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Use of Models with the MADS Algorithm for Blackbox Optimization

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Presentation outline

Blackbox optimization problems

Presentation outline

Blackbox optimization problems

The MADS algorithm

Presentation outline

Blackbox optimization problems

The MADS algorithm

MADS and models

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The MADS algorithm

MADS and models

Discussion

Blackbox optimization problems

The MADS algorithm

MADS and models

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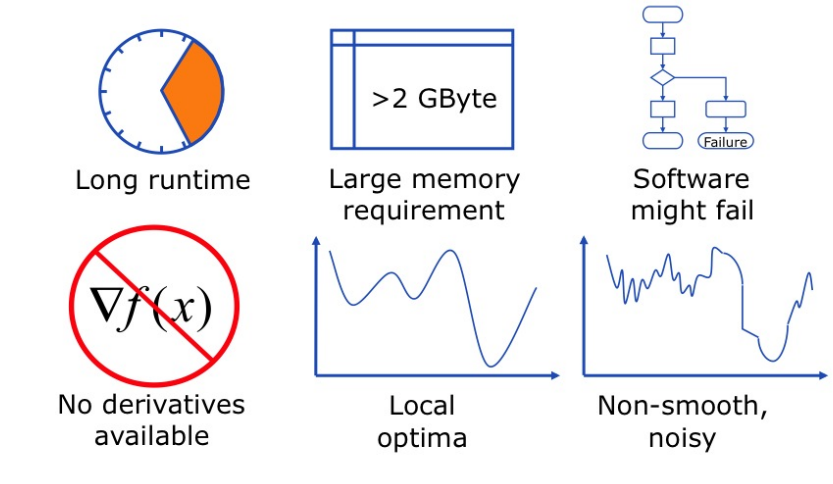
Blackbox optimization problems

We consider the optimization problem:

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

where evaluations of f and the functions defining Ω are usually the result of a computer code (a blackbox).

Blackboxes as illustrated by J. Simonis [ISMP 2009]



Long runtime

Large memory requirement

Software might fail

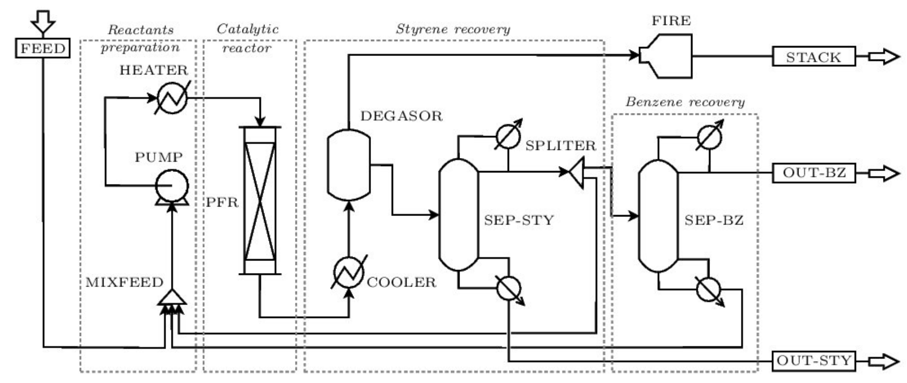
No derivatives available

Local optima

Non-smooth, noisy

Example of an engineering problem

STYRENE problem [Audet, Béchard, Le Digabel, JOGO 2008]



8 variables, 11 constraints, one evaluation $\simeq$ 3s, $\simeq$20% of failures.

Blackbox optimization problems

The MADS algorithm

MADS and models

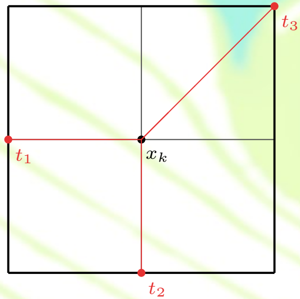
Discussion

Mesh Adaptive Direct Search (MADS)

- Audet and Dennis [SIOPT, 2006]
- Iterative algorithm that evaluates the blackbox at some trial points on a spatial discretization called the mesh.
- 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 iterate is found.
- Algorithm is backed by a convergence analysis based on the Clarke Calculus for nonsmooth functions.

Poll illustration (successive fails and mesh shrink)

$$\Delta_k^m = \Delta_k^p = 1$$



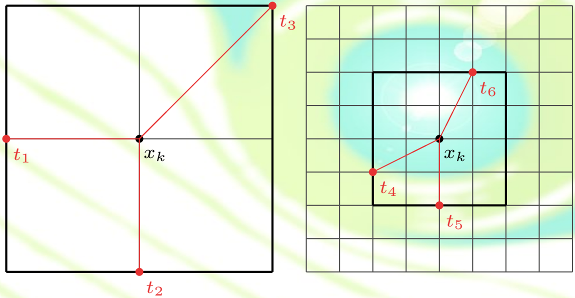
poll trial points=$\{t_1, t_2, t_3\}$

Poll illustration (successive fails and mesh shrink)

$\Delta_k^m = \Delta_k^p = 1$

$\Delta_{k+1}^m = 1/4$

$\Delta_{k+1}^p = 1/2$



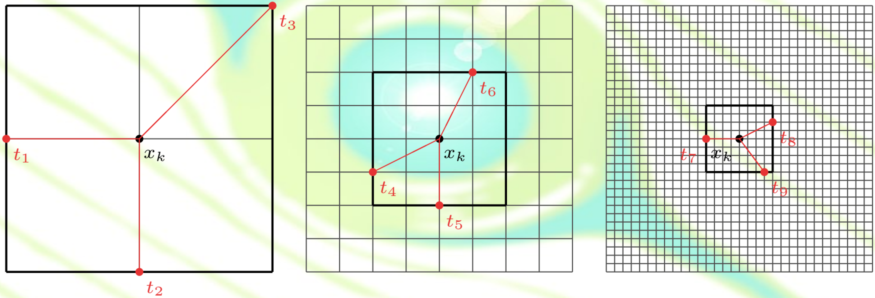
poll trial points=$\{t_1, t_2, t_3\}$ $= \{t_4, t_5, t_6\}$

Poll illustration (successive fails and mesh shrink)

$\Delta_k^m = \Delta_k^p = 1$

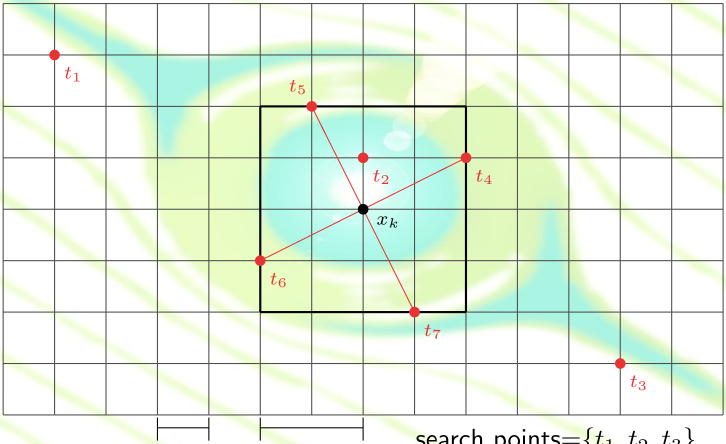
$\Delta_{k+1}^m = 1/4$
$\Delta_{k+1}^p = 1/2$

$\Delta_{k+2}^m = 1/16$
$\Delta_{k+2}^p = 1/4$



poll trial points$=\{t_1, t_2, t_3\}$ $=\{t_4, t_5, t_6\}$ $=\{t_7, t_8, t_9\}$

Poll and Search trial points



$\Delta_k^m = \frac{1}{4}$ $\Delta_k^p = \frac{1}{2}$

search points=$\{t_1, t_2, t_3\}$

poll points=$\{t_4, t_5, t_6, t_7\}$

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General framework

Only the additions to the MADS algorithm are reported.

```
[0] Initializations
[1] Iteration $k$
        [1.1] Model Search
                select data points from cache
                construct one model for each output (obj + cstrs)
                select points for model improvement
                optimize model to determine oracle points
                project candidates to the mesh
                evaluate candidates opportunistically
        [1.2] Poll (if the Search failed)
                Model Ordering: use models to sort trial points
[2] Updates
```

Constraints handling (Filter-type method)

- Constraint set $\Omega = \{x \in R : c_j(x) \leq 0, j \in J = \{1, \ldots, m\}\}$.
- Constraint violation function:

$$h(x) = \begin{cases} \sum_{j \in J} (\max(c_j(x), 0))^2 & \text{if } x \in R, \\ \infty & \text{otherwise.} \end{cases} \tag{1}$$

- x dominates y if $f(x) \leq f(y)$ and $h(x) \leq h(y)$ with at least one strict inequality.
- One model for each output: $f^s \simeq f$ and $c_j^s \simeq c_j$, $j \in J$.
- A model h^s for the violation is computed as in (1).
- No model for R (yet).

Model Ordering

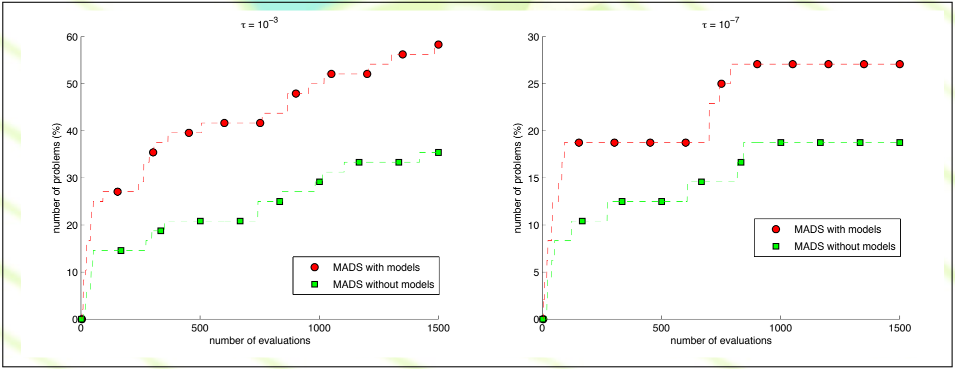
- Exploits the opportunistic strategy which consists to interrupt a series of evaluation as soon as a success is made.
- Points with $h^s = 0$ are given the highest priority.
- Predicted infeasible points are sorted accordingly to the dominance relation. Priority is given to smallest h^s values.
- Not limited to the Poll step.

Quadratic Models

- Local: data points are collected inside the ball of radius $\rho\Delta_k^p$ centered at the current solution (typically $\rho = 2$).
- The more smooth the functions are, the better the models.
- Cheap to construct (because in general $n \leq 20$).
- Under and over-determined cases:
  - If the number of data points is larger than the number of points necessary for exact quadratic interpolation, regression in the least square sense is used.
  - Otherwise (most likely), Minimum Frobenius Norm (MFN) interpolation is chosen.
- Well-poisedness (quality of the geometry of the data set) seems not to be an issue in the MADS context.

Results for quadratic models

Data profiles on a set of 48 problems (mostly academic).

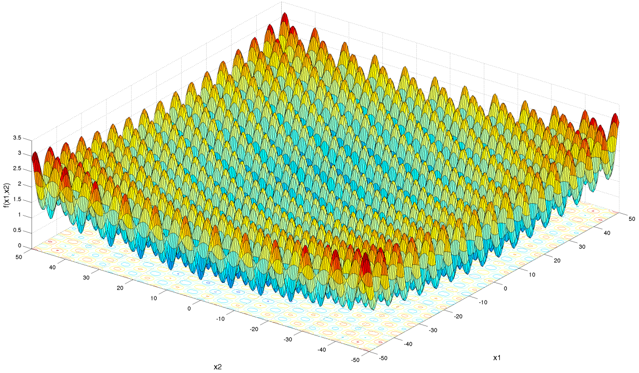


TGP Surrogates

- TGP: Treed Gaussian Processes [Gramacy and Lee, 2008]
- Space is partitioned as a tree. A Gaussian Process model is implemented at each leaf of this tree.
- Global model.
- More computationally costly.
- In addition to predictions for each output, TGP provides:
  - Expected improvement.
  - Expected reduction of variance.
- This gives other candidates in addition to the model optimization solutions.

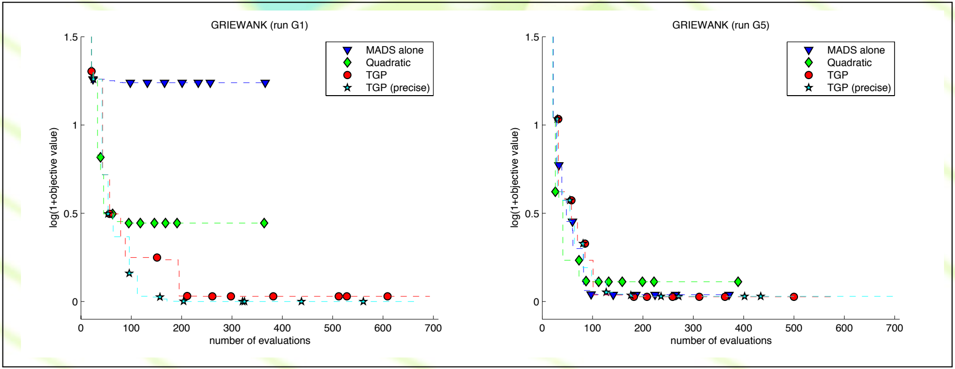
Results for TGP (1/3)

Griewank function, $n = 2$, $m = 0$, many local optima.



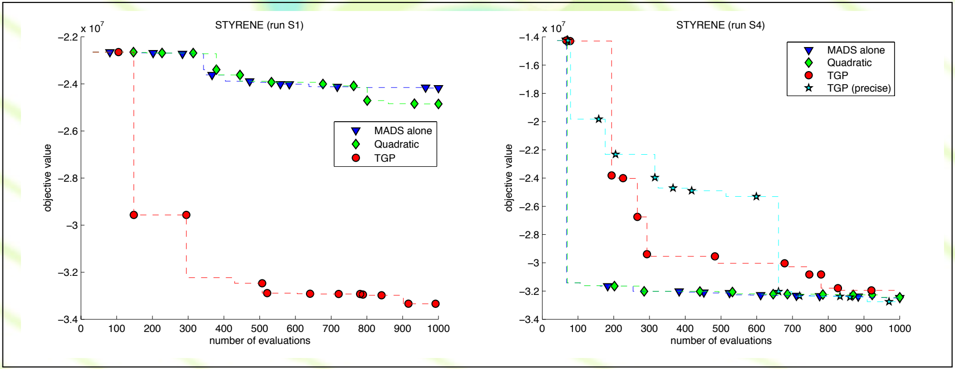
Results for TGP (2/3)

Best and worse TGP executions out of 10 runs with different seeds.
The same 20 LH points are chosen as starting solutions.



Results for TGP (3/3)

On the STYRENE problem. Out of 5 runs, the worse solution given by TGP has a 32% improvement versus 6% with quadratic models.



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- Improvement of the MADS algorithm for constrained blackbox optimization with the addition of models.
- Two types of models: quadratic and TGP.
- One or the other seems more adapted depending on the situation:
  - TGP for costly and real applications with hidden constraints.
  - TGP for simple problems with many local optima.
  - Quadratic models for all other situations (default in NOMAD).