Blackbox optimization with the NOMAD software

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Team

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Presentation outline

Blackbox optimization

Examples from hydrology

The MADS algorithm

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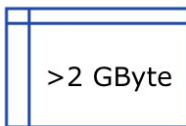## Blackbox optimization problems

▶ 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.

▶ $\Omega = \left\{ x \in \mathcal{X} : c_j(x) \leq 0, j \in \{1, 2, \ldots, m\} \right\} \subseteq \mathbb{R}^n$.

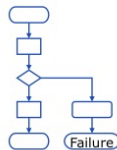▶ $\mathcal{X}$: Bounds and/or nonquantifiable constraints.

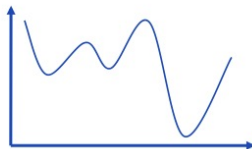# Blackboxes as illustrated by J. Simonis [ISMP 2009]

Long runtime

Large memory requirement

Software might fail

No derivatives available

Local optima

Non-smooth, noisy

Blackbox optimization

Examples from hydrology

The MADS algorithm

The NOMAD software package

References

Collaborators

▶ Snow Water Equivalent estimation [Alarie et al., 2013]:

  ▶ **IREQ**: Stéphane Alarie, Louis-Alexandre Leclaire.

  ▶ **GERAD**: Vincent Garnier, Charles Audet, SLD.

▶ Calibration of a hydrologic model [Minville et al., 2014]:

  ▶ **IREQ**: Marie Minville, Catherine Guay, Louis-Alexandre Leclaire, James Merlau.

  ▶ **GERAD**: Dominique Cartier, Charles Audet, SLD.

Snow Water Equivalent (SWE) estimation

▶ Accurate estimate of water stored in snow is crucial to optimize hydroelectric plants management.

▶ Exact snow measurement is impossible.

▶ SWE is measured at specific sites and next interpolated over the territory.

▶ Territory is huge: Hydro-Québec (HQ) operates 565 dams, 75 reservoirs, and 56 hydroelectric power plants, located over 90 watersheds and covering more than 550,000 km^2.

Previous SWE estimation

▶ Done manually by weighing snow cores at specific sites.

▶ Each measurement campaign requires 2 weeks.

▶ Missing measurements due to adverse meteorological conditions.

GMON device

▶ A new measuring instrument that provides daily automatic SWE.
▶ GMON for Gamma-MONitoring device: it measures the natural Gamma radiation emitted from the soil.
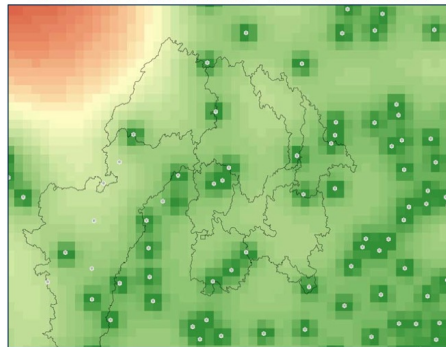▶ Communicates via satellites.

SWE estimation from GMON measures

▶ Kriging interpolation is used to obtain SWE estimation together with an error map.

▶ How to find the device locations that minimize the kriging interpolation error of the SWE?
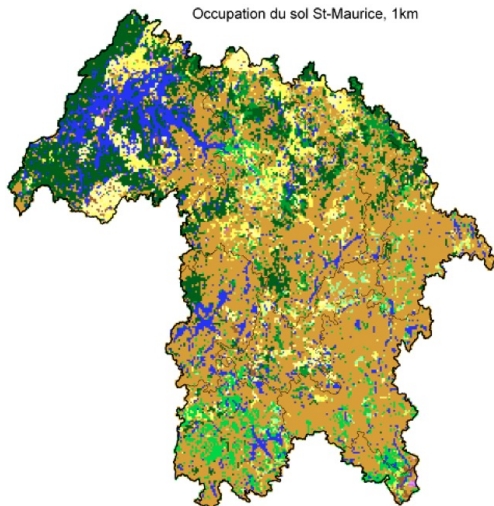
SWE estimation
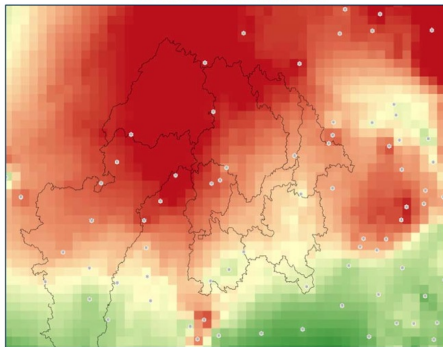
standard deviation of estimation

Problem formulation

- $x \in \mathbb{R}^{2N}$ are the locations of N stations.

- Typically, $N \leq 10$, so we do not consider it as a variable.

- $\Omega \subseteq \mathbb{R}^2$ is the feasible domain where the stations can be located.

- $f(x)$ is a score based on the standard deviation map obtained by the kriging simulation and is considered as a blackbox.

- Each simulation requires $\simeq 2$ seconds, and can only be launched within the Hydro-Québec research center (IREQ).

Constraints

Occupation du sol St-Maurice, 1km

▶ GMON stations cannot be
  located anywhere.

▶ Restrictions on:
  ▶ subsoil properties,
  ▶ slope,
  ▶ vegetation,
  ▶ exploitation,
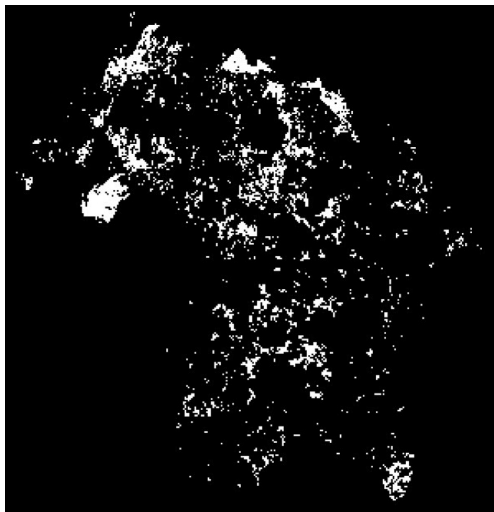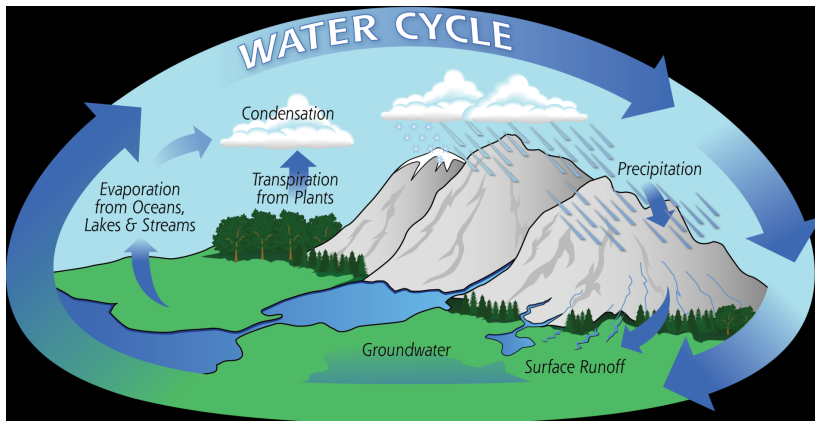 ▶ etc.

Constraints

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- ▶ Restrictions on:
  - ▶ subsoil properties,
  - ▶ slope,
  - ▶ vegetation,
  - ▶ exploitation,
  - ▶ etc.
- ▶ Highly fragmented domain.

Calibration of a hydrologic model

credit: NASA.

Evaporation + Transpiration = Evapotranspiration (ETR).

Objectives

▶ Define a calibration (= parameters optimization) approach in order to improve the transposability of the hydrologic model.

▶ A transposable model should adequately reproduce hydrologic processes when they are employed with other data than those used to obtain the parameters (e.g. climate change).

▶ Emphasis on a realistic representation of ETR.

▶ Characteristics of the optimization problem: Nonsmoothness, multiple regions of attraction, and many local optima within each region of attraction.

The model

▶ HSAMI (*Service hydrométéorologique apports modulés intermédiaires*) [Bisson and Roberge, 1983, Fortin, 1999].

▶ Hydrologic model developed by and used at Hydro-Québec.

▶ 23 parameters: optimization variables.

▶ One evaluation takes $\simeq$ 1-2 seconds.
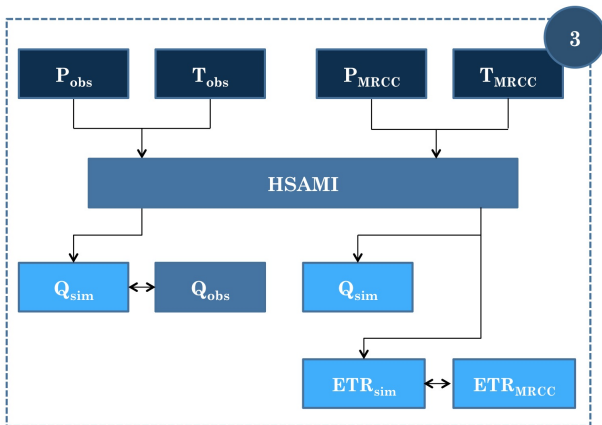
▶ We compare the simulated and observed streamflows and minimize the Nash-Sutcliffe criteria $\dfrac{\sum\limits_{t=1}^{T}(Q_t^o-Q_t^s)^2}{\sum\limits_{t=1}^{T}(Q_t^o-\overline{Q^o})^2}$.

▶ Cross-validation typically over half the data.

Definition of the ETR constraint

Calibration of the ETR is achieved by considering a climatic model (MRCC) for known values of P, T, and ETR.

Some applications related to buildings

▶ *Optimization of dampers for adjacent buildings under seismic excitations* [Bigdeli et al., 2012].

▶ *Review of algorithms for the optimization of building design* [Machairas et al., 2014].

▶ *Minimization of the annual energy consumption for lighting, cooling, and heating of an office building in Houston* [Polak and Wetter, 2006]; Based on the BuildOpt simulator [Wetter, 2005].

▶ *Meta-model based approach for integrated building energy simulation* [Manfren et al., 2013].

▶ *Building energy performance analysis* [Buonomano and Palombo, 2014].

Blackbox optimization

Examples from hydrology

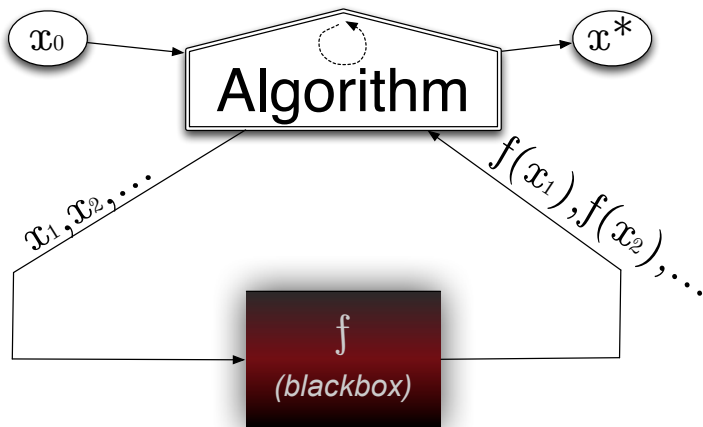## The MADS algorithm

The NOMAD software package

References

MADS and direct search principle

Mesh Adaptive Direct Search (MADS)

▶ [Audet and Dennis, Jr., 2006].

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- ▶ 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.
- ▶ At the end of the iteration, the mesh size is reduced if no new success point is found.
- ▶ Algorithm is backed by a convergence analysis based on the calculus for nonsmooth functions [Clarke, 1983].

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

[2] Updates

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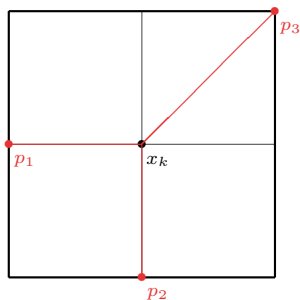>
> else
> > $x_{k+1} \leftarrow x_k$
> > decrease Δ_k^m
>
> $k \leftarrow k + 1$, stop or go to **[1]**

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)

$$\Delta_k = 1 \qquad\qquad \Delta_{k+1} = 1/4$$
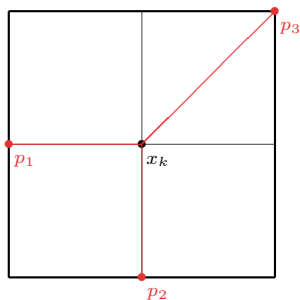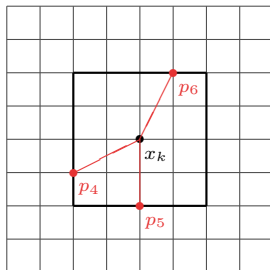
trial points$=\{p_1, p_2, p_3\}$ $\qquad = \{p_4, p_5, p_6\}$

Poll illustration (successive fails and mesh shrink)

$$\Delta_k = 1 \qquad\qquad \Delta_{k+1} = 1/4 \qquad\qquad \Delta_{k+2} = 1/16$$
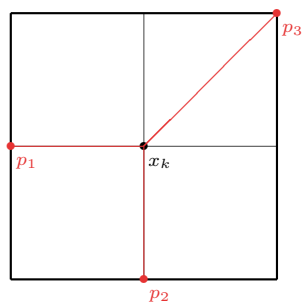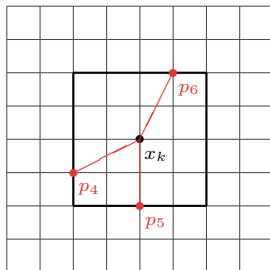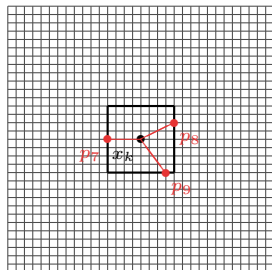
trial points=$\{p_1, p_2, p_3\}$ $\qquad = \{p_4, p_5, p_6\} \qquad = \{p_7, p_8, p_9\}$

MADS extensions

▶ Constraints handling with the Progressive Barrier technique [Audet and Dennis, Jr., 2009].

▶ Surrogates [Talgorn et al., 2015].

▶ Categorical variables [Abramson, 2004].

▶ 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].

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NOMAD (Nonlinear Optimization with MADS)

▶ C++ implementation of MADS.

▶ Standard C++, no other package needed.

▶ Parallel versions with MPI.

▶ Runs on Linux, Unix, Mac OS X and Windows.

▶ MATLAB versions.

▶ 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: 3.7.

- ▶ Algorithm designers:
    - ▶ M. Abramson, C. Audet, J. Dennis, S. Le Digabel, and C. Tribes.

- ▶ Developers:
    - ▶ Versions 1 and 2: G. Couture.
    - ▶ Version 3 (2008): S. Le Digabel and C. Tribes.

- ▶ Support at nomad@gerad.ca.

More than 6,000 certified downloads since 2008.
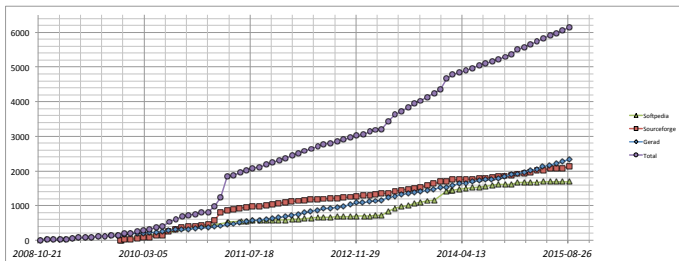
Users from Sept. 2014 to Sept. 2015

(downloads from the GERAD website only)

- ▶ **Industries:** Hydro-Québec (IREQ), Rio Tinto Alcan, 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:
  - ▶ Extreme Barrier.
  - ▶ Progressive Barrier (default).
  - ▶ 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,
   ▶ Latin-Hypercube sampling,
   ▶ Seeds.

▶ See the user guide for the description of all parameters, or use the nomad -h option.

Run NOMAD

```
> nomad parameters.txt
```

```
delta:2 sebld$ nomad param.txt

NOMAD - version 3.5.1.TGP - www.gerad.ca/nomad

Copyright (C) 2001-2012 {
        Mark A. Abramson     - The Boeing Company
        Charles Audet        - Ecole Polytechnique de Montreal
        Gilles Couture       - Ecole Polytechnique de Montreal
        John E. Dennis, Jr.  - Rice University
        Sebastien Le Digabel - Ecole Polytechnique de Montreal
        Christophe Tribes    - Ecole Polytechnique de Montreal
}

Funded in part 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

MADS run {

        BBE       SOL        OBJ

          1                 1             1     0.589738091176242
          7                31             1     0.545072064762882
         10                31             1     0.545072064762882

} end of run (max number of blackbox evaluations)

blackbox evaluations   : 10
best feasible solution : ( 31 1 ) h=0 f=0.5450720648
```

Advanced functionalities (library mode)

▶ No system calls: the code executes faster (more than twice).

▶ Easy to program multiple runs in parallel with different seeds.

▶ 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 indicate user-functions that will be called at some events (new success, new iteration, new MADS run in bi-objective optimization)

Examples included in the NOMAD package

These examples illustrate other possibilities:

- ▶ Multi-start from points generated with LH sampling.

- ▶ Compatibility with previous versions of NOMAD.

- ▶ 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

- ▶ Available in the MATLAB Optimization Toolbox.
  Old version, not maintained.

- ▶ MATLAB version within the Opti Toolbox package.
  http://www.i2c2.aut.ac.nz/Wiki/OPTI.

- ▶ 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.

- ▶ LGPL license.

- ▶ Features: Constraints, biobjective, global opt., surrogates, several types of variables, parallelism.

- ▶ NOMAD is rigorously supported.

- ▶ NOMAD can be customized through collaborations.

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