabel, C. Tribes.
  - **Version 4 (2019)**: C. Tribes, V. Rochon-Montplaisir.
- Support at nomad@gerad.ca.
- Related article in TOMS [Le Digabel, 2011].

More than 9,000 certified downloads since 2008.





Users from Sept. 2014 to Sept. 2015

(downloads from the GERAD website only)

- **Industries:** Hydro-Québec (IREQ), Rio Tinto, Bombardier, Airbus, Boeing, United Airlines, Siemens, Schneider Electric, GHD Toronto, Energen, Skyconseil, German Aerospace Center, Moscow Power Engineering Institute, Newmerical Technologies, Disney Research, US Federal Reserve Board, Softree, Aditazz, Essar Steel, Tatura Milk Industries, Westrock, Market Appeal, Corona Insights, The Climate Corporation.
- **National Labs:** Argonne, Sandia, Los Alamos.
- **Universities.**

Main functionalities (1/2)

- Single or biobjective optimization.
- Variables:
  - Continuous, integer, binary, categorical.
  - Periodic.
  - Fixed.
  - Groups of variables.
- Searches:
  - Latin-Hypercube (LH).
  - Variable Neighborhood Search (VNS).
  - 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).

NOMAD installation

- Pre-compiled executables are available for Windows and Mac.
- Installation programs copy these executables.
- On Unix/Linux, after download, launch an installation script.
- Two ways to use NOMAD: batch mode or library mode.

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).

Important parameters

- Necessary parameters: Blackbox characteristics (dimension n, number of constraints, etc.), starting point (x_0).
- All algorithmic parameters have default values. The most important are:
  - Maximum number of blackbox evaluations,
  - Starting point (more than one can be defined),
  - Types of directions (more than one can be defined),
  - Initial mesh size,
  - Constraint types,
  - Surrogate searches,
  - Seeds.
- See the user guide for the description of all parameters, or use the `nomad -h` option.

Run NOMAD

```
> nomad parameters.txt
```

```
[iota ~/Desktop/2018_UQAC_NOMAD/demo_NOMAD/mac] > ../nomad.3.8.1/bin/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 {
        Sebastien Le Digabel - Ecole Polytechnique de Montreal
        Christophe Tribes    - Ecole Polytechnique de Montreal
}

NOMAD v3 has been funded by AFOSR, Exxon Mobil, Hydro Québec, Rio Tinto and
IVADO.

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 AFOSR 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 {

        BBE     OBJ

        4       0.0000000000
        21      -1.0000000000
        23      -3.0000000000
        51      -4.0000000000
        563     -4.0000000000

} end of run (mesh size reached NOMAD precision)

blackbox evaluations                    : 563
best infeasible solution (min. violation): ( 1.000000013 1.000000048 0.9999999797 0.999999992 -4 ) h=1.10134e-13 f=-4
best feasible solution                  : ( 1 1 1 1 -4 ) h=0 f=-4
```

Advanced functionalities (library mode)

- No system calls: the code executes faster.
- The user can program a custom search strategy.
- The user can pre-process all evaluation points before they are evaluated.
- The user can decide the priority in which trial points are evaluated.
- The user can define callback functions that will be called at some specific events (new success, new iteration, new MADS run in bi-objective optimization)

Examples included in the NOMAD package

Simple examples:

- How to run NOMAD.
- Usage of parallellism.
- Categorical variables.
- MATLAB/Python interfaces.

Advanced examples to illustrate additional possibilities:

- Multi-start from points generated with LH sampling.
- Problems used in library mode and coded as:
  - A Windows DLL.
  - A GAMS program.
  - A CUTEst problem.
  - A FORTRAN code.
- A GUI prototype in JAVA.

Other MADS distributions

- MATLAB version within the Opti Toolbox package.
  http://www.i2c2.aut.ac.nz/Wiki/OPTI.
- Available in the MATLAB Optimization Toolbox.
  Old version, not maintained.
- NOMADM by M. Abramson. Old version, not maintained.
- Excel with the OpenSolver tool.
  http://www.opensolver.org (GPLv3).

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.
- Fast support at nomad@gerad.ca.
- NOMAD can be customized through collaborations.

References I

Abramson, M. (2004).
Mixed variable optimization of a Load-Bearing thermal insulation system using a filter pattern search algorithm.
Optimization and Engineering, 5(2):157–177.

Audet, C., Béchard, V., and Le Digabel, S. (2008a).
Nonsmooth optimization through mesh adaptive direct search and variable neighborhood search.
Journal of Global Optimization, 41(2):299–318.

Audet, C. and Dennis, Jr., J. (2006).
Mesh adaptive direct search algorithms for constrained optimization.
SIAM Journal on Optimization, 17(1):188–217.

Audet, C. and Dennis, Jr., J. (2009).
A Progressive Barrier for Derivative-Free Nonlinear Programming.
SIAM Journal on Optimization, 20(1):445–472.

Audet, C., Dennis, Jr., J., and Le Digabel, S. (2008b).
Parallel space decomposition of the mesh adaptive direct search algorithm.
SIAM Journal on Optimization, 19(3):1150–1170.

Audet, C., Dennis, Jr., J., and Le Digabel, S. (2012).
Trade-off studies in blackbox optimization.
Optimization Methods and Software, 27(4–5):613–624.

References II

Audet, C., Digabel, S. L., and Tribes, C. (2018).
The mesh adaptive direct search algorithm for granular and discrete variables.
Technical Report G-2018-16, Les cahiers du GERAD.

Audet, C., Savard, G., and Zghal, W. (2008c).
Multiobjective optimization through a series of single-objective formulations.
SIAM Journal on Optimization, 19(1):188–210.

Le Digabel, S. (2011).
Algorithm 909: NOMAD: Nonlinear Optimization with the MADS algorithm.
ACM Transactions on Mathematical Software, 37(4):44:1–44:15.

Le Digabel, S., Abramson, M., Audet, C., and Dennis, Jr., J. (2010).
Parallel Versions of the MADS Algorithm for Black-Box Optimization.
In *Optimization days*, Montreal. GERAD.
Slides available at `https://www.gerad.ca/Sebastien.Le.Digabel/talks/2010_JOPT_25mins.pdf`.

Talgorn, B., Le Digabel, S., and Kokkolaras, M. (2015).
Statistical Surrogate Formulations for Simulation-Based Design Optimization.
Journal of Mechanical Design, 137(2):021405–1–021405–18.