Blackbox Optimization: Algorithm and Applications

Sébastien Le Digabel

GERAD and École Polytechnique de Montréal

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Team and collaborators

- Profs: Charles Audet, Michael Kokkolaras, SLD.
- Research associate: Christophe Tribes.
- Students: Bastien Talgorn, Nadir Amaioua, Stéphane Jacquet, Mathilde Peyrega, Sara Séguin, Vincent Garnier, Amina Ihaddadène, Mathieu Lemyre Garneau, Loïc Sarrazin.
- Hydro-Québec: Stéphane Alarie, Louis-Alexandre Leclaire.
- LANL: Jerawan C. Armstrong, Brian A. Temple, Kevin L. Buescher.
- Airbus: O. Babando, C. Bes, J. Chaptal, J.-B. Hiriart-Urruty, B. Talgorn, B. Tessier, R. Torres.

Presentation outline

Blackbox optimization

Snow Water Equivalent estimation

Characterization of objects from radiographs

Biobjective optimization of aircraft takeoff trajectories

The MADS algorithm

The NOMAD software package

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Blackbox optimization (BBO) problems

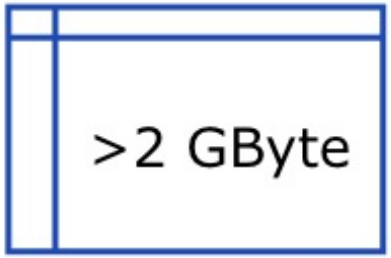
- Optimization problem:

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

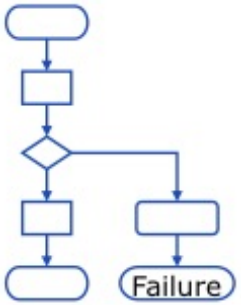
- Evaluations of f (the objective function) and of the functions defining Ω are usually the result of a computer code (a blackbox).
- n variables, m general constraints.
- $\Omega = \{x \in \mathcal{X} : c_j(x) \leq 0, j \in \{1, 2, \ldots, m\}\} \subseteq \mathbb{R}^n$.
- $\mathcal{X}$: Bounds and/or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

Blackboxes as illustrated by J. Simonis [ISMP 2009]

Long runtime

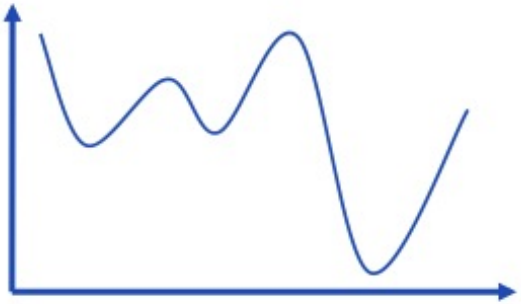


Large memory requirement



Software might fail

No derivatives available



Local optima

Non-smooth, noisy

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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.



source: Hydro-Québec.

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.



source: Hydro-Québec.

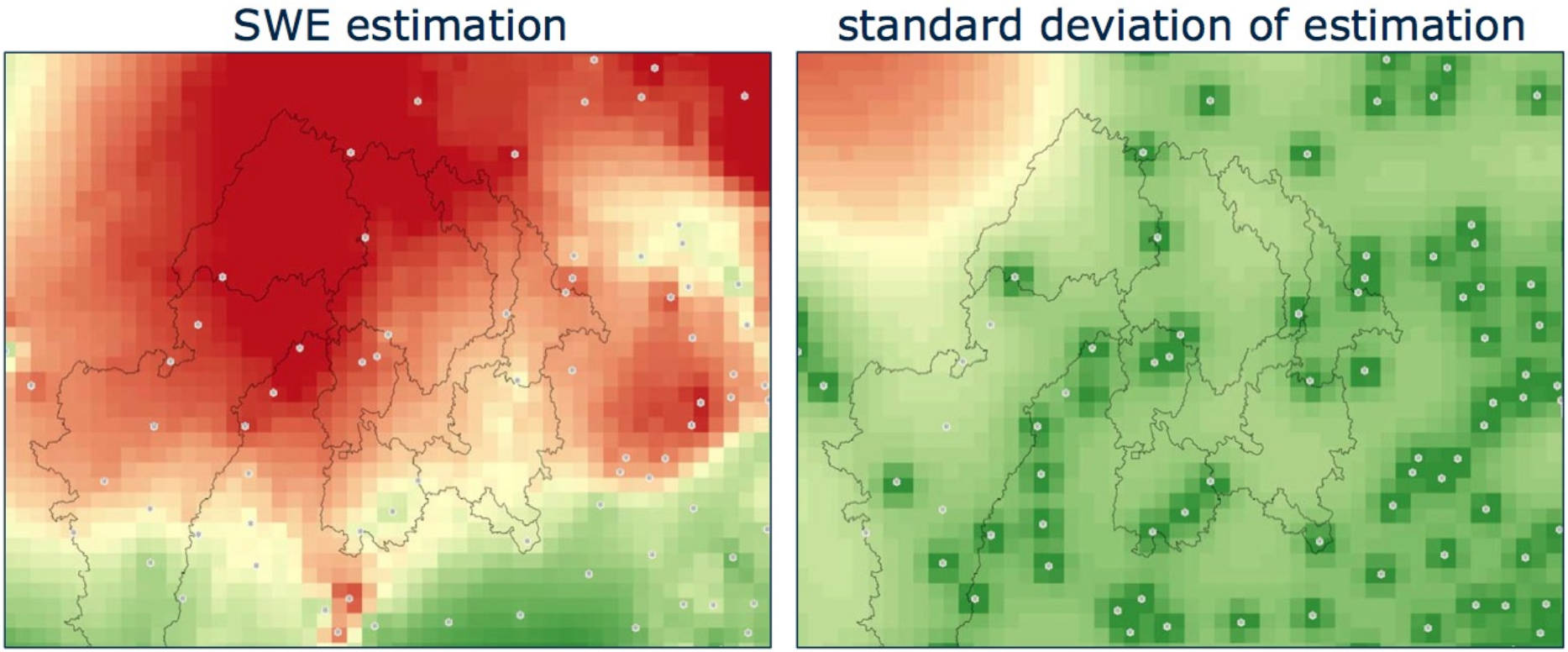
GMON device

- 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.


source: Hydro-Québec.

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?

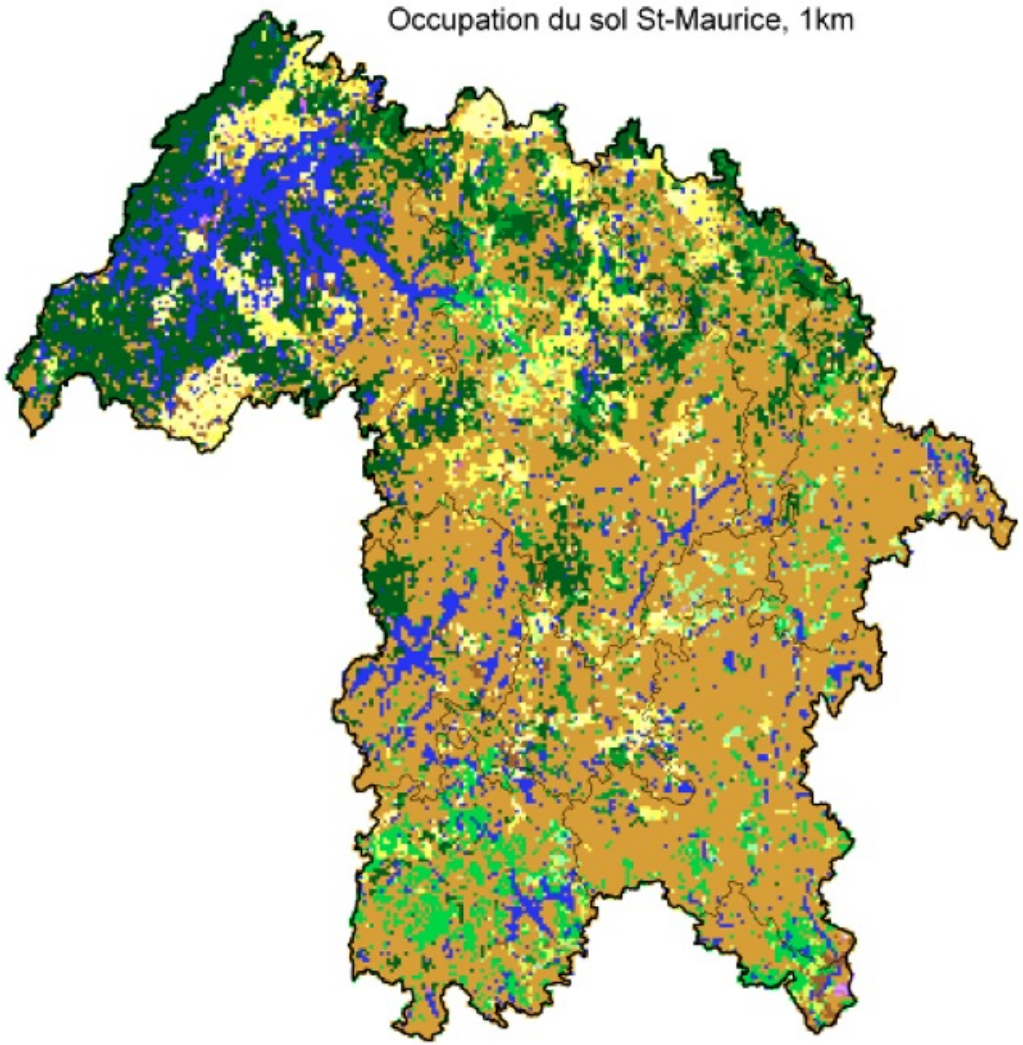


Problem formulation

- $x \in \mathbb{R}^{2N}$ 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).

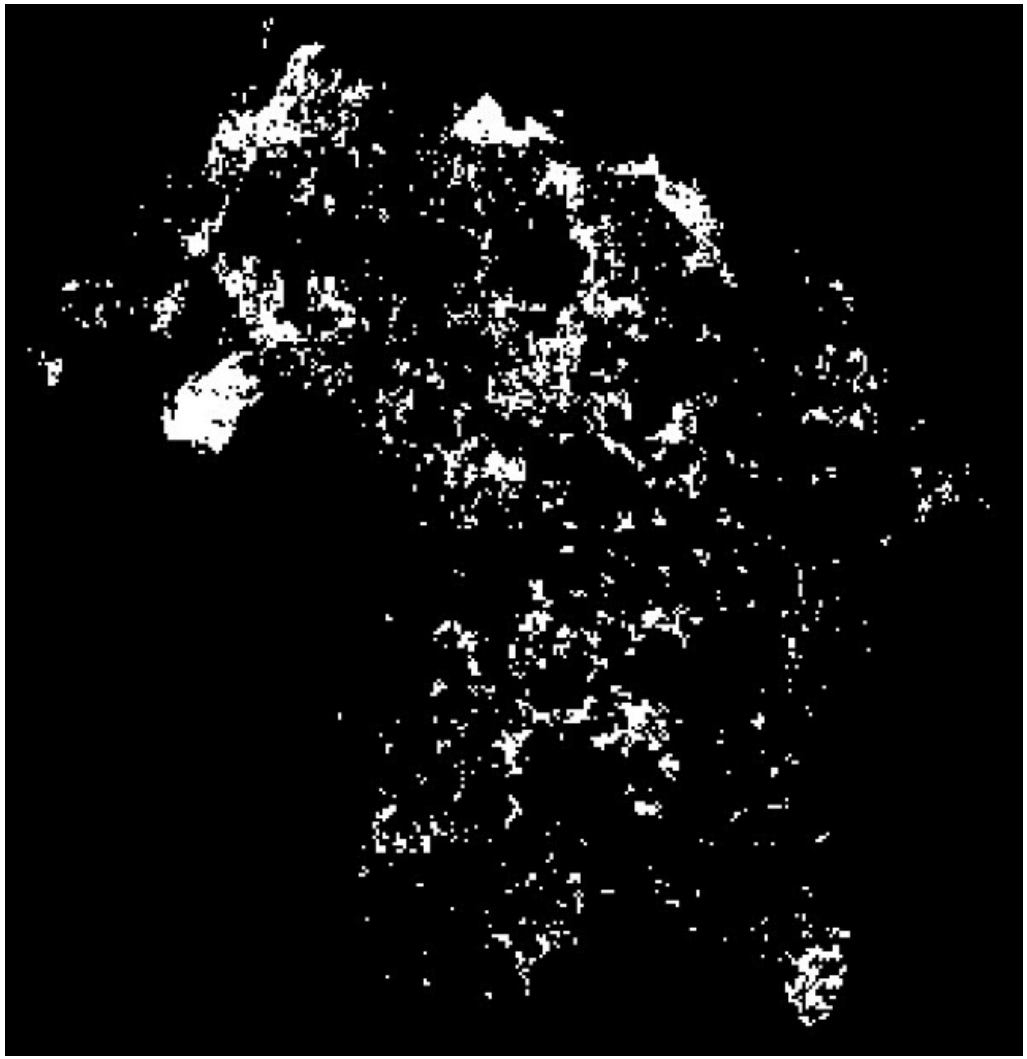
Constraints

- GMON stations cannot be located anywhere.
- Restrictions on:
  - subsoil properties,
  - slope,
  - vegetation,
  - exploitation,
  - etc.



Constraints

- GMON stations cannot be located anywhere.
- Restrictions on:
  - subsoil properties,
  - slope,
  - vegetation,
  - exploitation,
  - etc.
- Highly fragmented domain.



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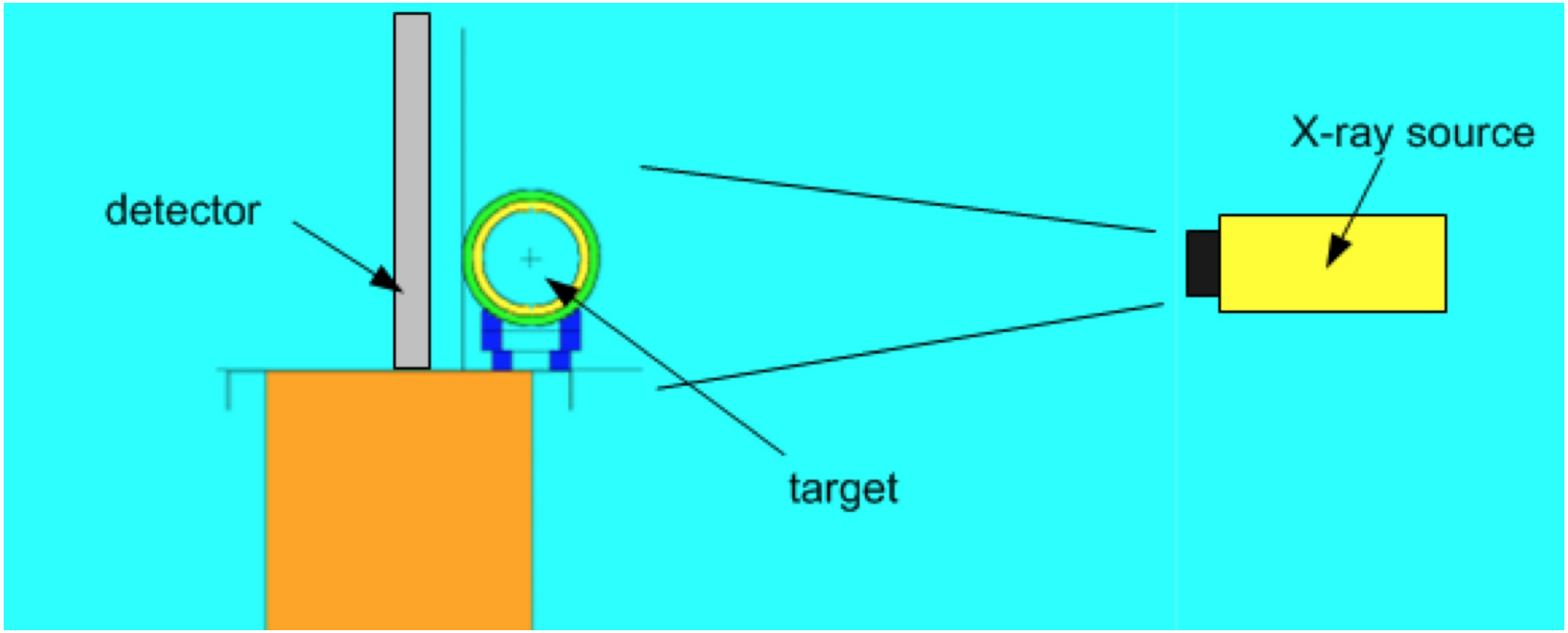
Setting

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

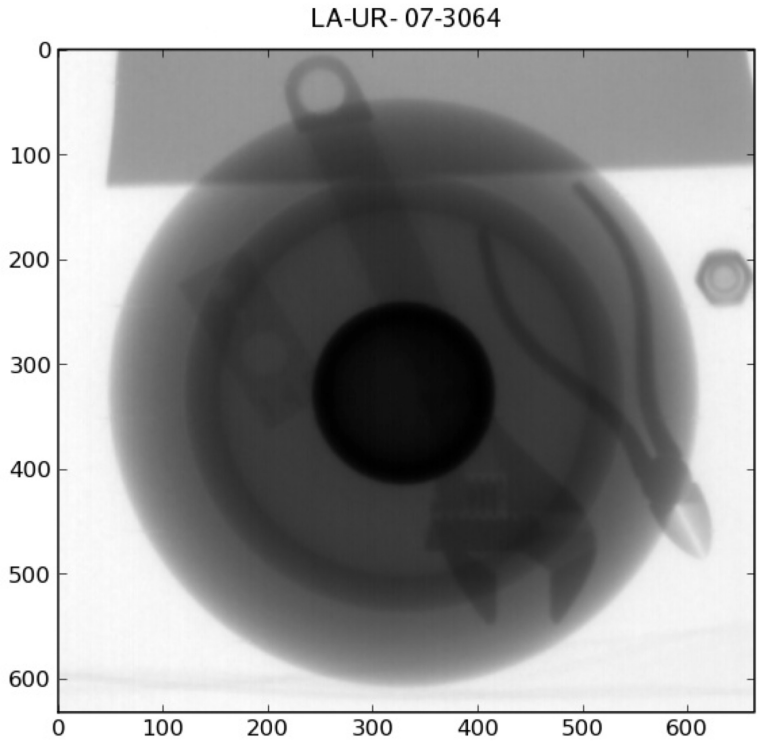


Source: LANL – LA-UR-11-0342

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

Radiograph

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



source: LANL.

Description of the problem

- The problem consists 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.

Definition of the optimization problem

- **Variables:**
  - They represent a spherical object in 1D.
  - Categorical variables: Number of layers and type of material of each layer.
  - Continuous variables: Radius of each layer.
  - The number of variables can change depending on the number of layers.
- **Objective function**:
  - A score associated to the difference between the observed image on the detector, and a simulated image obtained from the candidate object.
  - A numerical code – the blackbox – produces this simulated radiograph, using raytracing.
  - Quick to compute.

Motivations for MADS and NOMAD

- A blackbox is involved.
- Presence of categorical variables.
- Robustness of the code regarding the uncertainty and noise in the data.

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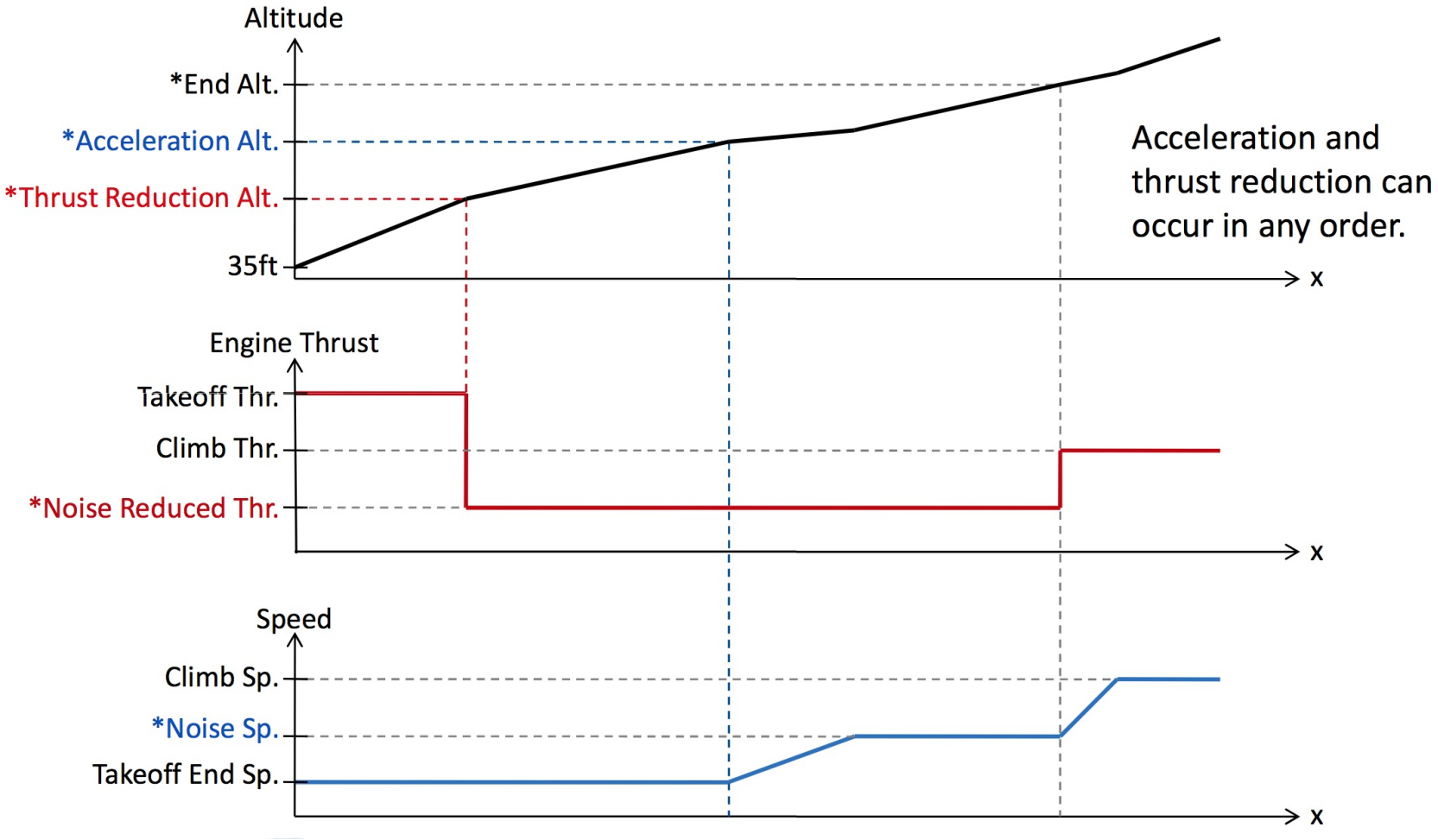
Aircraft takeoff trajectories

- Collaboration with Airbus mainly via Bastien Talgorn.
- Motivations for MADS and NOMAD:
  - A blackbox is involved.
  - Biobjective optimization.
  - Free software.
  - Must execute on different platforms including some old Solaris distributions.

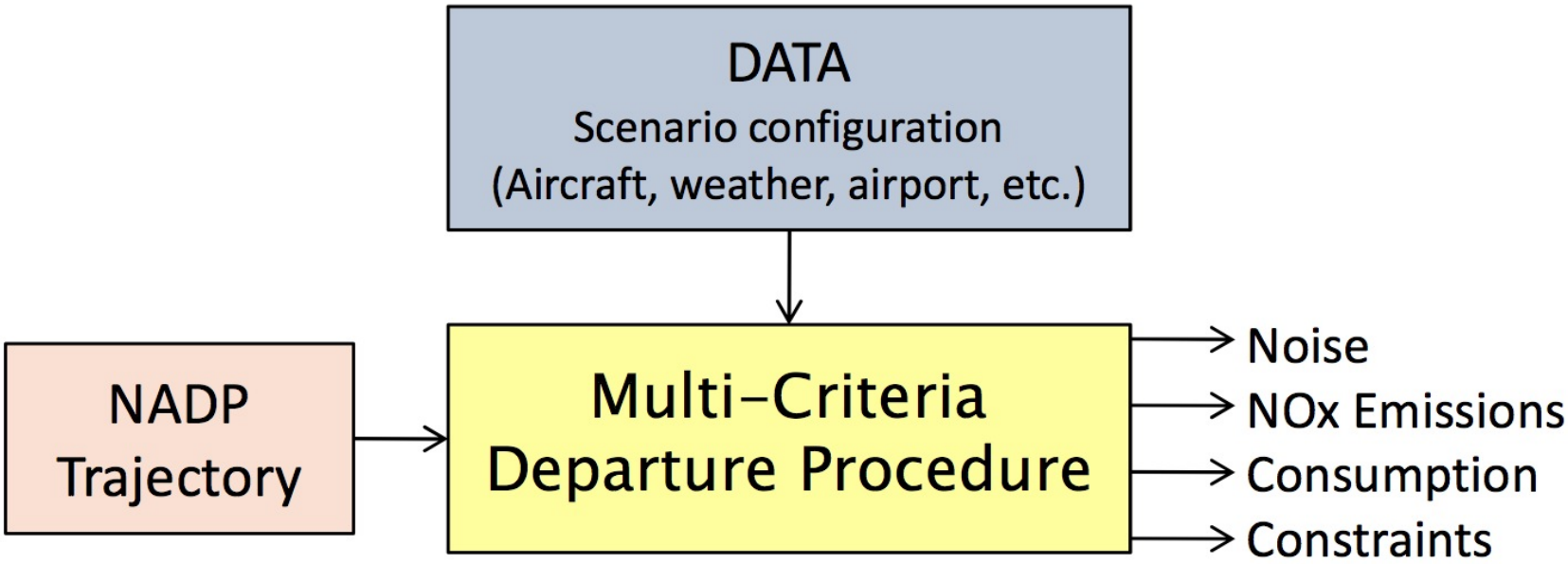
Definition of the optimization problem

- 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.

Parametric Trajectory: 5 optimization variables (*)



The blackbox: MCDP: Multi-Criteria Departure Procedure



One evaluation $\simeq$ 2 seconds.

Special features

- The best trajectory parameters are returned to the pilot who enters them in the aircraft system manually.
- Finite precision on optimization parameters: Discretization of optimization variables (100 to 1000 different values for each parameter).
- The variables have been defined as integers in `NOMAD` (minimum mesh size of 1 and rounding of directions).

BBO challenges

- In general:
  - A blackbox is involved, nonsmoothness, noise $\longrightarrow$ no derivatives.
  - Runtimes, software failures, several local optima.
- In particular, for the three examples:
  - Disconnected feasible domain.
  - Discrete and categorical variables.
  - Two objectives.
  - Solutions with limited precision (granularity).

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Mesh Adaptive Direct Search (MADS)

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Mesh Adaptive Direct Search (MADS)

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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, Δ_0)

[1] Iteration k

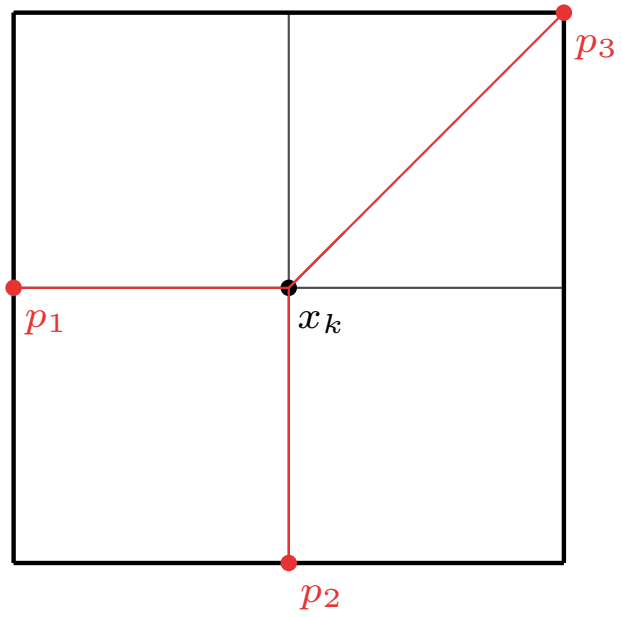
- **[1.1] Search**
  - select a finite number of mesh points
  - evaluate candidates opportunistically
- **[1.2] Poll** (if the Search failed)
  - construct poll set $P_k = \{x_k + \Delta_k d : d \in D_k\}$
  - sort(P_k)
  - evaluate candidates opportunistically

[2] Updates

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

Poll illustration (successive fails and mesh shrinks)

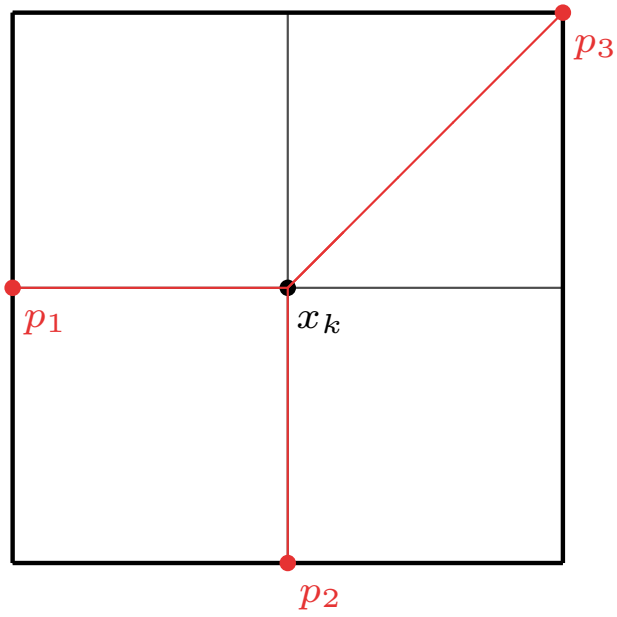
$$\Delta_k = 1$$

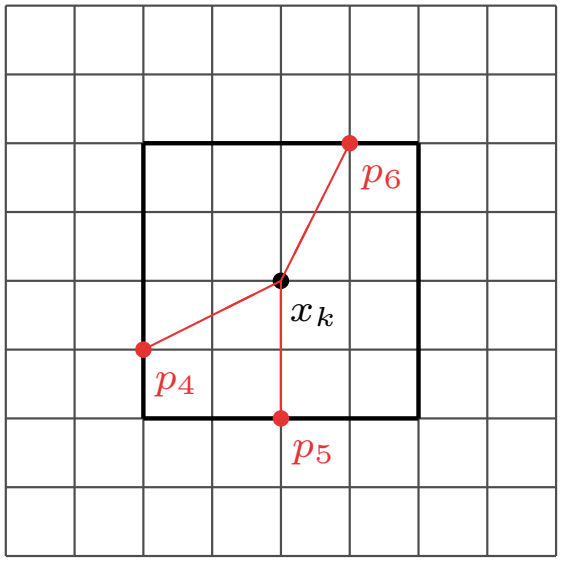


trial points$=\{p_1, p_2, p_3\}$

Poll illustration (successive fails and mesh shrinks)

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

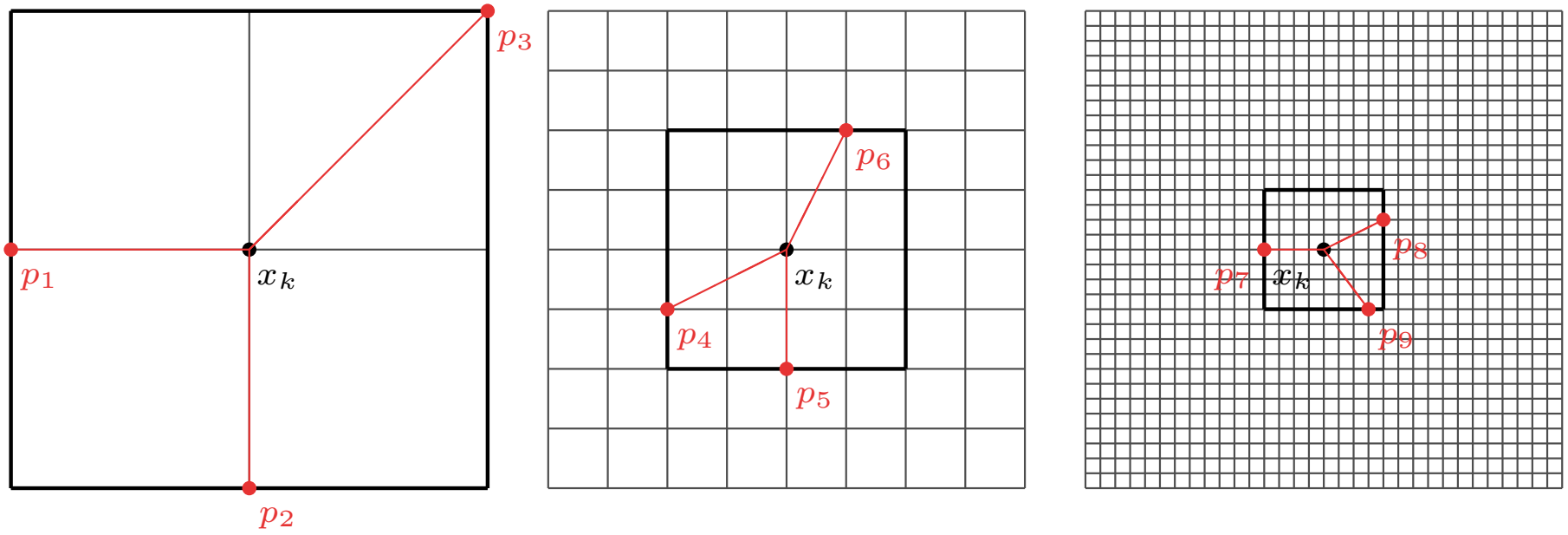




trial points$=\{p_1, p_2, p_3\}$ $= \{p_4, p_5, p_6\}$

Poll illustration (successive fails and mesh shrinks)

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



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

Convergence results

- MADS is backed by a convergence analysis based on the calculus for nonsmooth functions [Clarke, 1983].
- It produces solutions satisfying optimality conditions "proportional" to the smoothness of the problem.
- Summary of the results:

	Unconstrained	Constrained
Smooth	$\nabla f(x) = 0$	$f'(x;d) \geq 0$ for all $d \in T_\Omega(x)$
Nonsmooth	$0 \in \partial f(x)$	$f^\circ(x;d) \geq 0$ for all $d \in T_\Omega^H(x)$

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].
- Dynamic scaling [Audet et al., 2016].

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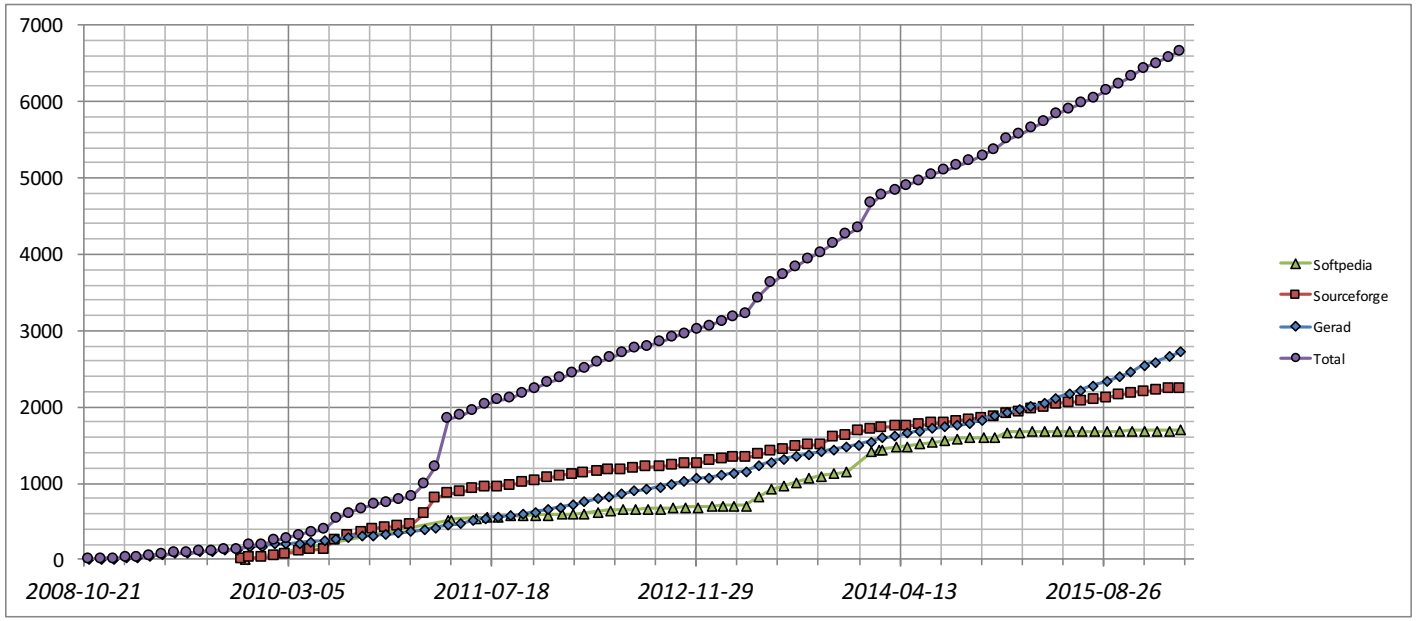
NOMAD (Nonlinear Optimization with MADS)

- 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 6,500 certified downloads since 2008.



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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