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Machine Learning Assisted Cyclic Coordinate Descent Algorithm For Scalable Black-box Optimization

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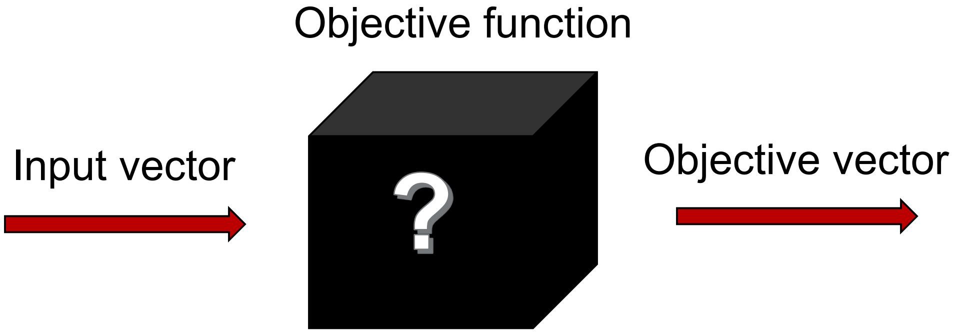
Contents

Introduction and Motivation

Black-box optimization

- Given a set of potential power plant layouts, how do we find the best layout defined against a set of Quantities of Interest?
- Given a steam turbine, how do we configure its geometry to achieve the best efficiency?
- Given design variables of a machine, how do we know its life? And how do they connect to the damage?



Introduction and Motivation

Traditional optimization

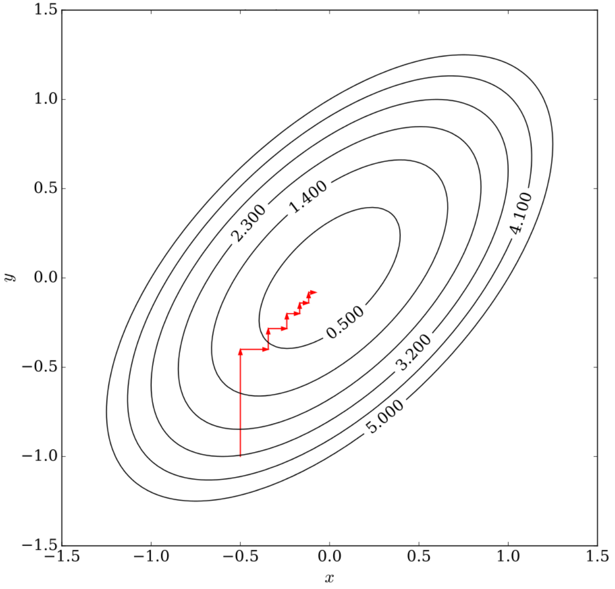
- A physical problem can be mathematically expressed as a function
- Optimum solution (either minimum or maximum) of the objective function can be obtained using the concept of derivative
- Common methods:
  - Direct search
  - Gradient-based search

Black-box optimization

- Unsolvable using conventional approaches because of non-smoothness or discontinuities, etc
- Unaffordable cost of function evaluations (experimental or industrial situations)

Proposed Algorithm

Cyclic Coordinate



Set a tolerance $\epsilon > 0$;
Let $d^1, d^2, \ldots, d^n$ be the coordinate directions;
Initialize starting point x^0;
Set $k = 1$ and $i = 1$;
while $||x^{k+1} - x^k|| \geqslant \epsilon$ **do**
  Set $y_1 = x_k$;
  for $i = 1, 2, \ldots, n$ **do**
    $x_i^k = \underset{x_i}{argmin} f(x_1^k, \ldots, x_{i-1}^k, x_i, x_{i+1}^{k-1}, \ldots, x_n^{k-1})$;
    $y_{i+1} = y_i + \lambda_i d_i$;
  end for
  Let $X_{k+1} = y_{k+1}$;
  $k = k + 1$;
end while

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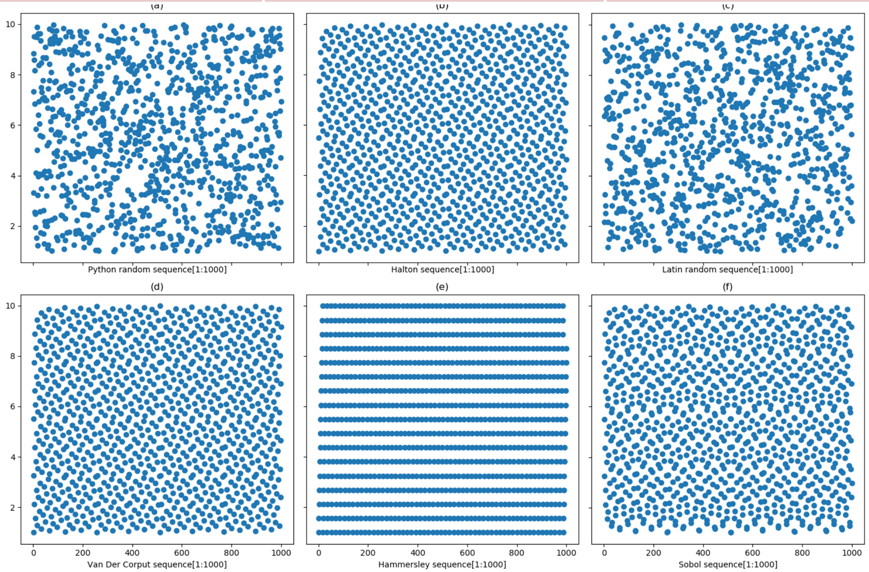
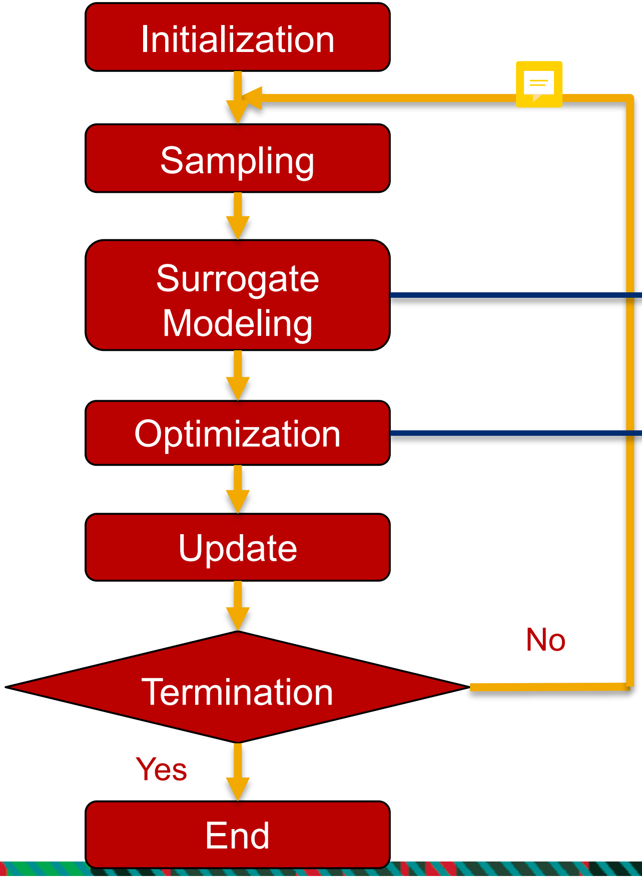
Proposed Algorithm

Sampling Methods

Python random	Halton sequence	Latin square
Van Der Corput sequence	Hammersly sequence	Sobol sequence



Proposed Algorithm



Tools

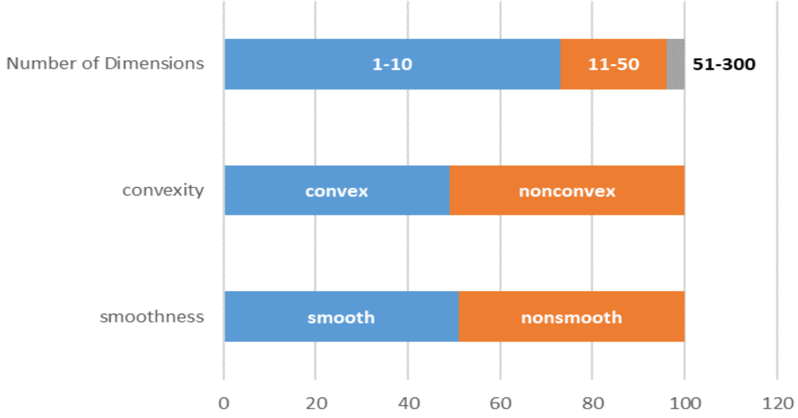
ALAMO
- Adaptive sampling
- Surrogate modeling

BARON
- Mixed-Integer nonlinear optimization solver

Problem Statement

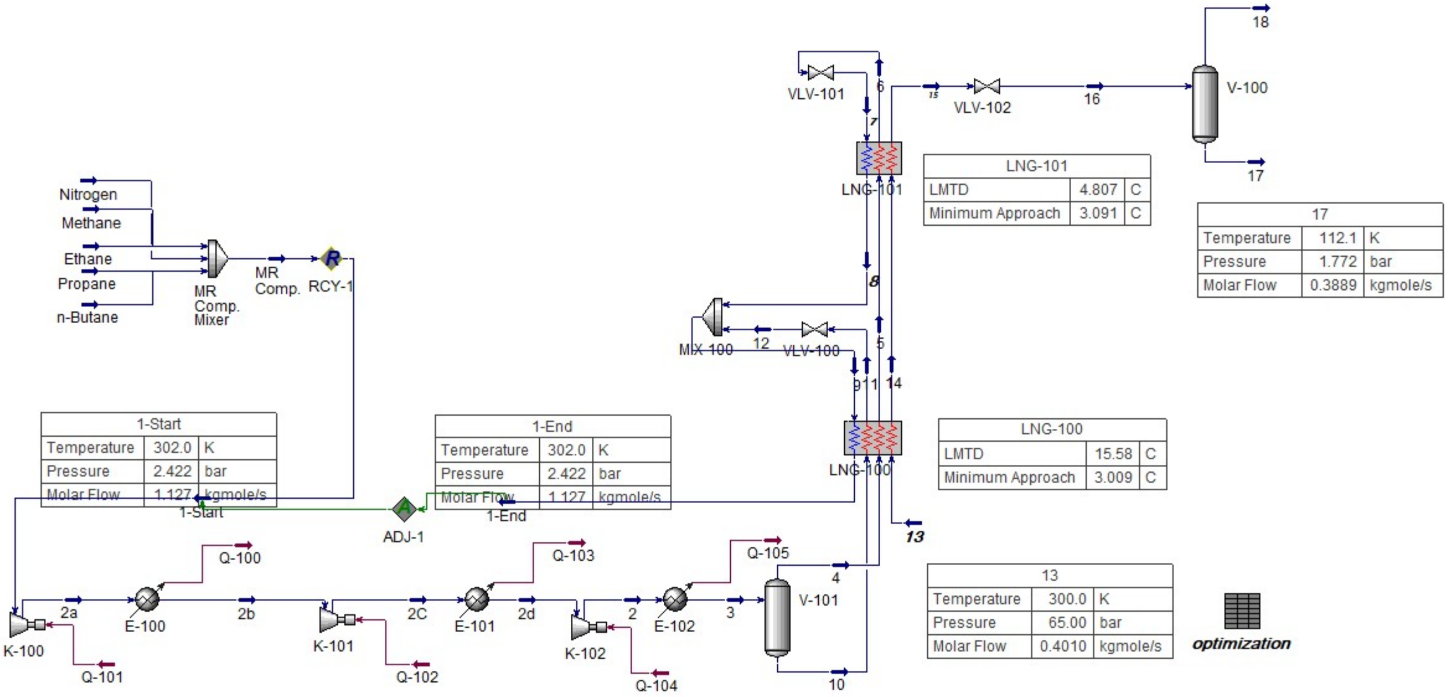
100 Black box models

Variables	smoothness		Convexity		total
	Smooth	Nonsmooth	Convex	Nonconvex	
1-10	36	37	28	45	73
10-50	11	12	18	5	23
50-300	4	0	3	1	4



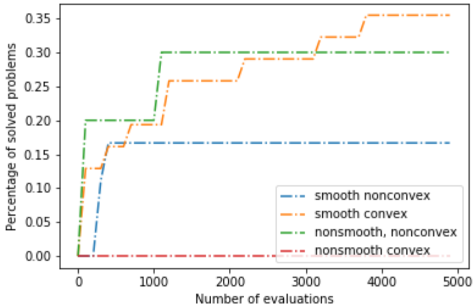
Problem Statement

The Single Mixed Refrigerant Liquefaction Process Simulation

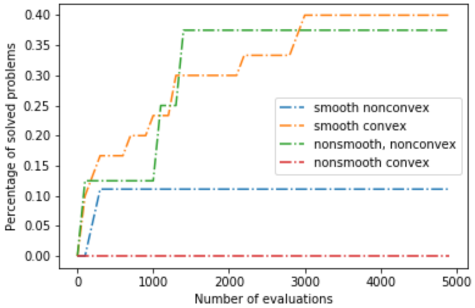


Results and Discussion

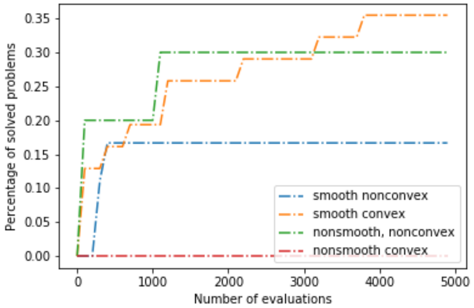
Percentage of solved problems v.s. Number of evaluations



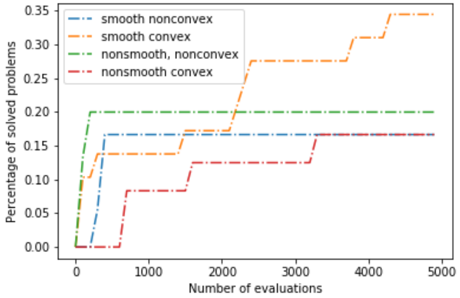
Halton



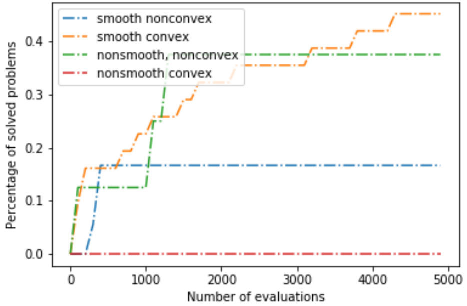
Hammersley



Van Der Corput



Latin



Sobol

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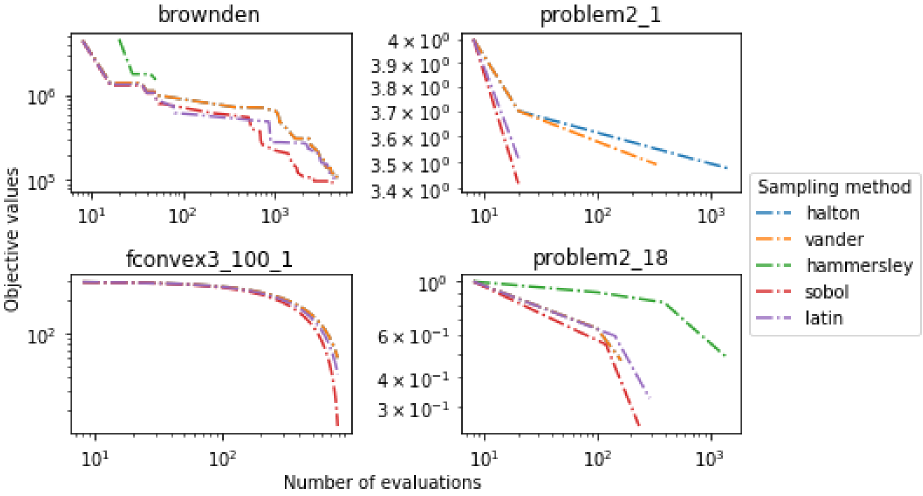
Results and Discussion



Observations:

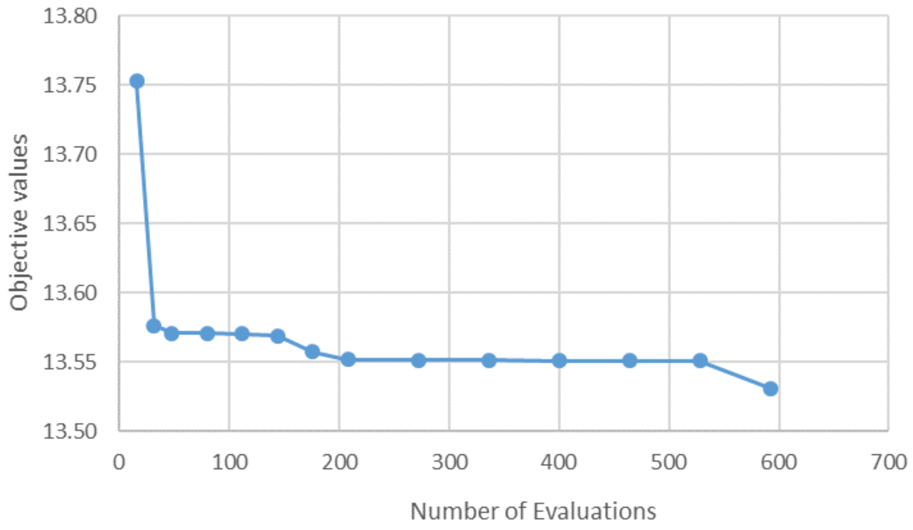
- Better performance in smooth models
- Tend to be stuck in local optimal points in nonsmooth models
- Global optimal can be expected for smooth-convex models

Discussions:

- Difference performances of quasi-random sequence sampling
- Impact from smoothness and convexity

Results and Discussion

SMR liquefaction process simulation result



Fail to optimize the SMR simulator

Discussions:

- Discontinuous hidden constraints
- Pre-defined constraints from relationship between variables based on physical configuration

Potential solutions:

- Search globally
- Block coordinate search

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Conclusions

- Surrogate modeling has been proved that it is a flexible and useful method in black-box optimization problems
- Different sampling methods has shown different performances depending on smoothness, convexity and the dimensions of surrogate model
- Sobol sequence has the best solutions combining with cyclic coordinate search algorithm
- Proposed algorithm is not able to solve problems with discontinuous hidden constraints and linked variables deriving from industrial problem; global sampling and block coordinate search probably are expected to be applied

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Question and Answer