

Blackbox optimization: Algorithms and applications

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Presentation outline

- 1** Introduction
- 2** The MADS algorithm
- 3** The NOMAD software package
- 4** Example 1: Solar thermal power plant
- 5** Example 2: Wind farm optimization
- 6** Example 3: Distribution network reconfiguration
- 7** Summary and references

1 Introduction

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3 The NOMAD software package

4 Example 1: Solar thermal power plant

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6 Example 3: Distribution network reconfiguration

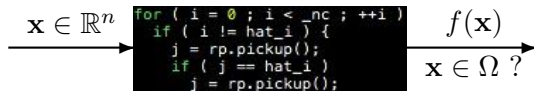
7 Summary and references

Blackbox / Derivative-Free Optimization

We consider

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

where the evaluations of f and the functions defining Ω are the result of a computer simulation (a **blackbox**)

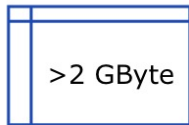


- Each call to the simulation may be expensive
- The simulation can fail
- Sometimes $f(\mathbf{x}) \neq f(\mathbf{x})$
- Derivatives are not available and cannot be approximated

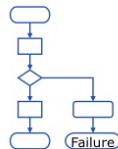
Blackboxes as illustrated by a Boeing engineer



Long runtime



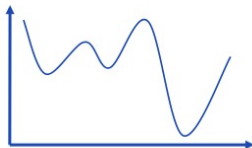
Large memory requirement



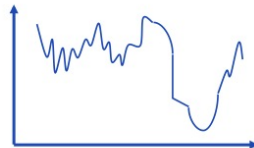
Software might fail



No derivatives available



Local optima

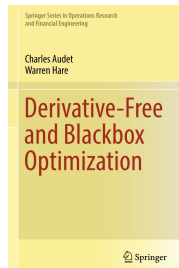


Non-smooth, noisy

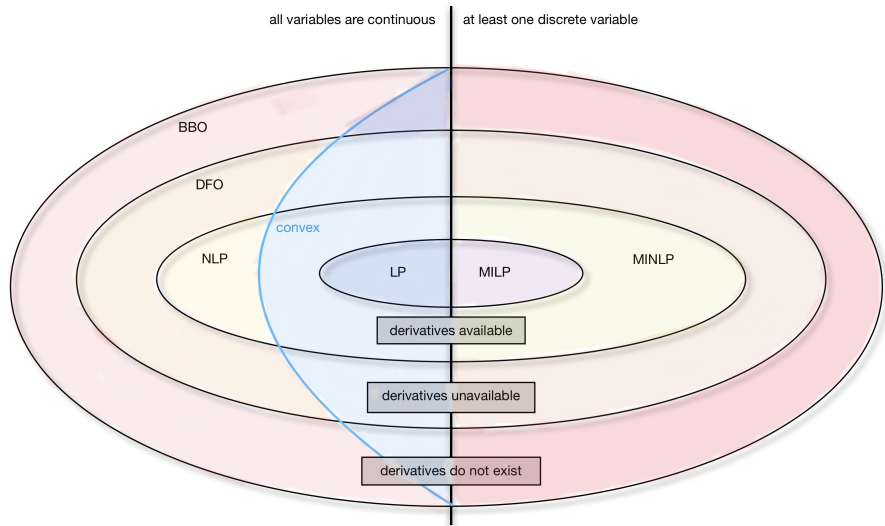
Terms

- “*Derivative-Free Optimization (DFO)* is the mathematical study of optimization algorithms that do not use derivatives” [Audet and Hare, 2017]
 - Optimization without using derivatives
 - Derivatives may exist but are not available
 - Obj./constraints may be analytical or given by a blackbox

- “*Blackbox Optimization (BBO)* is the study of design and analysis of algorithms that assume the objective and/or constraints functions are given by blackboxes” [Audet and Hare, 2017]
 - A simulation, or a blackbox, is involved
 - Obj./constraints may be analytical functions of the outputs
 - Derivatives may be available (ex.: PDEs)
 - Sometimes referred as *Simulation-Based Optimization (SBO)*



Optimization: Global view



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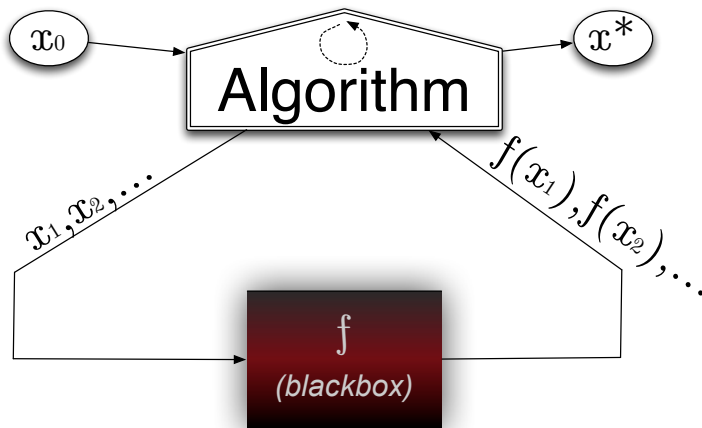
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Typical setting



Unconstrained case, with one initial starting solution

Algorithms for blackbox optimization

A method for blackbox optimization should ideally:

- Be efficient given a **limited budget of evaluations**
- Be **robust** to noise and blackbox failures
- Natively handle **general constraints**
- Deal with **multiobjective optimization**
- Deal with **integer and categorical variables**
- Easily exploit **parallelism**
- Have a publicly available **implementation**
- Have **convergence properties** ensuring first-order local optimality in the smooth case – otherwise why using it on more complicated problems?

Families of methods

- “*Computer science*” methods:
 - Heuristics such as genetic algorithms
 - No convergence properties
 - Cost a **lot** of evaluations
 - Should be used only in **last resort** for desperate cases
- Statistical methods:
 - Design of experiments
 - Bayesian optimization: EGO algorithm based on **surrogates** and **expected improvement**
 - Still limited in terms of dimension
 - Does not natively handle constraints
 - Good to use these tools in conjunction with DFO methods
- **Derivative-Free Optimization methods (DFO)**

DFO methods

■ Model-based methods:

- Derivative-Free Trust-Region methods
- Based on quadratic models or radial-basis functions
- Use of a trust-region
- Better for { DFO \ BBO }
- Not resilient to noise and *hidden constraints*
- Not easy to parallelize

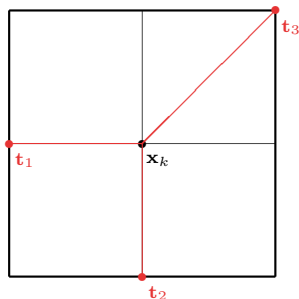
■ Direct-search methods:

- Classical methods: Coordinate search, Nelder-Mead – the *other* simplex method
- Modern methods: Generalized Pattern Search, Generating Set Search, Mesh Adaptive Direct Search (MADS)

So far, the size of the instances (variables and constraints) is typically limited to $\simeq 50$, and we target local optimization

MADS illustration with $n = 2$: Poll step

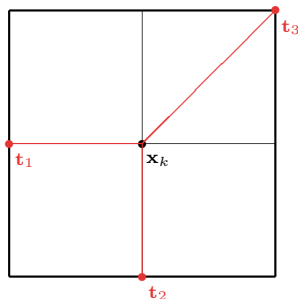
$$\delta^k = \Delta^k = 1$$



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

MADS illustration with $n = 2$: Poll step

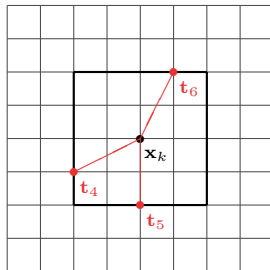
$$\delta^k = \Delta^k = 1$$



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

$$\delta^{k+1} = 1/4$$

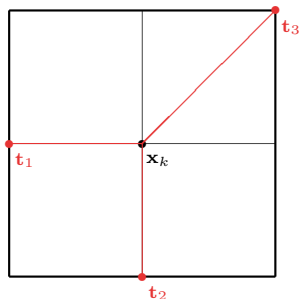
$$\Delta^{k+1} = 1/2$$



= $\{t_4, t_5, t_6\}$

MADS illustration with $n = 2$: Poll step

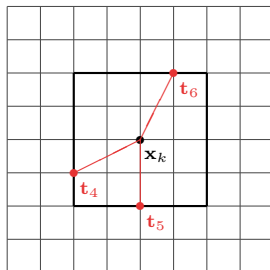
$$\delta^k = \Delta^k = 1$$



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

$$\delta^{k+1} = 1/4$$

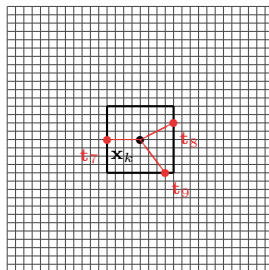
$$\Delta^{k+1} = 1/2$$



= $\{t_4, t_5, t_6\}$

$$\delta^{k+2} = 1/16$$

$$\Delta^{k+2} = 1/4$$



= $\{t_7, t_8, t_9\}$

[0] Initializations (\mathbf{x}_0, δ^0)

[1] Iteration k

[1.1] Search (flexible part)

select a finite number of **mesh** points
evaluate candidates opportunistically

[1.2] Poll (if Search failed) (“rigid” part)

construct poll set $P_k = \{\mathbf{x}_k + \delta^k \mathbf{d} : \mathbf{d} \in D_k\}$
sort(P_k)
evaluate candidates opportunistically

[2] Updates

if success

$\mathbf{x}_{k+1} \leftarrow$ success point
increase δ^k

else

$\mathbf{x}_{k+1} \leftarrow \mathbf{x}_k$
decrease δ^k

$k \leftarrow k + 1$, stop or go to **[1]**

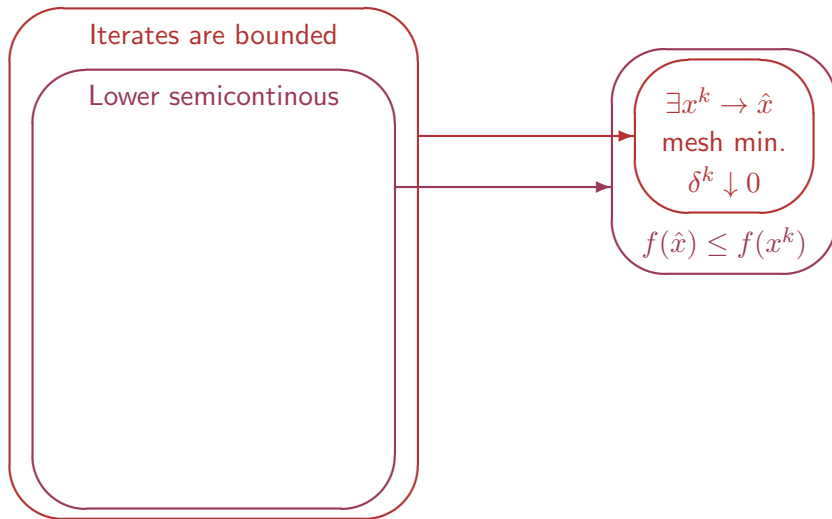
The MADS algorithm [Audet and Dennis, Jr., 2006]

Hierarchical convergence

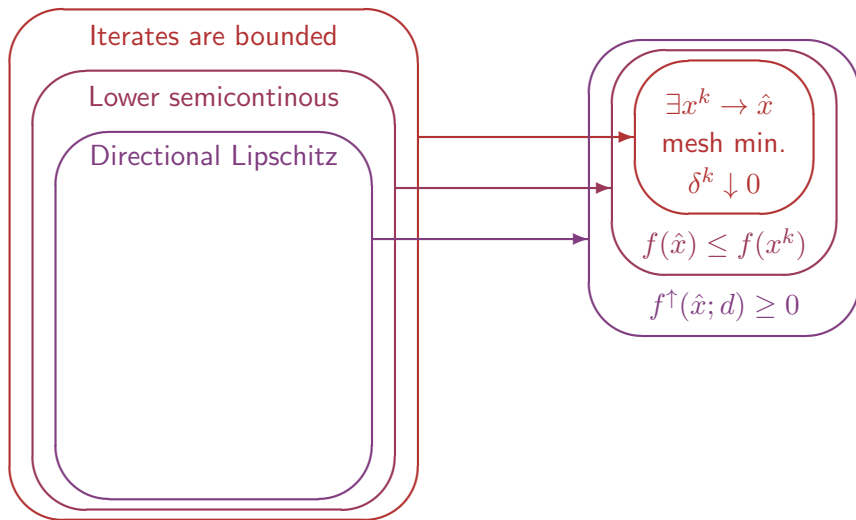
Iterates are bounded

$\exists x^k \rightarrow \hat{x}$
mesh min.
 $\delta^k \downarrow 0$

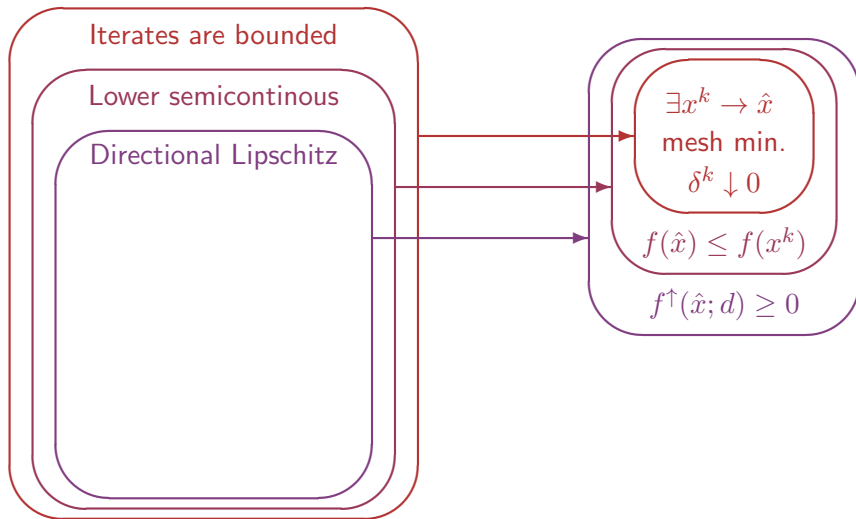
Hierarchical convergence



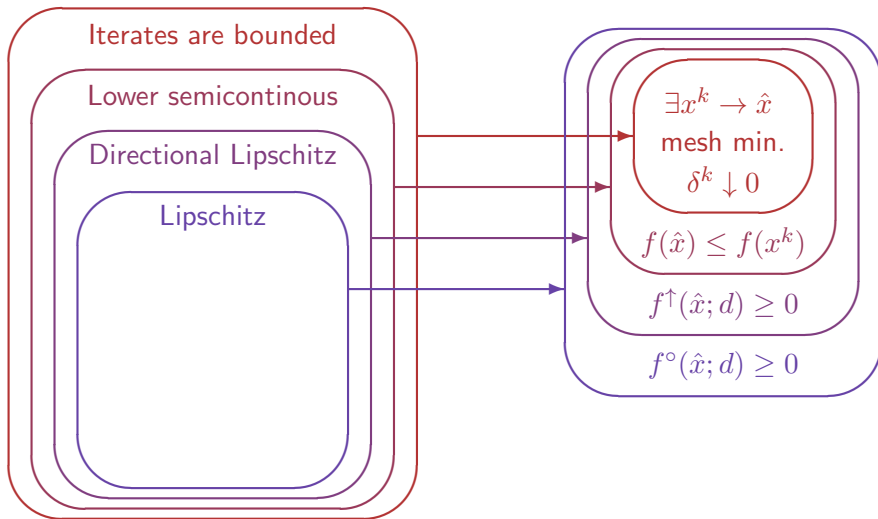
Hierarchical convergence



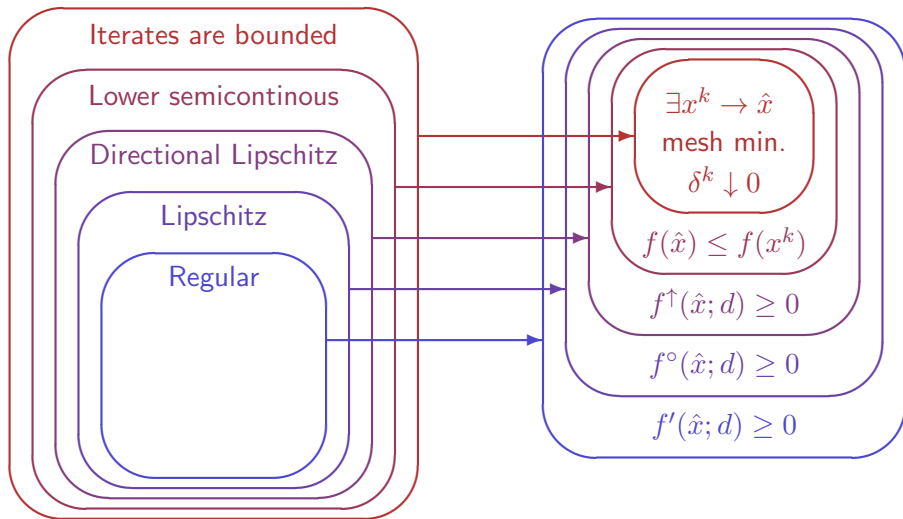
Hierarchical convergence



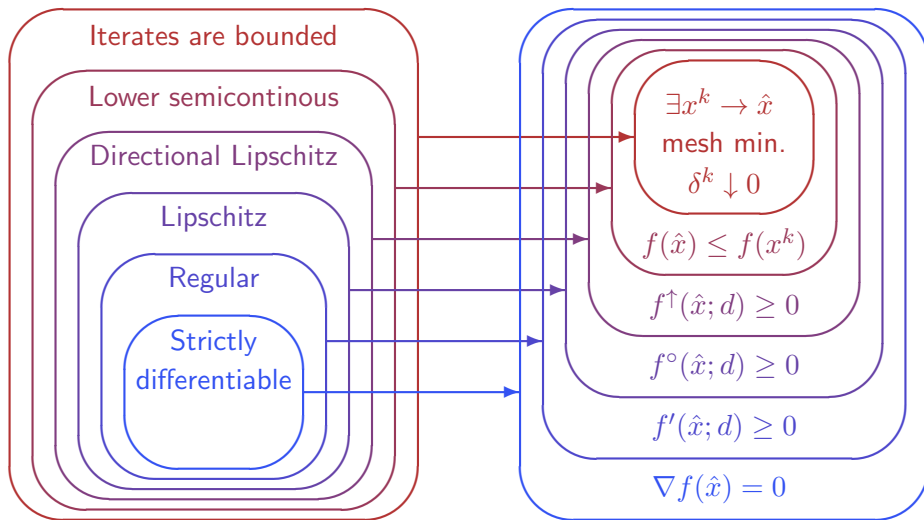
Hierarchical convergence



Hierarchical convergence



Hierarchical convergence



Features and evolution of MADS [Audet and Dennis, Jr., 2006]

- **Constraints** handling [Audet and Dennis, Jr., 2009, Audet et al., 2015, Le Digabel and Wild, 2024]
- **Core of MADS** [Abramson et al., 2009, Audet et al., 2014, Audet et al., 2016, Audet et al., 2025a]
- **Global optimization** [Audet et al., 2008a]
- **Parallelism** [Audet et al., 2008b, Le Digabel et al., 2010]
- **Sensitivity analysis** [Audet et al., 2012]
- **Surrogates** [Conn and Le Digabel, 2013, Gramacy and Le Digabel, 2015, Talgorn et al., 2015, Audet et al., 2018b, Talgorn et al., 2018, Amaioua et al., 2018, Audet et al., 2022b]
- **Hyperparameters tuning** [Lakhmire et al., 2021, Lakhmire and Le Digabel, 2022]
- **Discrete/Categorical/Meta variables** [Audet et al., 2019, Audet et al., 2023, Hallé-Hannan et al., 2025a, Hallé-Hannan et al., 2025b, Audet et al., 2025b]
- **Multiobjective optimization** [Audet et al., 2008c, Bigeon et al., 2021, Audet et al., 2021a, Bigeon et al., 2024, Le Digabel et al., 2025]
- **Multifidelity** [Alarie et al., 2022, Alarie et al., 2025]
- **Stochastic blackboxes** [Audet et al., 2018a, Alarie et al., 2021, Audet et al., 2021b, Audet et al., 2021b, Dzahini, 2022, Dzahini et al., 2023]
- **NOMAD** [Le Digabel, 2011, Audet et al., 2022a]
- **Large dimension**

Constraints – with **taxonomy** of [Le Digabel and Wild, 2024]

Domain: $\Omega = \{\mathbf{x} \in \mathcal{X} : c_j(\mathbf{x}) \leq 0, j \in J\} \subset \mathbb{R}^n$

- \mathcal{X} corresponds to **unrelaxable** constraints

Cannot be violated;

Example: $x > 0$ when $\log x$ is used inside the simulation

Constraints – with **taxonomy** of [Le Digabel and Wild, 2024]

Domain: $\Omega = \{\mathbf{x} \in \mathcal{X} : c_j(\mathbf{x}) \leq 0, j \in J\} \subset \mathbb{R}^n$

- \mathcal{X} corresponds to **unrelaxable** constraints
- $c_j(\mathbf{x}) \leq 0$: **Relaxable** and **quantifiable** constraints

May be violated at intermediate designs

$c_j(\mathbf{x})$ measures the violation

Example: cost \leq budget

Constraints – with **taxonomy** of [Le Digabel and Wild, 2024]

Domain: $\Omega = \{\mathbf{x} \in \mathcal{X} : c_j(\mathbf{x}) \leq 0, j \in J\} \subset \mathbb{R}^n$

- \mathcal{X} corresponds to **unrelaxable** constraints
- $c_j(\mathbf{x}) \leq 0$: **Relaxable** and **quantifiable** constraints
- **Hidden** constraints

when the simulation fails, even for points in Ω

Example:

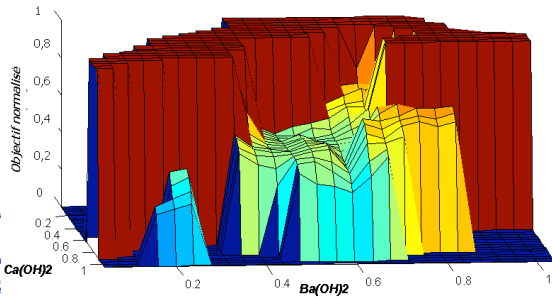
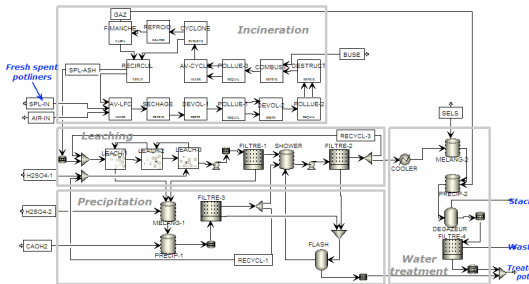
Segmentation fault
Bus error
ERROR 42
DIVISION BY ZERO

Constraints – with **taxonomy** of [Le Digabel and Wild, 2024]

Domain: $\Omega = \{\mathbf{x} \in \mathcal{X} : c_j(\mathbf{x}) \leq 0, j \in J\} \subset \mathbb{R}^n$

- \mathcal{X} corresponds to **unrelaxable** constraints
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- **Hidden** constraints

Example: Chemical process:



7 variables, 4 constraints. The ASPEN software fails on 43% of the calls

Two strategies to deal with constraints

■ Extreme barrier (EB)

Treats the problem as being unconstrained,
by replacing the objective function $f(\mathbf{x})$ by

$$f_{\Omega}(\mathbf{x}) := \begin{cases} f(\mathbf{x}) & \text{if } \mathbf{x} \in \Omega \\ \infty & \text{otherwise} \end{cases}$$

The problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f_{\Omega}(\mathbf{x})$$

is then solved.

Remark: this strategy can also be applied to **a priori** constraints in order to avoid the costly evaluation of $f(\mathbf{x})$

Two strategies to deal with constraints

- Extreme barrier (EB)
- Progressive barrier (PB)

Defined for relaxable and quantifiable constraints.

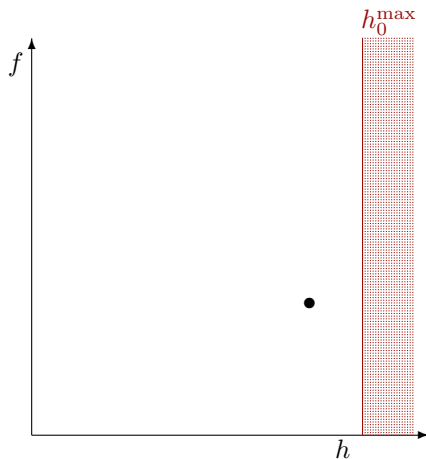
As in the filter methods of Fletcher and Leyffer, it uses the non-negative constraint violation function $h : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{\infty\}$

$$h(\mathbf{x}) := \begin{cases} \sum_{j \in J} (\max(c_j(\mathbf{x}), 0))^2 & \text{if } \mathbf{x} \in \mathcal{X} \\ \infty & \text{otherwise} \end{cases}$$

At iteration k , points with $h(\mathbf{x}) > h_k^{\max}$ are rejected by the algorithm, and h_k^{\max} decreases toward 0 as $k \rightarrow \infty$

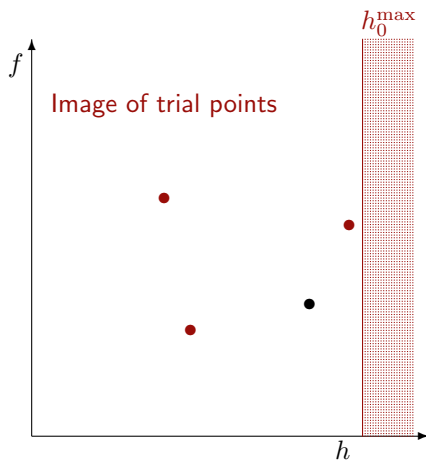
Two strategies to deal with constraints

- Extreme barrier (EB)
- Progressive barrier (PB)



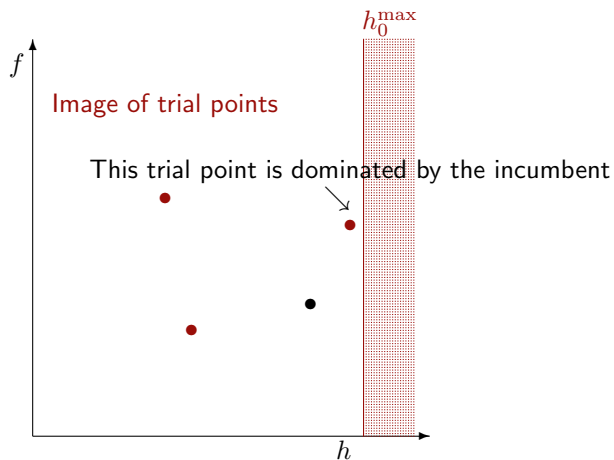
Two strategies to deal with constraints

- Extreme barrier (EB)
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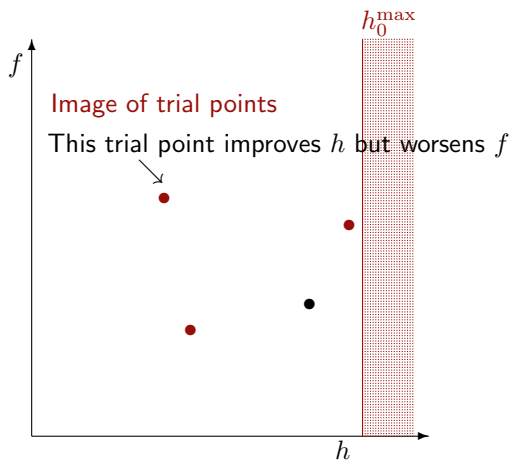
Two strategies to deal with constraints

- Extreme barrier (EB)
- Progressive barrier (PB)



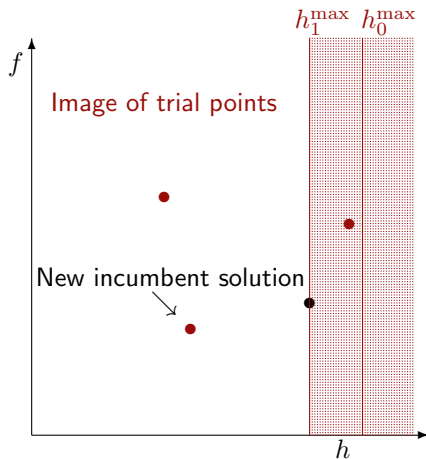
Two strategies to deal with constraints

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Two strategies to deal with constraints

- Extreme barrier (EB)
- Progressive barrier (PB)



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NOMAD (Nonlinear Optimization with MADS)

- C++ implementation of the MADS algorithm [Audet and Dennis, Jr., 2006]
- Standard C++. Runs on Linux, Mac OS X and Windows
- Parallel versions
- PyNomad.py and NOMAD.jl versions
- Open and free – LGPL license
- Download at <https://www.gerad.ca/nomad> or <https://github.com/bbopt/nomad>
- Support at nomad@gerad.ca
- Related articles in TOMS [Le Digabel, 2011] and [Audet et al., 2022a]



Main functionalities (1/2)

- Single or biobjective optimization
- Variables:
 - Continuous, integer, binary, categorical, granular
 - Periodic
 - Fixed
 - Groups of variables
- Searches:
 - Latin-Hypercube
 - Variable Neighborhood Search
 - Nelder-Mead Search
 - 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
- default values for all parameters
- all items correspond to published or submitted papers

Blackbox conception (batch mode)

- Command-line program that takes in argument a file containing \mathbf{x} , and displays the values of $f(\mathbf{x})$ and the $c_j(\mathbf{x})$'s
- Can be coded in any language
- Typically: `> bb.exe x.txt` displays `f c1 c2` (objective and two constraints)

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): ( 1.0000000013 1.0000000048 0.9999999797 0.9999999992 -4 ) h=1.10134e-13 f=-4
best feasible solution        : ( 1 1 1 -4 ) h=0 f=-4
```

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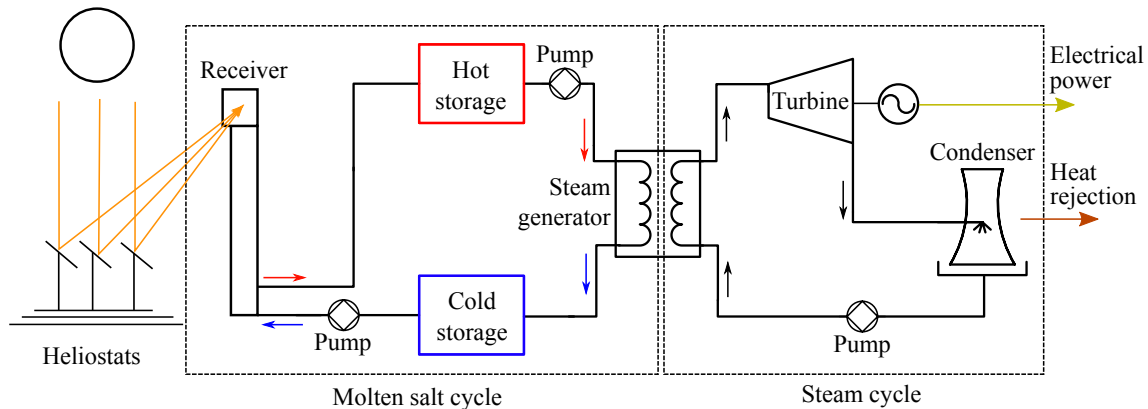
CSP power plant with molten salt thermal energy storage

- Work published in [Andrés-Thió et al., 2025]
- A large number of mirrors (**heliostats**) reflects solar radiation on a receiver at the top of a tower
- The heat collected from the concentrated solar flux is removed from the receiver by a stream of molten salt
- Hot molten salt is then used to feed thermal power to a conventional power block
- The photo shows the Thémis CSP power plant, the first built with this design

Source: https://commons.wikimedia.org/wiki/File:Themis_2.jpg



System dynamics



Features for BBO benchmarking

- Several numerical methods: real-world blackbox
- Reproducibility across all platforms
- Continuous and discrete variables
- Different types of constraints (quantifiable, relaxable, a priori, hidden)
- Stochastic and deterministic outputs
- Static surrogates with variable fidelity
- Number of replications is controllable

Ten instances

Instance	# of variables			# of obj. <i>p</i>	# of constraints			# of stoch. outputs (obj. or constr.)	Static surrogate
	cont.	discr.	(cat.) <i>n</i>		simu.	a priori (lin.)	<i>m</i>		
solar1	8	1 (0)	9	1	2	3 (2)	5	1	no
solar2 ¹	12	2 (0)	14	1	9	4 (2)	13	3	yes
solar3	17	3 (1)	20	1	8	5 (3)	13	5	yes
solar4	22	7 (1)	29	1	9	7 (5)	16	6	yes
solar5	14	6 (1)	20	1	8	4 (3)	12	0	no
solar6	5	0 (0)	5	1	6	0 (0)	6	0	no
solar7	6	1 (0)	7	1	4	2 (1)	6	3	yes
solar8	11	2 (0)	13	2	4	5 (3)	9	3	yes
solar9	22	7 (1)	29	2	10	7 (5)	17	6	yes
solar10 ²	5	0 (0)	5	1	0	0 (0)	0	0	yes

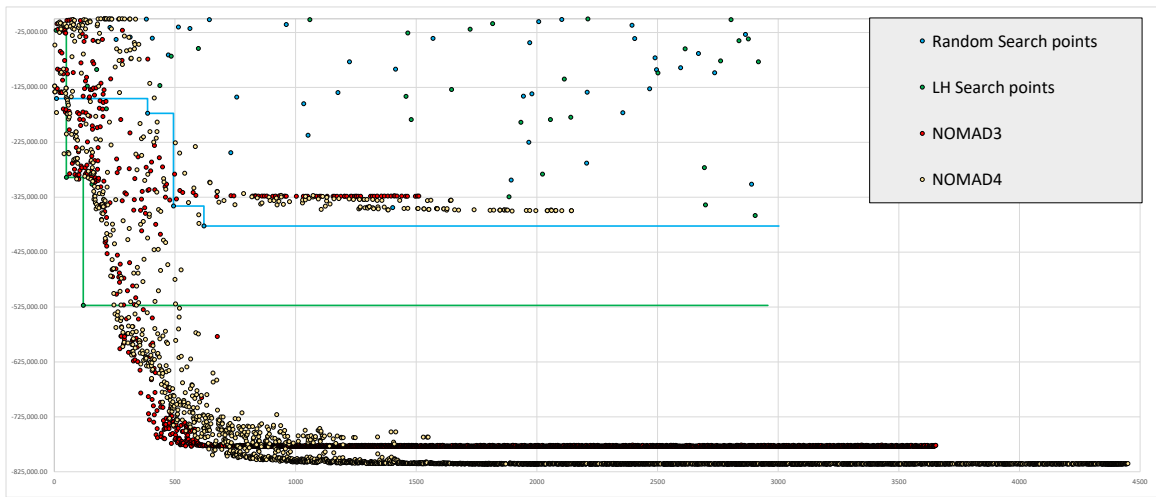
¹analytic objective

²unconstrained

Feasibility with sampling and NOMAD

Instance	LH search (10k points)		NOMAD3		
	satisf. ap constr.	feas. pts	satisf. ap constr.	feas. pts	number of eval.
solar1	30%	0.35%	96%	74%	3,792
solar2	0%	0%	97%	0%	1,635
solar3	0.49%	0%	99%	9%	30,525
solar4	0%	0%	83%	0%	44,303
solar5	0%	0%	83%	59%	3,405
solar6	90%	5%	99%	0%	3,539
solar7	2%	1%	74%	72%	2,224
solar8	1%	0.03%			
solar9	1%	0%			

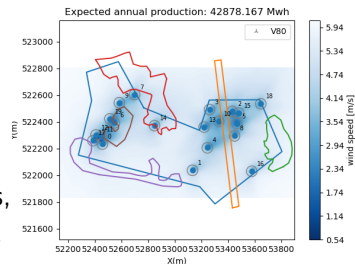
Optimization on solar1



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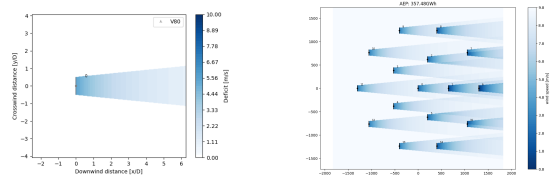
Wind farm layout optimization

- Joint work with [Joséphine Gobert](#), [Léon Biner](#), [Antoine Lesage-Landry](#), [Merlin Keller](#) and [Julien Pelamatti](#).
- **Context:** Minimizing the **Levelized Cost of Energy** requires maximizing the **Annual Energy Production (AEP)**, which depends on turbine layout
- **Problem:** Given a wind site and a fixed number of turbines, find the **layout** (positions) that **maximizes the AEP**, subject to placement and spacing constraints
- **Simulator:** **PyWake** [Pedersen et al., 2023] (DTU), an open-source wind farm flow simulator



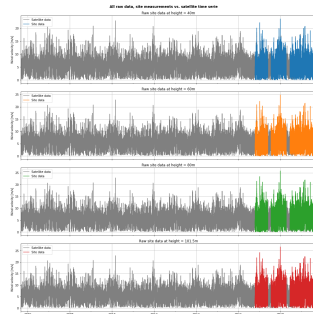
Wind farm model: PyWake and wind speed modeling

- Inputs: onsite wind speed time-series (uncertain) and turbine layout (design variable)
- Output: power production time-series
- Simulator: PyWake + power curve of the turbine



PyWake:

- Superposition of wake deficit functions
- Static: each time-step treated independently
- Faster (but less accurate) than CFD solvers



BBO Model: Objective, Variables, and Constraints

Decision variables:

- Positions (coordinates) of the turbines
- Continuous variables only

Objective: maximize the AEP, computed as a weighted sum of turbine power outputs over all wind direction and speed combinations, using probabilities from a wind rose

Constraints:

1. *Placement in constructible zone:*
 - **A priori**, binary: each turbine position must be admissible (checked before PyWake call)
 - Or relaxable/quantifiable: sum of distances to the constructible zone
2. *Minimal spacing between turbines:*
 - Each pair of turbines must be at least 2 diameters apart
 - **A priori** and quantifiable; treated as relaxable or unrelaxable

NOMAD vs Monte Carlo

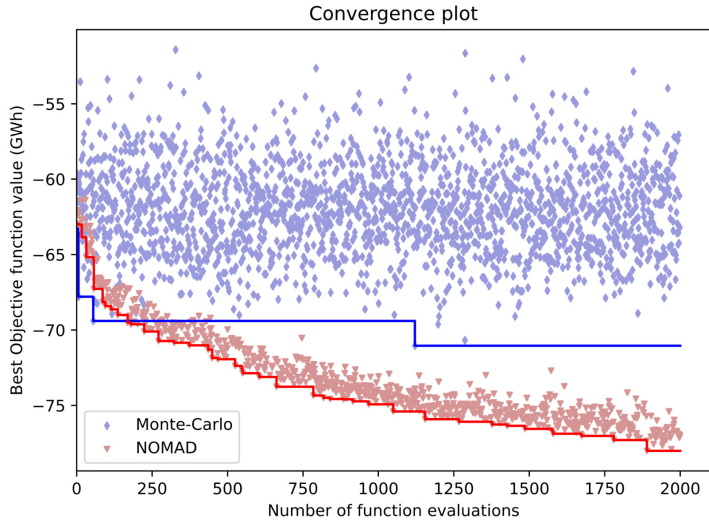
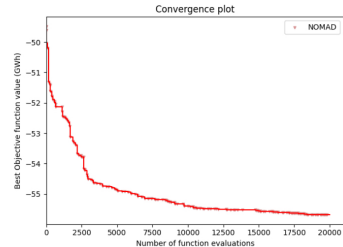
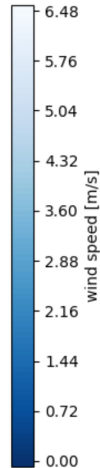
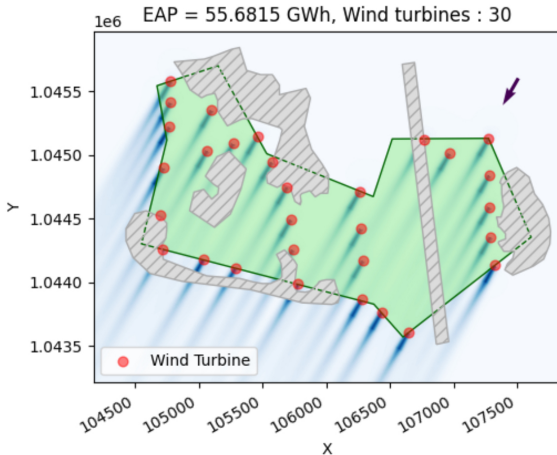


Illustration of a solution



The amon package

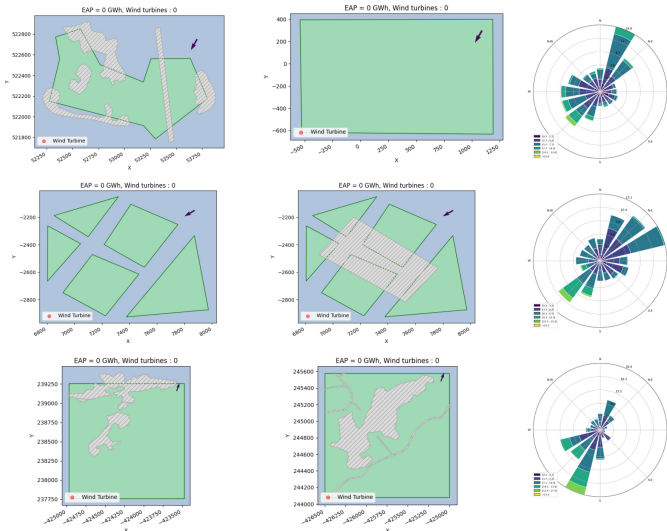
- Available at <https://github.com/josephinegobert/AMON>
- Several instances have been defined as realistic benchmarking instances for the BBO community

The screenshot shows the GitHub repository page for 'AMON' by 'josephinegobert'. The repository is public and has 8 branches and 0 tags. The main branch is selected. The file list includes:

File Name	Last Commit	Time Ago
__pycache__	fix_instances	3 weeks ago
bb_example	bug fix	3 weeks ago
data	fix_instance	3 weeks ago
instances	spacing constr updated	3 weeks ago
README.md	Update README.md	8 minutes ago
blackbox.py	flow map	3 weeks ago
constraints.py	spacing constr updated	3 weeks ago
data.py	Comments finished	last month
initial_solution.py	spacing constr updated	3 weeks ago
plotting_functions.py	flow map	3 weeks ago
requirements.txt	bug fix	3 weeks ago
windfarm_eval.py	flow map	3 weeks ago

The right sidebar shows the 'About' section with no description, website, or topics provided. It also shows 'Releases' (no releases published), 'Packages' (no packages published), and 'Languages' (Python 100.0%).

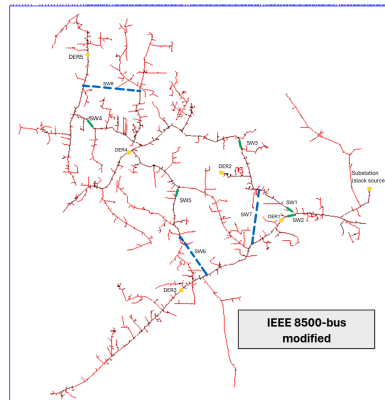
The amon package: Instances



- 1 Introduction
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- 4 Example 1: Solar thermal power plant
- 5 Example 2: Wind farm optimization
- 6 Example 3: Distribution network reconfiguration**
- 7 Summary and references

Distribution network reconfiguration with DERs³

- PhD project of [Christina Soldati](#)
- Collaboration with [Miguel Anjos](#) and [Antoine Lesage-Landry](#)
- Presentation at [SIAM OP26](#) (Wednesday 9:15am)
- **Problem:** **Unbalanced phases** in power distribution networks, amplified by **DER integration**, increase power losses
- **Goal:** Reconfigure the network topology (switch states) and DER injections to **minimize total generation losses**



³Distributed Energy Resources

The BBO Model

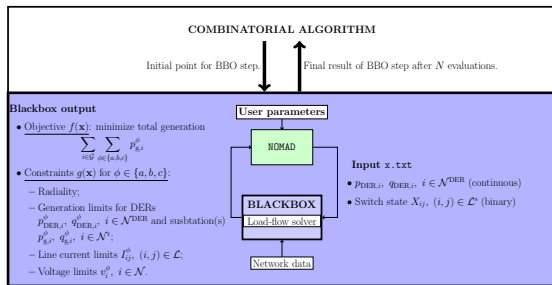
Decision variables :

- **Continuous:** active/reactive DER power injections
- **Binary:** switch states: drives the combinatorial complexity

Objective: minimize total active power generation (losses)

Constraints: via the **EMTP**⁴ load-flow solver:

- Connectivity
- Radiality
- Voltage limits



⁴[Mahseredjian et al., 2007]

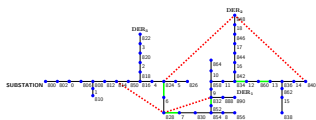
Resolution Methods

NOMAD is the **core** of all methods. The **binary variables** are handled by combining BBO with combinatorial strategies:

- BBO
- BBO-VNS
- BBO-B&B
- BBO-VNS-B&B
- BBO-B&B-VNS
- L-BBO-VNS
- L-BBO-MST
- **VNS**: randomly permutes binary variables (switch states) and re-optimizes continuous variables with BBO
- **B&B**: fixes one binary variable at a time, optimizes the rest with BBO
- **List-based**: pre-generates feasible topologies (spanning trees); (VNS or MST)-inspired heuristic selects the next topology

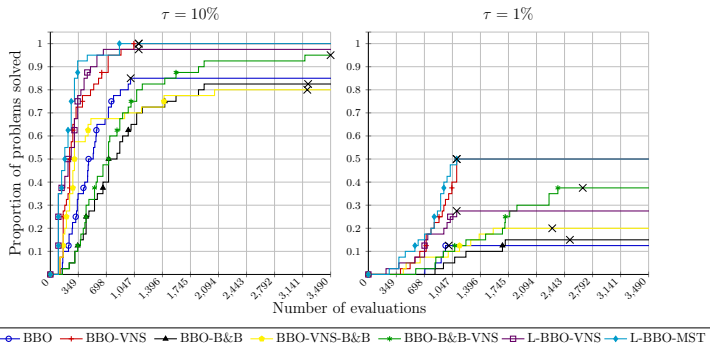
→ BBO serves as a **warm start** and **baseline**; combinatorial methods improve exploration of the binary space

IEEE 34-bus results

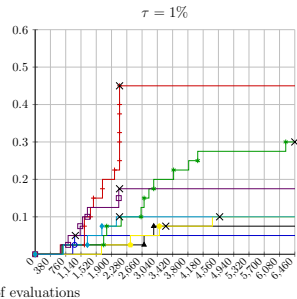
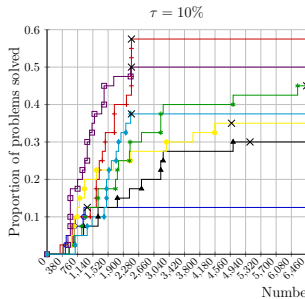
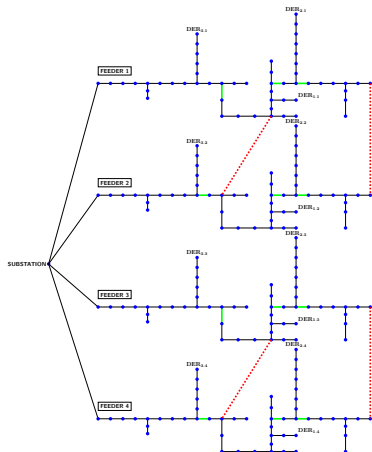


15 variables:

- 6 continuous
- 9 binary



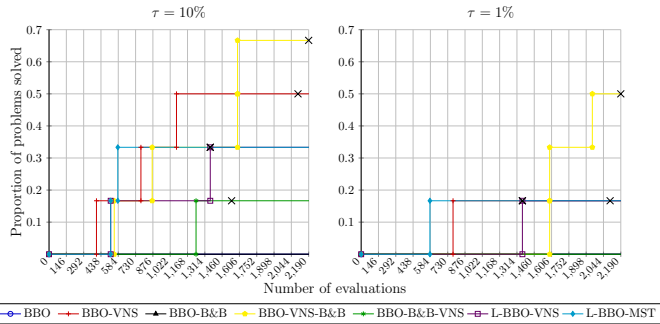
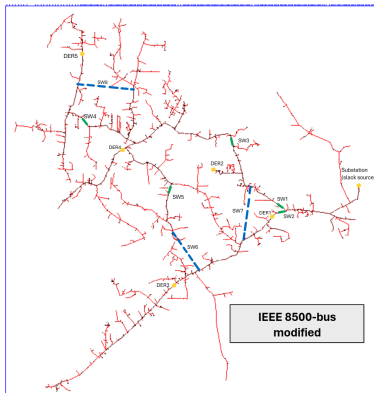
136-bus results



40 variables:

- 24 continuous
- 16 binary

IEEE 8500-bus results



18 variables:

- 10 continuous
- 8 binary

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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
- **Fast support** at nomad@gerad.ca
- NOMAD has become a **baseline** for benchmarking DFO algorithms
- MADS-related talks at SIAM OP26:
 - **MS126: Christina Soldati**, *Blackbox Optimization for Distribution Network Reconfiguration with Distributed Energy Resources*
 - **MS191: Tudor Buhut**, *Chance-constrained Blackbox Optimization*
 - **MS232: Charles Audet**, *Adaptive Direct Search Algorithms for Constrained Optimization*

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