Blackbox optimization: Part 3/4: Applications

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Presentation outline

Example 1: Aircraft takeoff trajectories

Example 2: Characterization of objects from radiographs

Example 3: Hyperparameters Optimization

Example 4: Solar thermal power plant

References

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Aircraft takeoff trajectories

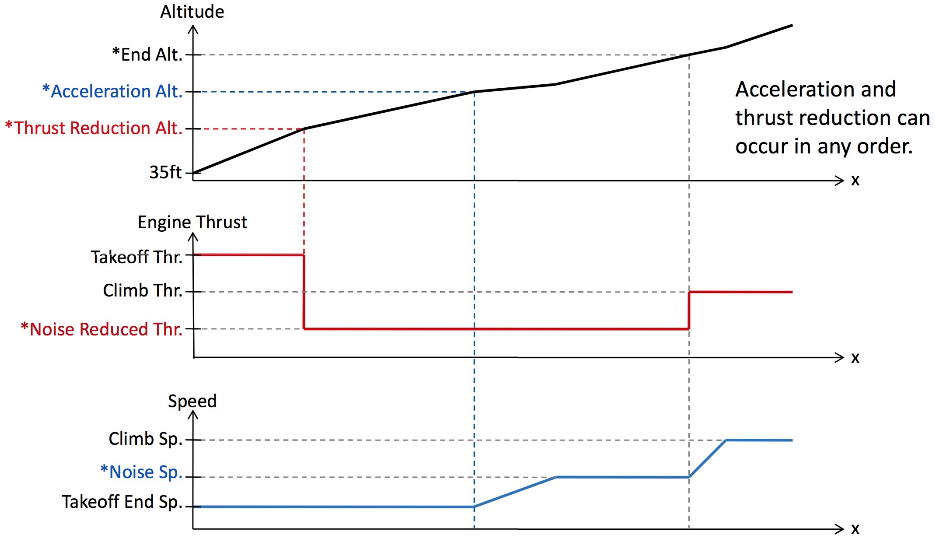
- [Torres et al., 2011]

- AIRBUS problem involving (among others): O. Babando, C. Bes, J. Chaptal, J.-B. Hiriart-Urruty, B. Talgorn, B. Tessier, and R. Torres
- Biobjective optimization problem

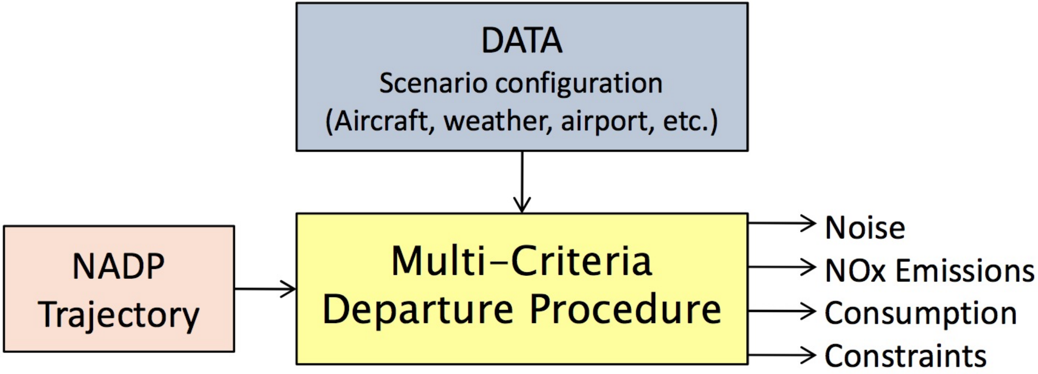
Definition of the optimization problem

- 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
- Variables define the NADP (Noise Abatement Departure Procedure): 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: Multi-Criteria Departure Procedure



One evaluation $\simeq$ 2 seconds

Special features

- Must execute on different platforms including some old Solaris distributions
- The best trajectory parameters are returned to the pilot who enters them in the aircraft system manually $\rightarrow$ the less decimals the better
- Finite precision on optimization parameters: Discretization of optimization variables $\rightarrow$ granular variables [Audet et al., 2019]

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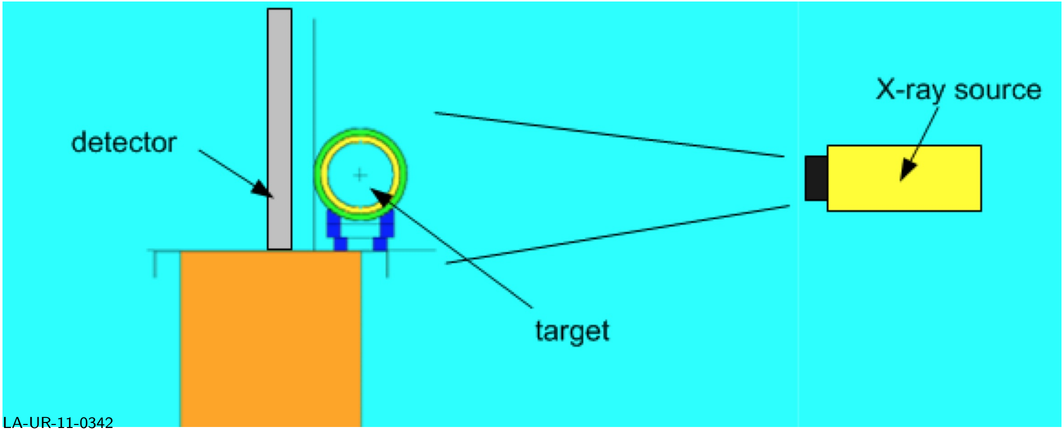
Characterization of objects from radiographs - LANL

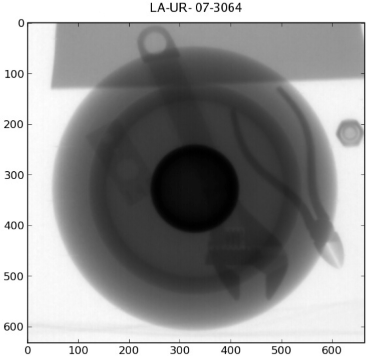
We want to identify an unknown object inside a box, using a x-ray source that gives an image on a detector



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

Radiograph

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



Description of the problem

- The problem consist 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
  - Meta 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 (inverse problem)
  - A numerical code – the blackbox – produces this simulated radiograph, using raytracing

Motivations for MADS and NOMAD

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

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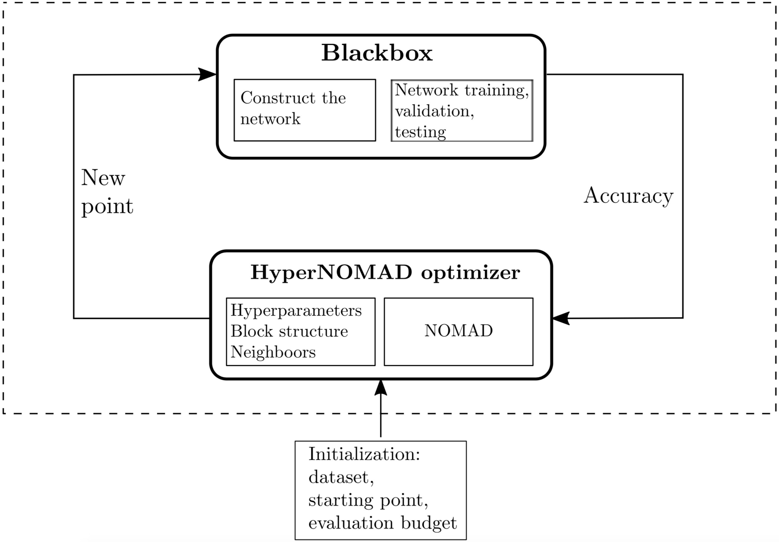
HPO with HyperNOMAD

- PhD project of Dounia Lakhmiri
- Published in TOMS [Lakhmiri et al., 2021]
- We focus on the HPO of deep neural networks
- Our advantages:
  - Blackbox optimization problem:
    One blackbox call = Training + validation + test, for a fixed set of hyperparameters
  - Presence of categorical variables *(ex.: number of layers)*
  - Existing methods are mostly heuristics
    (grid search, random search, GAs, etc.)
- Based on the NOMAD implementation of MADS

Principle


Blackbox
Construct the network
Network training, validation, testing
New point
Accuracy
HyperNOMAD optimizer
Hyperparameters
Block structure
Neighboors
NOMAD
Initialization:
dataset,
starting point,
evaluation budget

Hyperparameters for the architecture $(5n_1 + n_2 + 4)$

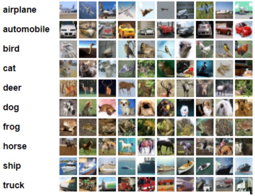
Hyperparameter	Type	Scope
Number of convolutional layers (n_1)	Meta	[0;20]
Number of output channels	Integer	[0;50]
Kernel size	Integer	[0;10]
Stride	Integer	[1;3]
Padding	Integer	[0;2]
Do a pooling	Boolean	0 or 1
Number of full layers (n_2)	Meta	[0;30]
Size of the full layer	Integer	[0;500]
Dropout rate	Real	[0;1]
Activation function	Categorical	ReLU, Sigmoid, Tanh

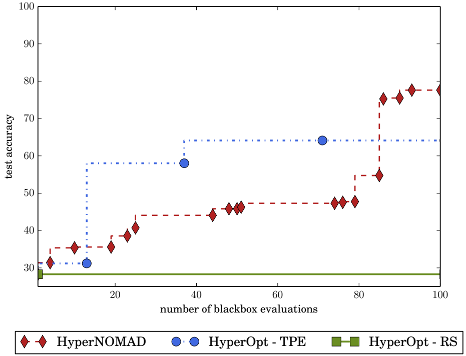
Hyperparameters for the optimizer (5)

Optimizer	Hyperparameter	Type	Scope
Stochastic Gradient Descent (SGD)	Learning rate	Real	[0;1]
	Momentum	Real	[0;1]
	Dampening	Real	[0;1]
	Weight decay	Real	[0;1]
Adam	Learning rate	Real	[0;1]
	β_1	Real	[0;1]
	β_2	Real	[0;1]
	Weight decay	Real	[0;1]
Adagrad	Learning rate	Real	[0;1]
	Learning rate decay	Real	[0;1]
	Initial accumulator	Real	[0;1]
	Weight decay	Real	[0;1]
RMSProp	Learning rate	Real	[0;1]
	Momentum	Real	[0;1]
	α	Real	[0;1]
	Weight decay	Real	[0;1]

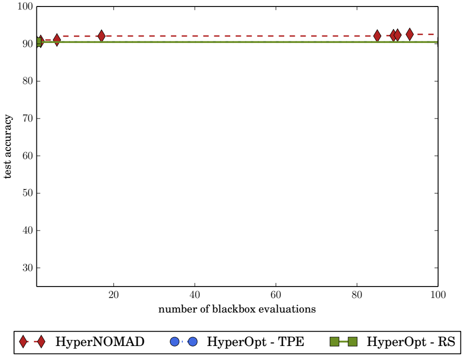
Results on CIFAR-10 (vs Hyperopt)

- Training with 40,000 images, validation/test on 10,000 images
- One evaluation (training+test) $\simeq$ 2 hours
  (i7-6700@3.4 GHz, GeForce GTX 1070)





(a) Default starting point



(b) From a VGG architecture

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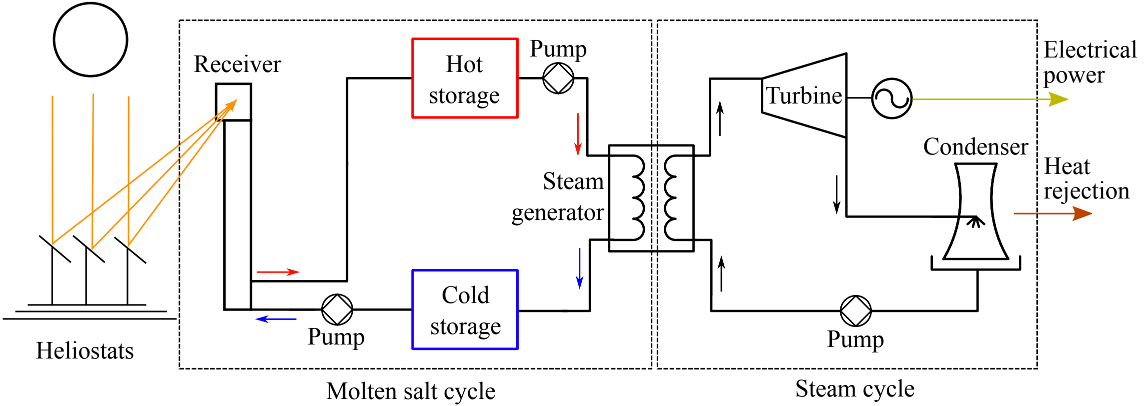
CSP tower plant with molten salt thermal energy storage

- 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



Ten instances

Instance	# of variables cont.	discr. (cat.)	n	# of obj. p	# of constraints simu.	a priori (lin.)	m	# of stoch. outputs (obj. or constr.)	Static surrogate
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

[1] analytic objective
[2] unconstrained

Features for BBO benchmarking

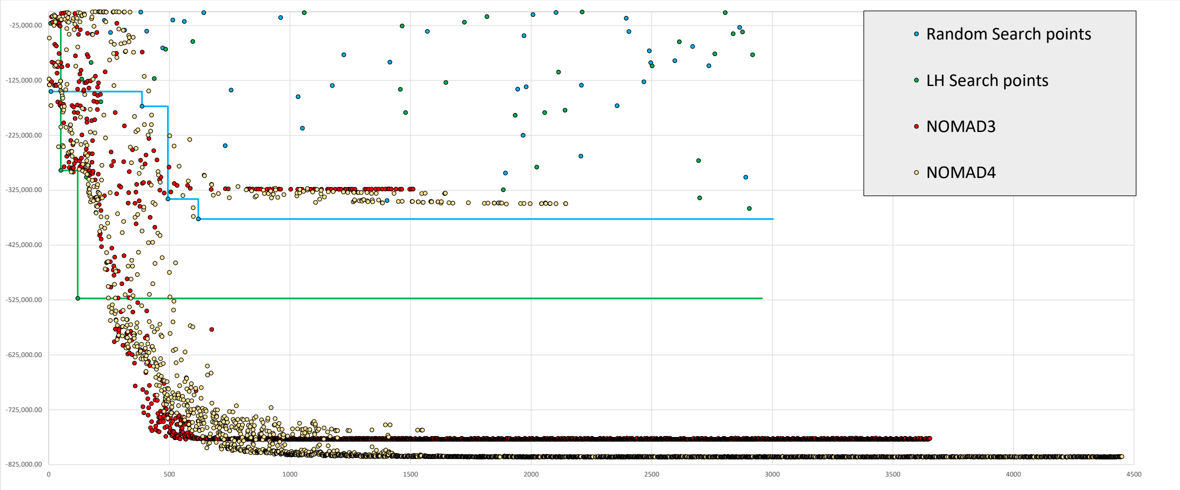
- Several numerical methods: real-world blackbox
- Reproducibility accros all platforms
- Continuous and discrete variables
- Different types of constraints (quantifiable, relaxable, a priori, hidden)
- Stochastic and deterministic outputs
- Static surrogates with variable fidelity
- Number of replications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

Feasibility with sampling and NOMAD

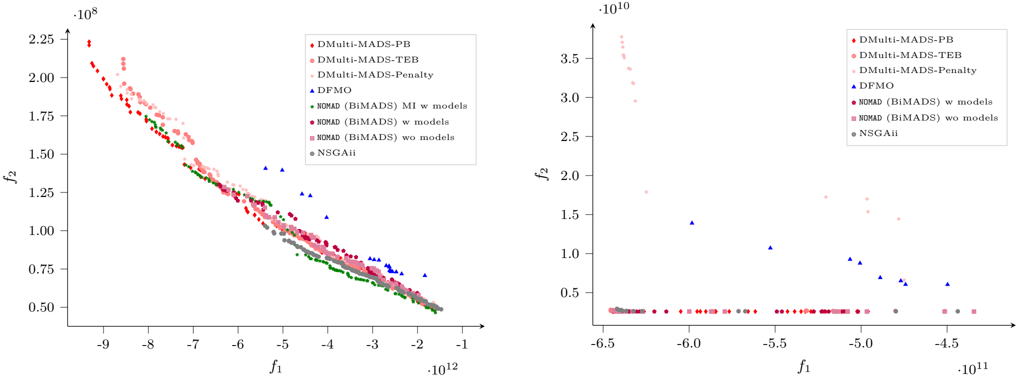
Instance	LH search (10k points)		NOMAD3		
	satisf. ap constr.	feas. pts	satisf. ap constr.	feas. pts	number of eval.
solar1	30%	0.35%	96%	74%	3,792
solar2	0%	0%	97%	0%	1,635
solar3	0.49%	0%	99%	9%	30,525
solar4	0%	0%	83%	0%	44,303
solar5	0%	0%	83%	59%	3,405
solar6	90%	5%	99%	0%	3,539
solar7	2%	1%	74%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

there has been no violation of hidden constraints during the construction of this table

Optimization on solar1



Biobjective optimization (by L. Salomon)



Pareto front approximations for solar8 (left) and solar9 (right) with different solvers with a budget of 5K evaluations. Taken from [Bigeon et al., 2022]

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References I

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