

Optimization days

Ecole Polytechnique de Montréal

Black Box Optimization with the NOMAD Software

Sébastien Le Digabel

Charles Audet

Mark Abramson

John Dennis

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Presentation outline

Context

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NOMAD

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Black box optimization problems

We consider the nonsmooth optimization problem:

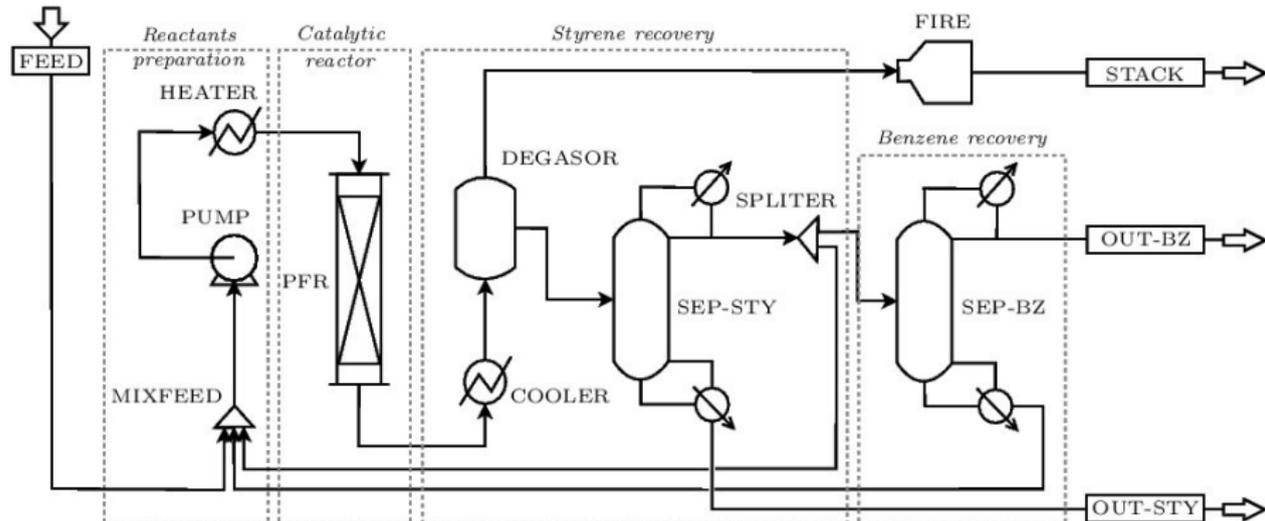
$$\begin{aligned} & \text{Minimize} && f(x) \\ & \text{subject to} && x \in \Omega = \{x \in X : c_j(x) \leq 0, j \in J\} \subset \mathbb{R}^n, \end{aligned}$$

where

- ▶ $f, c_j : X \rightarrow \mathbb{R} \cup \{\infty\}$ for all $j \in J = \{1, 2, \dots, m\}$.
- ▶ X is a subset of \mathbb{R}^n .
- ▶ Evaluation of the functions are usually the result of a computer code (a black box) costly to evaluate.

An engineering problem

Styrene production [Audet, Béchard, Le Digabel, JOGO 2008]



An engineering problem

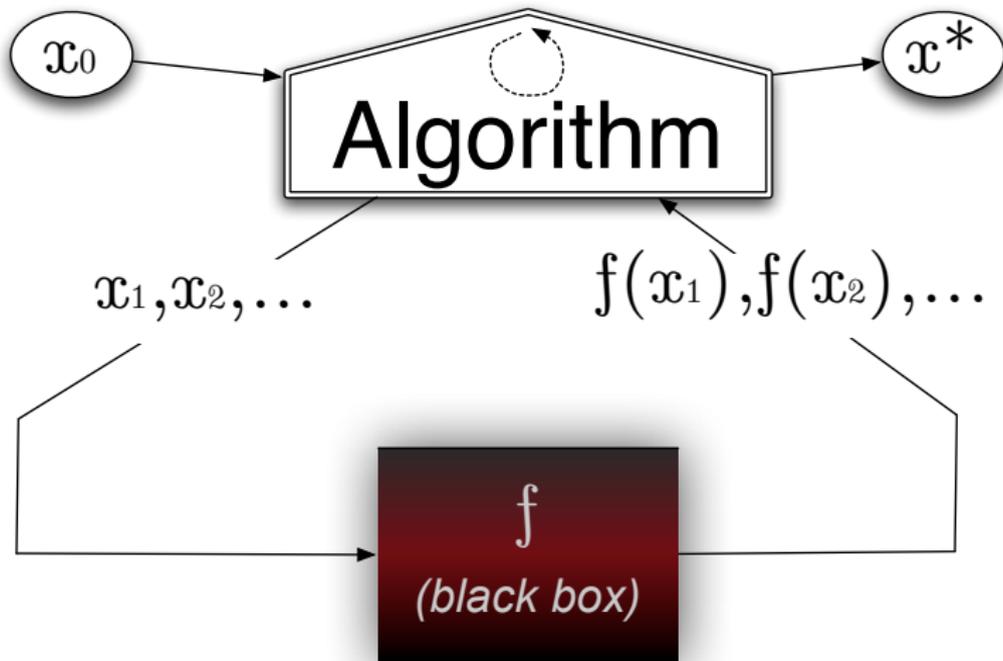
- ▶ Objective: maximize the Net Present Value.
- ▶ Constraints: satisfy industrial and environmental regulations.
- ▶ Written by a chemical engineer.
- ▶ Uses some common numerical methods: Runge-Kutta, Newton, fixed points, secant, bisection, ...
- ▶ 8 bound constrained variables,
4 boolean unrelaxable constraints,
7 relaxable constraints.
- ▶ A surrogate is obtained by using greater tolerances and smaller maximum number of iterations in the numerical methods.

Context

MADS overview

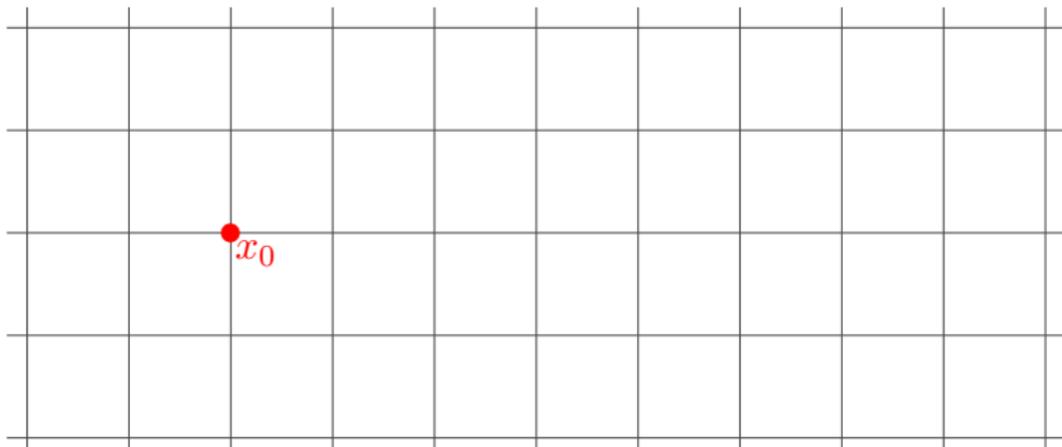
NOMAD

MADS and direct search principle



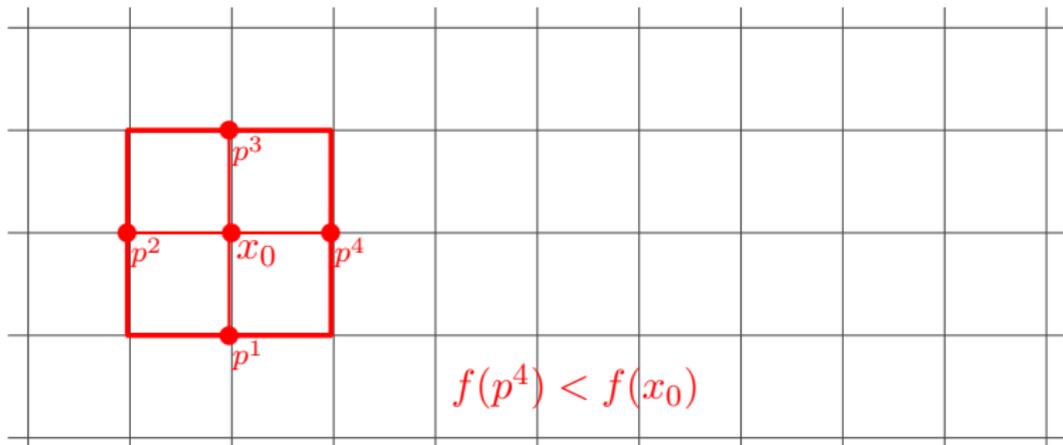
Mesh Adaptive Direct Search (MADS)

- ▶ GPS with coordinate search.



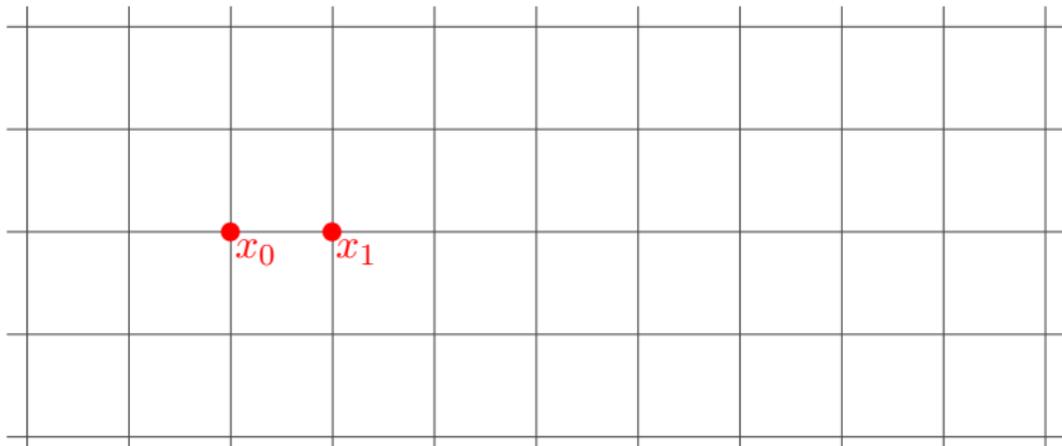
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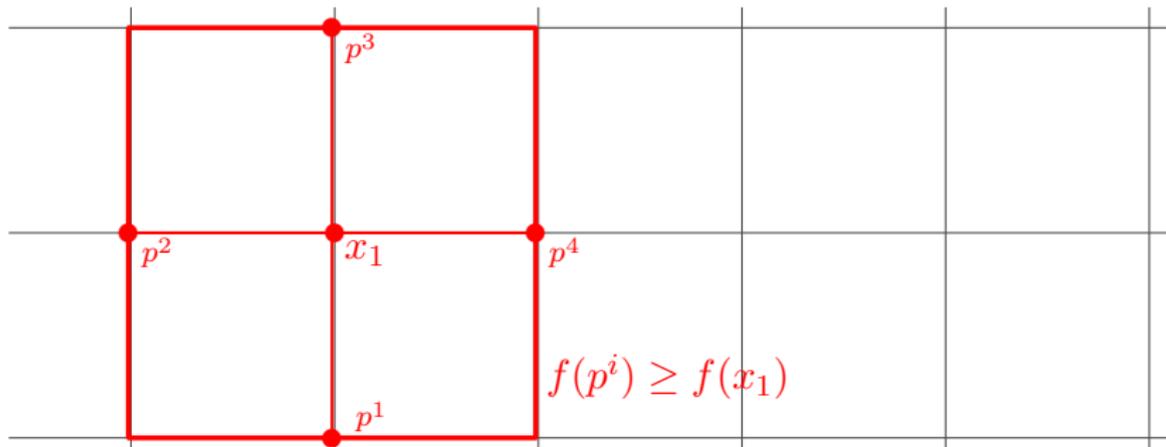
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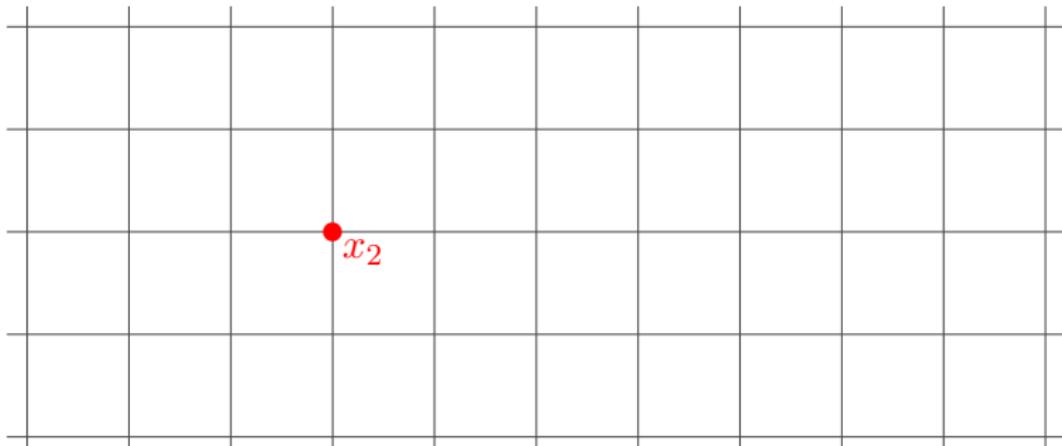
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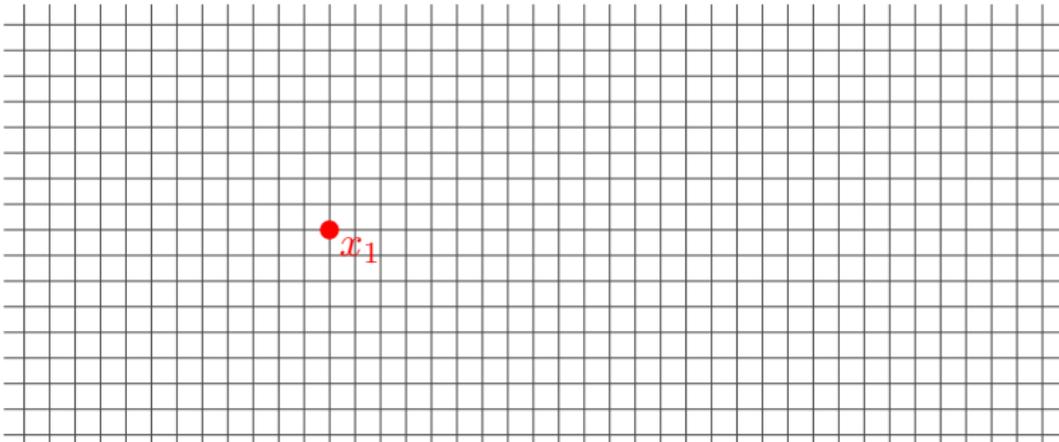
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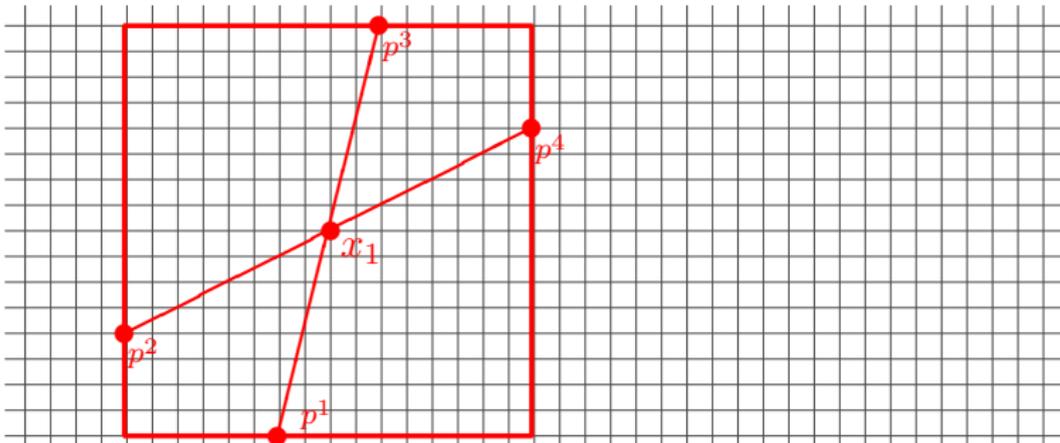
Mesh Adaptive Direct Search (MADS)

- ▶ **GPS** with coordinate search.
- ▶ **LT-MADS** a non-deterministic implementation of MADS.
Union of normalized polling directions grows dense in the unit sphere with probability one.



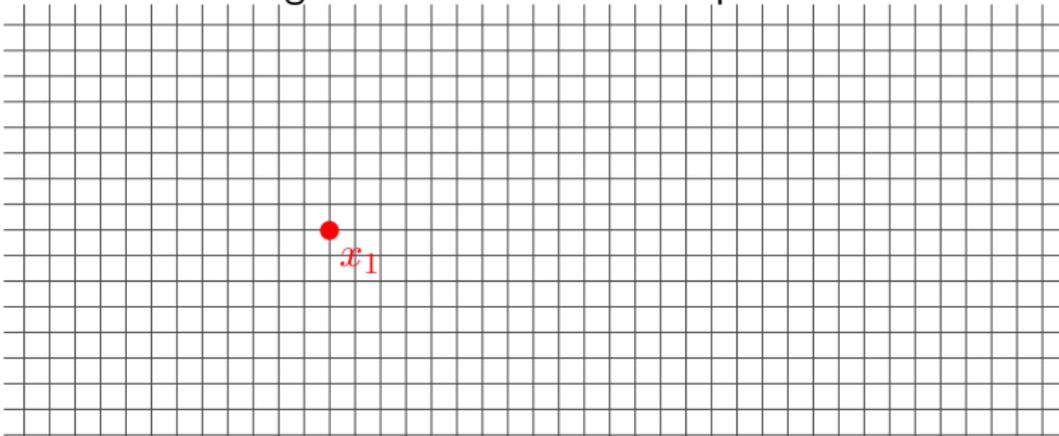
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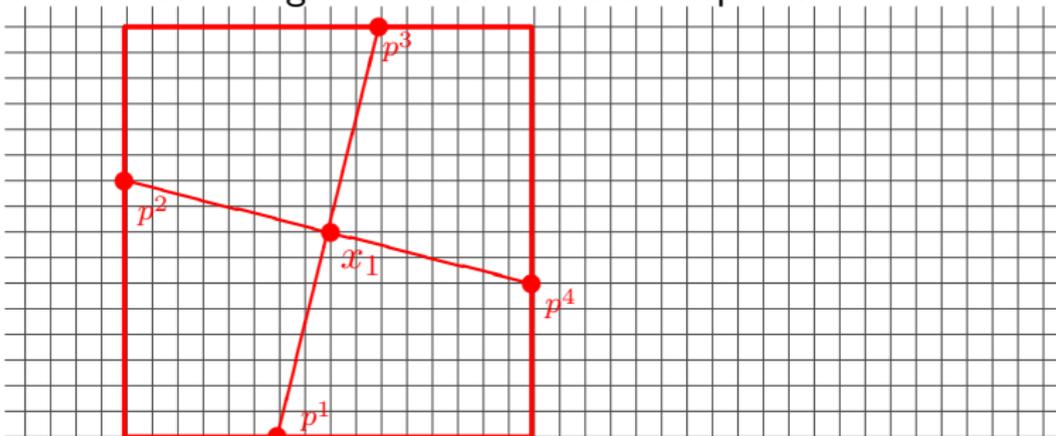
Mesh Adaptive Direct Search (MADS)

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- ▶ **LT-MADS** a non-deterministic implementation of MADS. Union of normalized polling directions grows dense in the unit sphere with probability one.
- ▶ **OrthoMADS** a deterministic implementation of MADS with orthogonal polling directions. Union of normalized polling directions grows dense in the unit sphere.



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NOMAD

NOMAD

- ▶ C++ implementation of MADS.
- ▶ Developed since 2000
- ▶ Current version: 3.1.
- ▶ Runs on Linux, Mac OS X and Windows.
- ▶ Distributed under the GPL license
- ▶ Command-line interface.
- ▶ In use at Airbus, Boeing, Exxon, GM, IREQ, ...

Main functionalities

- ▶ Mono or Biobjective optimization.
- ▶ Variables: continuous, integer, binary.
- ▶ Variables: periodic, fixed.
- ▶ Groups of variables.
- ▶ Constraints treated with 3 different methods (Extreme or Progressive Barrier, Filter).
- ▶ Surrogate functions.
- ▶ Several direction types (GPS, LT-MADS, OrthoMADS).

(all items correspond to published or submitted papers).

Batch/library

- ▶ Two ways to use NOMAD: batch mode or library mode.
- ▶ This presentation focuses on the batch mode.

Black box conception

- ▶ 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 g1 g2`.
- ▶ Example on the styrene problem:
`> ./black_box/truth/truth.exe points/x0.txt`.

Run NOMAD

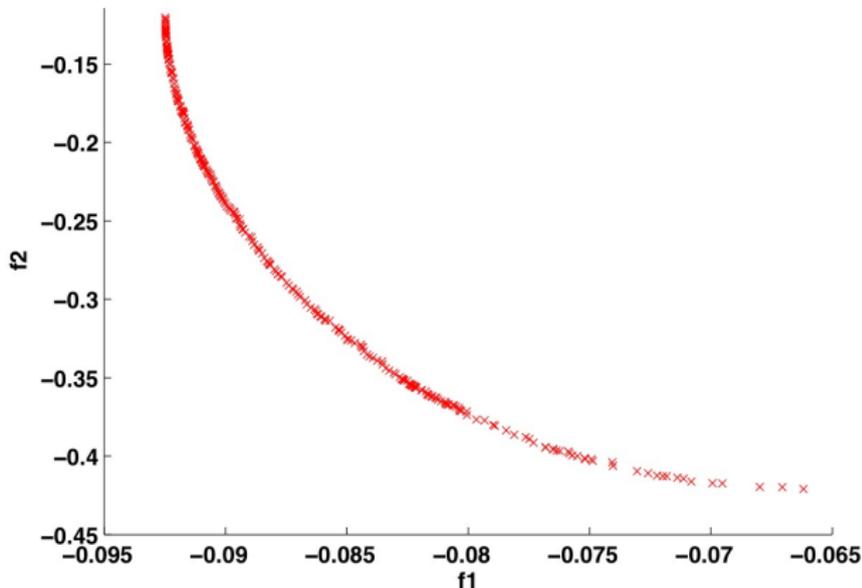
- ▶ Example on the styrene problem.
- ▶ `> nomad parameters.txt`

Important parameters

- ▶ Necessary parameters: dimension (n), the black box characteristics, and the starting point (x_0).
- ▶ All other parameters have default values. The most important (algorithmic) are:
 - ▶ Maximum number of black box evaluations,
 - ▶ Starting point (more than one can be defined),
 - ▶ Types of directions (more than one can be defined),
 - ▶ Initial mesh size,
 - ▶ Constraints types,
 - ▶ Latin-Hypercube sampling,
 - ▶ Seeds.
- ▶ See the user guide for the description of all parameters.

Biobjective optimization

- ▶ Example on a portfolio selection problem.
- ▶ Tradeoff solutions:



Advanced functionalities

- ▶ More advanced functionalities are available via the library mode.
- ▶ No more black box separated program: the code executes faster (more than twice).
- ▶ Easy to program multiple runs in parallel with different seeds.
- ▶ The user can pre-process all evaluation points before they are evaluated (exploited in the GMON problem).
- ▶ The user can program its own search strategy (version 3.2).

Future functionalities

- ▶ Version 3.2: installer program (Quentin Reynaud), generic user searches, VNS search.
- ▶ Versions 3.3 and above:
 - ▶ PMADS and PSD-MADS (parallel versions),
 - ▶ Compatibility with AMPL format,
 - ▶ Simplex gradients,
 - ▶ Dynamic surrogates,
 - ▶ Categorical variables.

Questions

