MS130: Derivative-Free Optimization Methods for Solving Expensive Global Black-Box Problems

Enhanced Kriging models within a Bayesian optimization framework to handle both continuous and categorical inputs

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Joseph Morlier (ISAE-SUPAERO)

ISAE Institut Supérieur de l'Aéronautique et de l'Espace SUPAERO

RÉPUBLIQUE FRANÇAISE *Liberté Égalité Fraternité*

ONERA THE FRENCH AEROSPACE LAB

Context

New aircraft configurations = Unknown behaviors

A. Lambe and J. R. R. A. Martins. “Extensions to the design structure matrix for the description of multidisciplinary design, analysis, and optimization processes". Structural and Multidisciplinary Optimization 46 (2012), pages 273-284.

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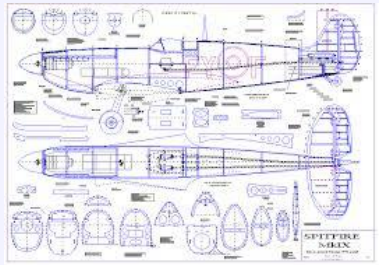

Aircraft design developments required:

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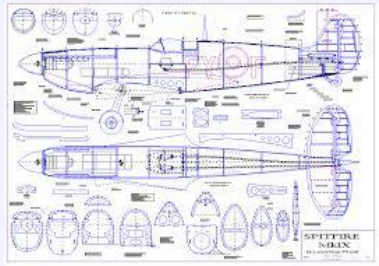
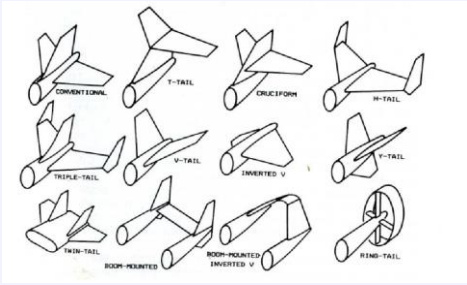


Discrete variables



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- mixed integer variables
- multimodal constraints (convex or non-convex, equality or inequality,…)

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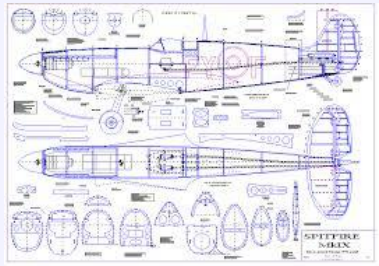

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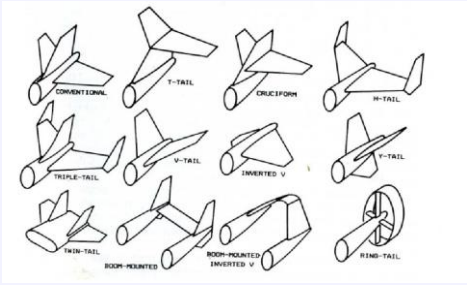
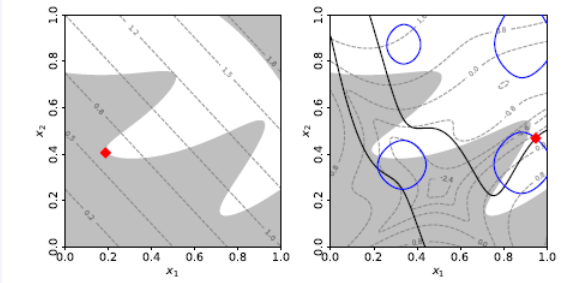


Multimodal constraints



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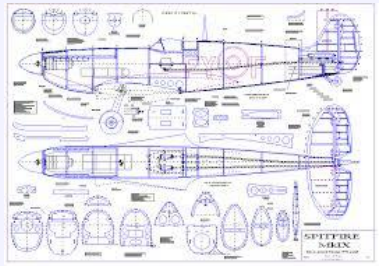
➔ Our objective is to solve **high dimensional mixed integer constrained optimization problems using Bayesian optimization**.

High-dimension



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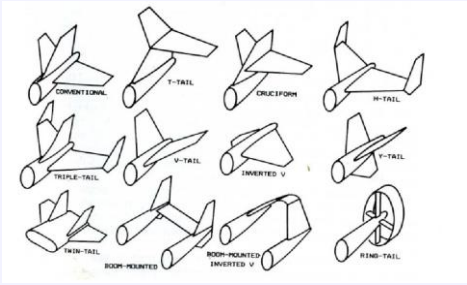

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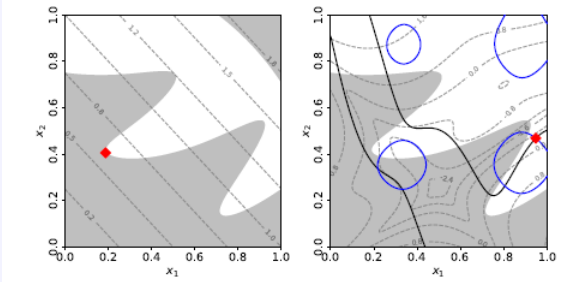

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Bayesian optimization applied to aircraft design

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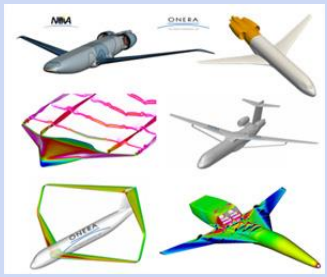
New concepts



Ω

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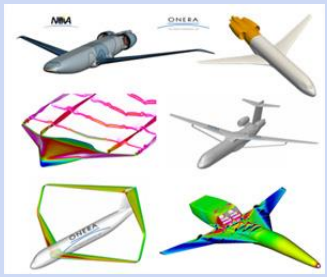

Ω

Analyze

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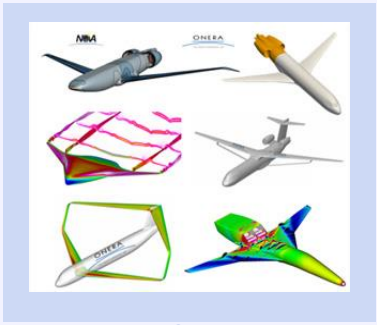
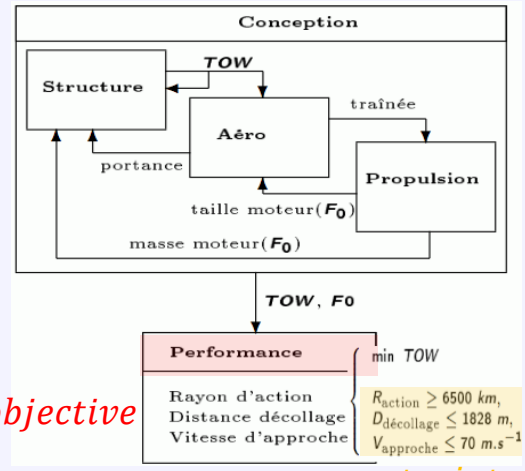


Ω

Analyze

Multidisciplinary Design Analysis



objective

constraints

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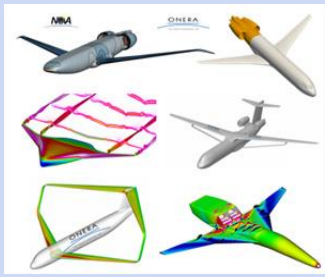

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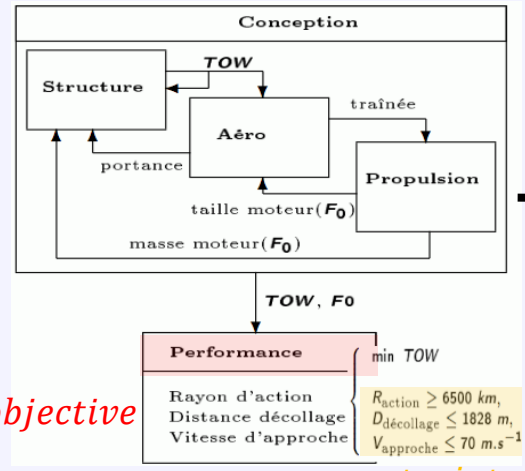

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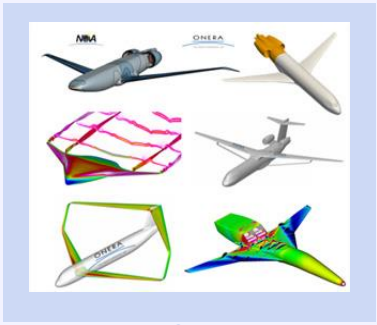

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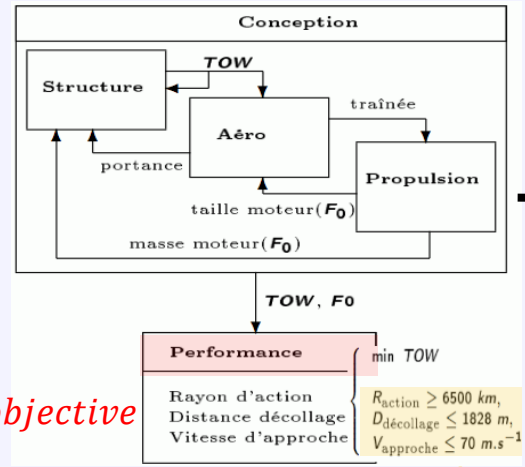

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Global optimization

MDF Formulation

$$\min_{inputs \in \Omega} \ objective\ (inputs)$$

$$s.t \quad constraints\ (inputs)$$

Bayesian optimization applied to aircraft design

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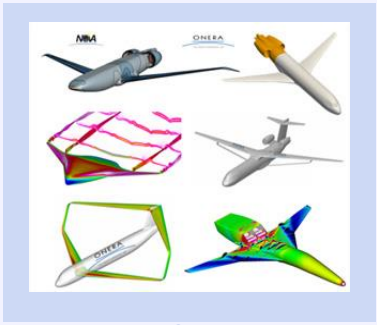

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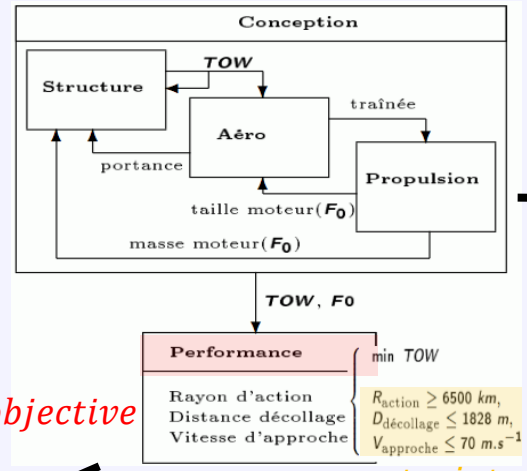

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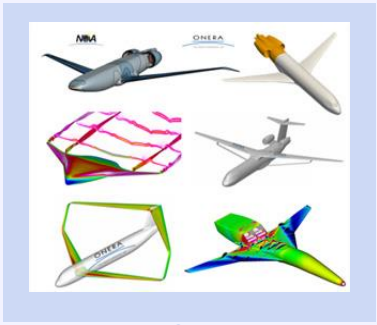

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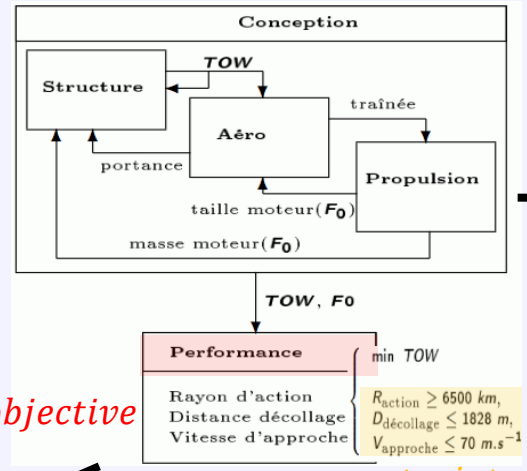

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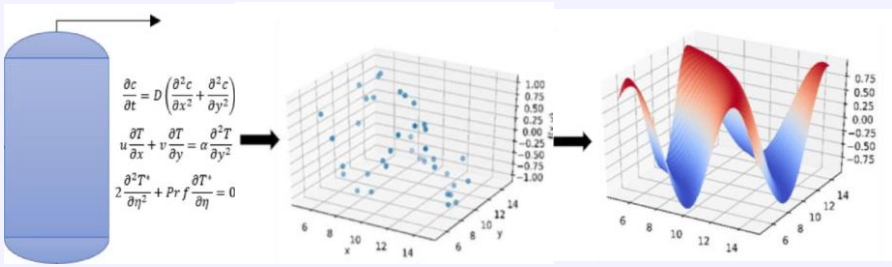
Surrogate model



Expensive black-box | Design of Experiments | Gaussian processes

Bayesian optimization applied to aircraft design

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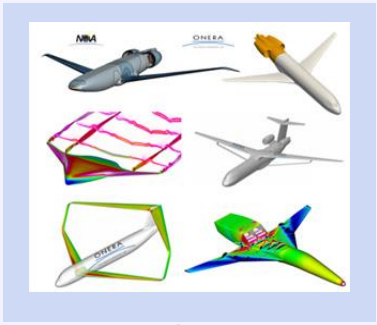

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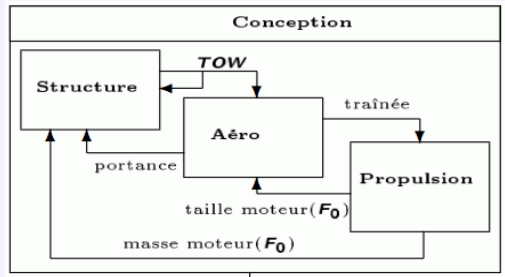

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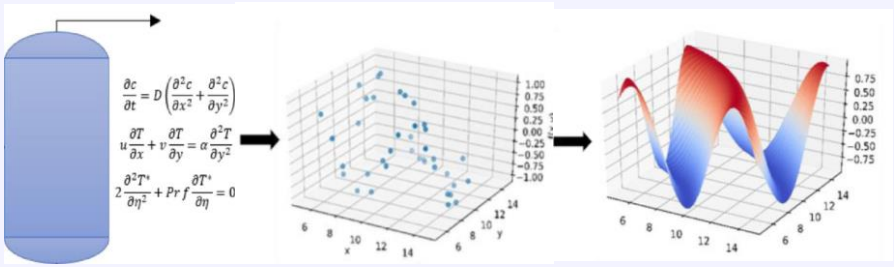
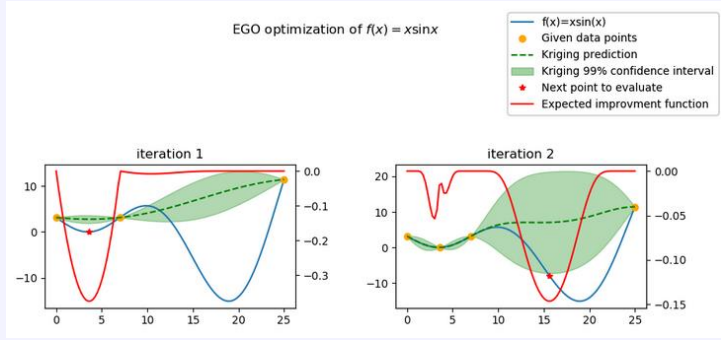


Expensive black-box — Design of Experiments — Gaussian processes

Efficient Global Optimization



State-of-the-art

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Baseline method ⇨ Super Efficient Global Optimizer (SEGO)

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High-Dimension ☺

Mixed integer ☹

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Garrido-Merchán and Hernández-Lobato

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The proposed approach:

- **Continuous relaxation** to tackle mixed integer but increase the number of dimensions.
- **Kriging with Partial Least Squares (KPLS)** to tackle high-dimension.
- **SEGO** to tackle constrained optimization.

A. M. Bouhlel, N. Bartoli, A. Otsmane, and J. Morlier. “Improving kriging surrogates of high-dimensional design models by Partial Least Squares dimension reduction". Structural and Multidisciplinary Optimization 53 (2016), pages 935-952

Proposed approach: the surrogate model (1/2)

i. Relax continuously integer/categorical input variables

$\boldsymbol{if}\ integer$

|relax continuously within the bounds

$\boldsymbol{if}\ categorical$

|Add a dimension by level with bounds $[0,1]$

D. R. Jones, M. Schonlau, and W. J. Welch. “Efficient Global Optimization of Expensive Black-Box Functions”. Journal of Global Optimization, vol. 13 (1998), pages 455–492.

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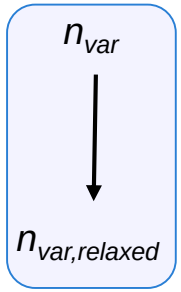

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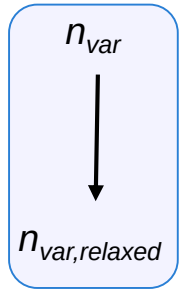
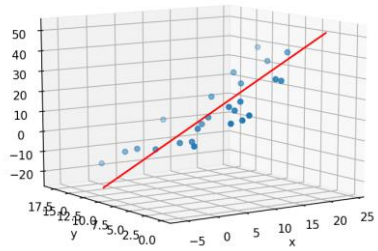


ii. Use PLS to reduce the dimension $n_{var,relaxed}$ to h principal components ($h \ll n_{var,relaxed}$)



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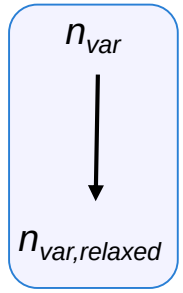

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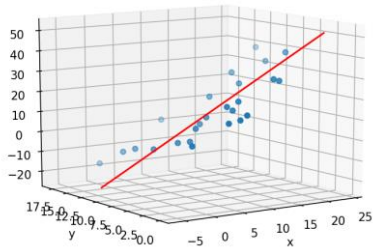

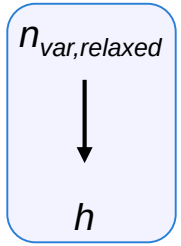

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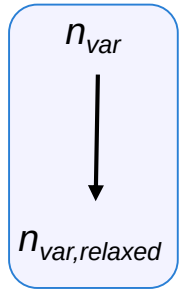

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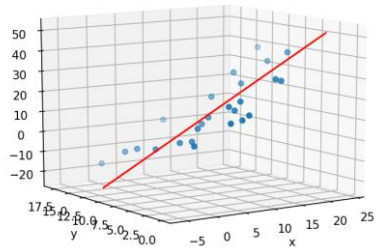

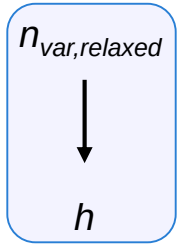

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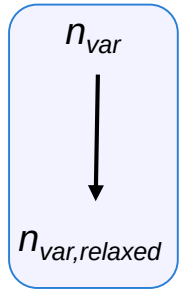

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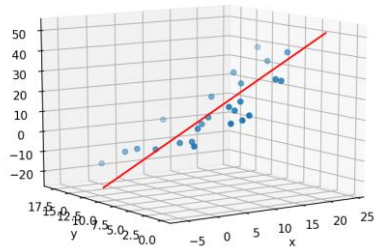

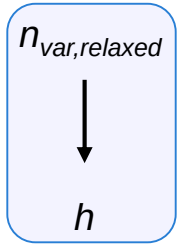

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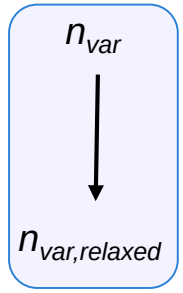

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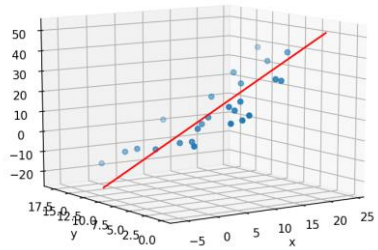

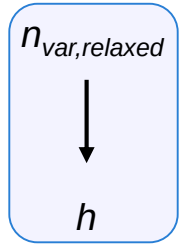

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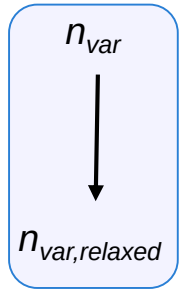

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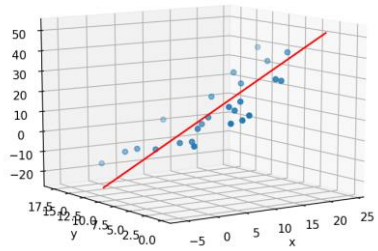

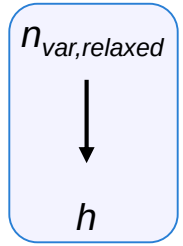

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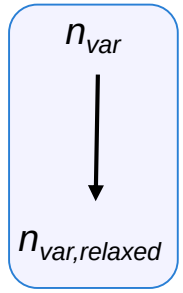

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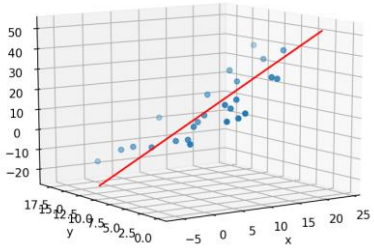

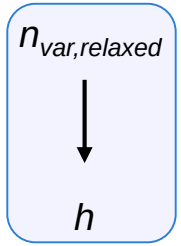

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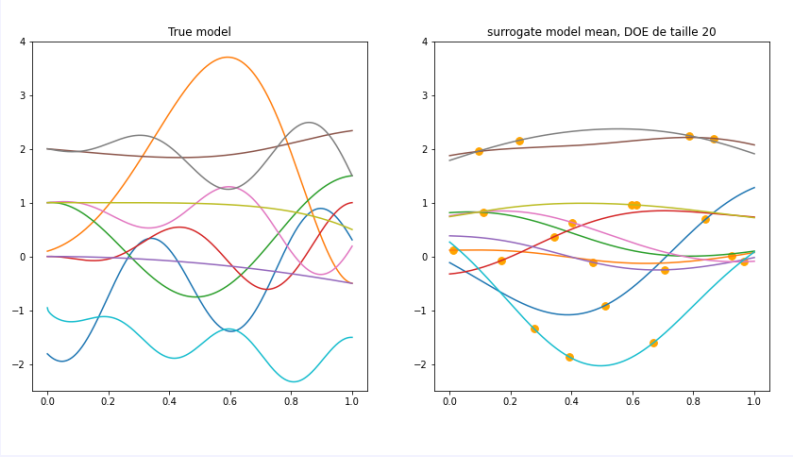
Validation problem $n_{var} = 2$

- Variable types: continuous and categorical with 10 levels. $n_{var,relaxed} = 11$



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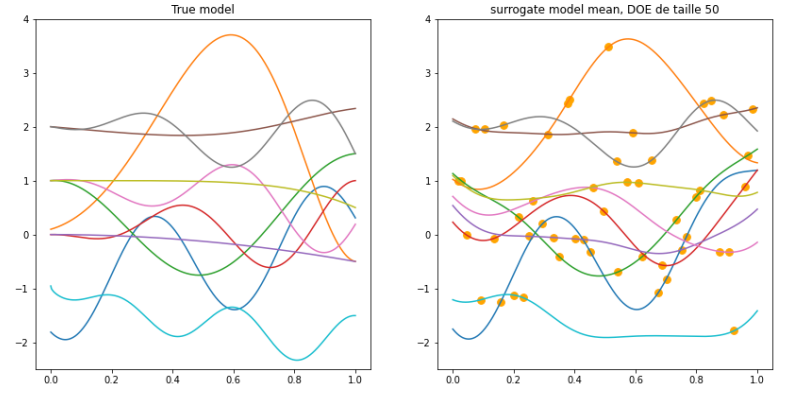

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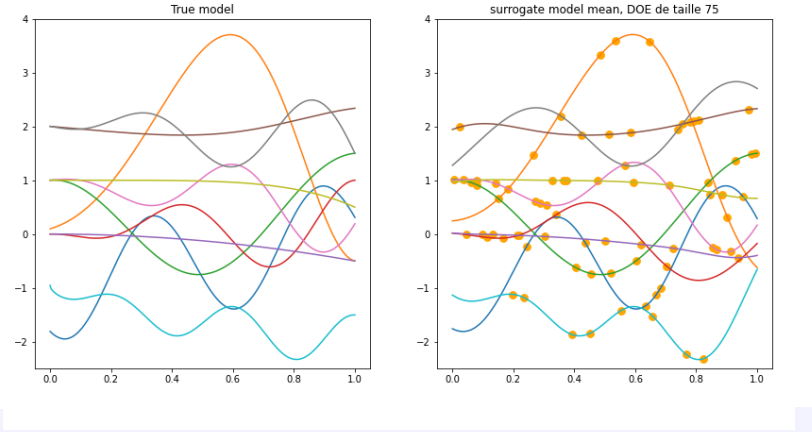

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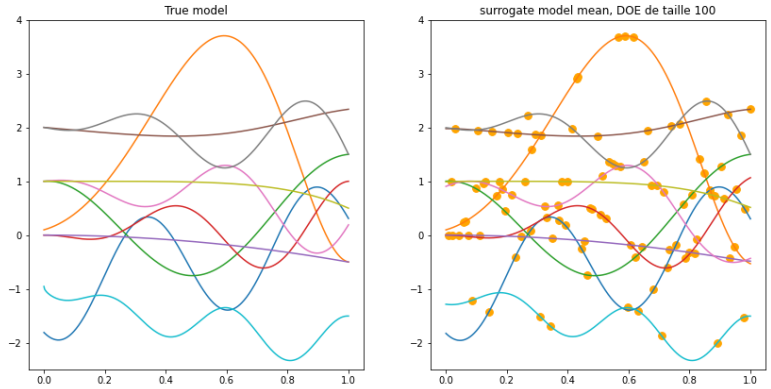

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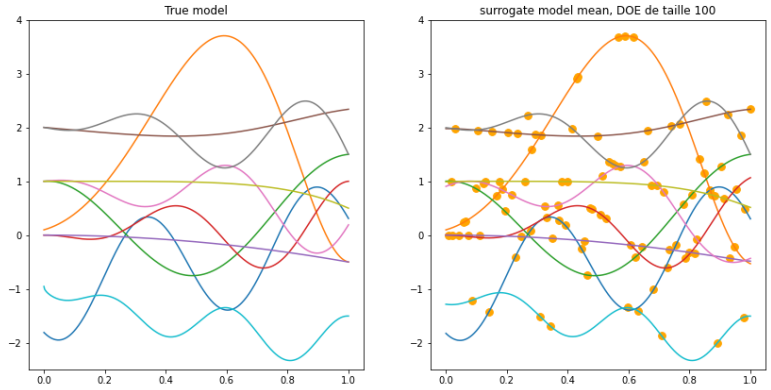

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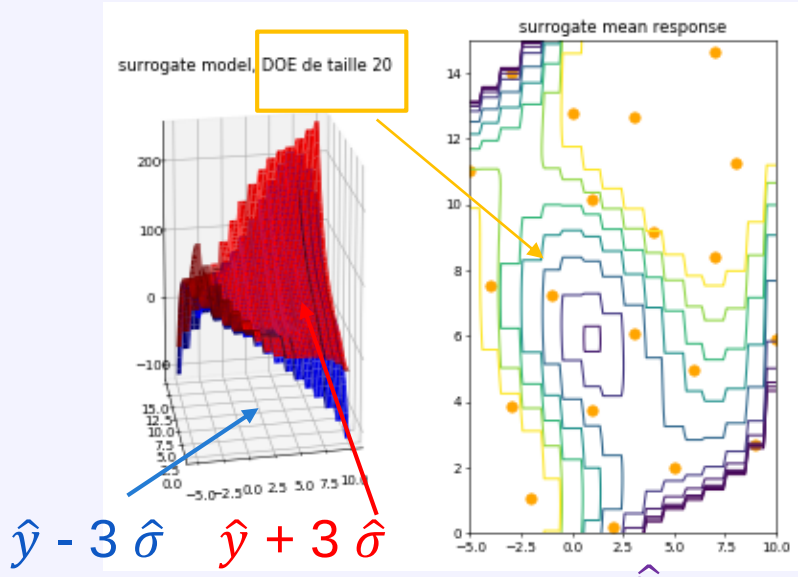

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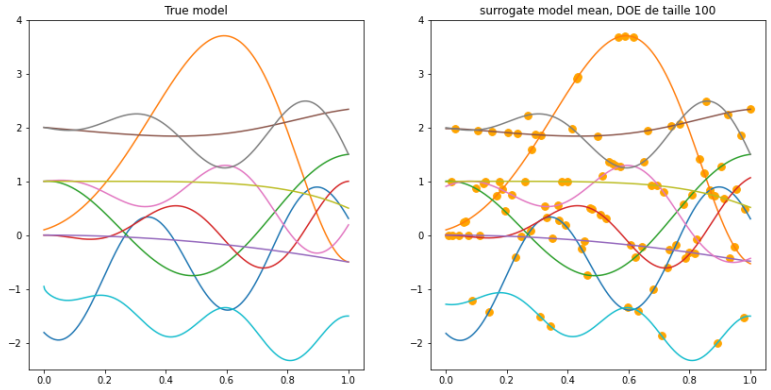

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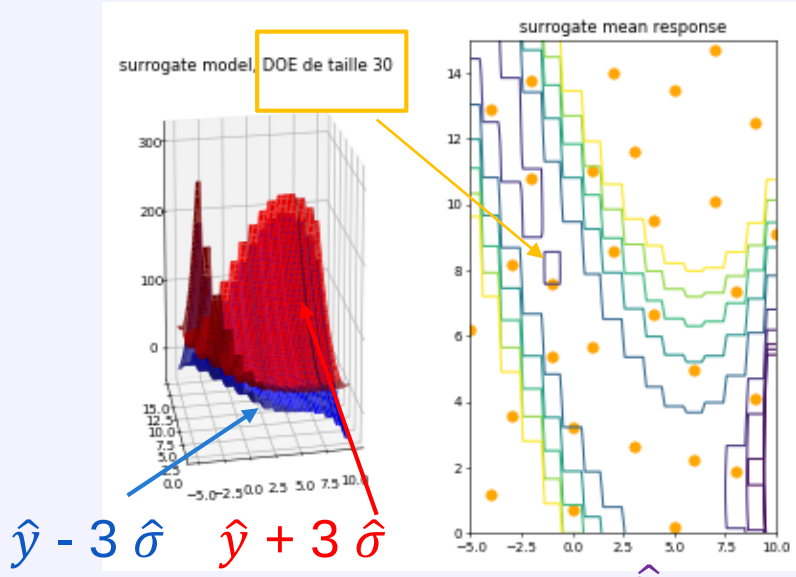

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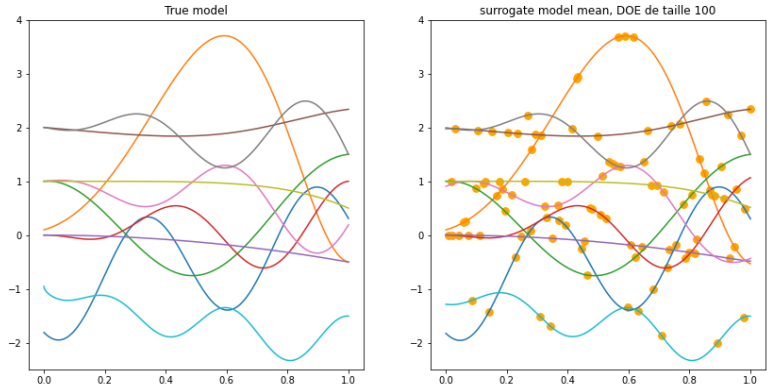

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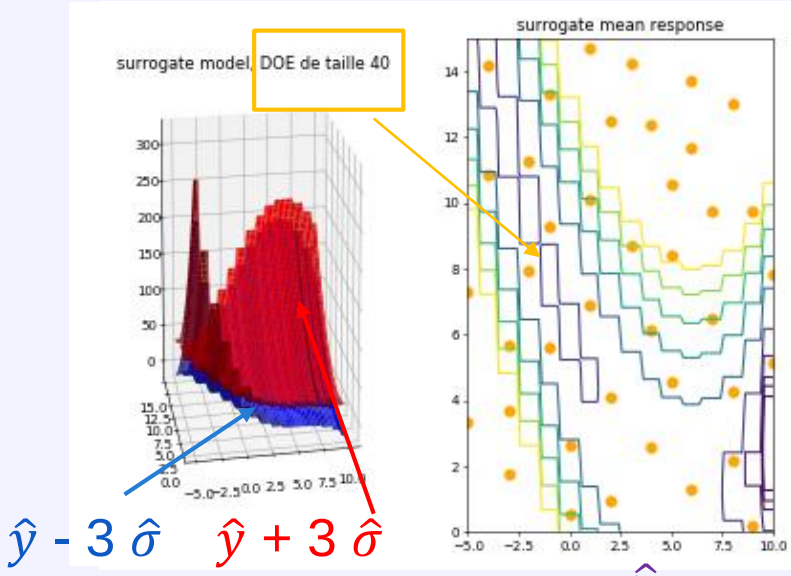

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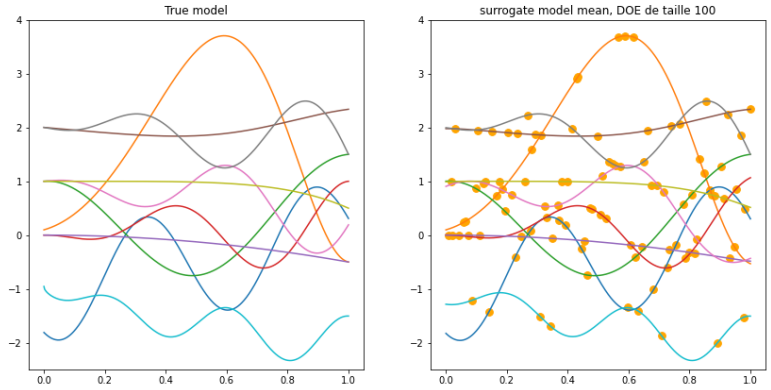

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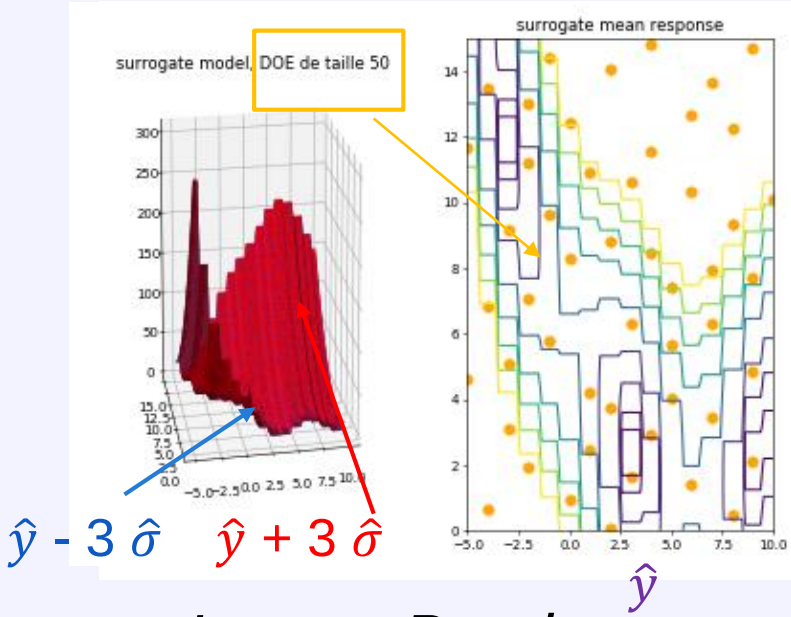

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iv. Compute $\mathrm{y}_{new} = f\left(\arg\max_{x \in \Omega_f} WB2s(x)\right)$.

R. Priem, N. Bartoli, Y. Diouane, A. Sgueglia. “Upper Trust Bound Feasibility Criterion for Mixed Constrained Bayesian Optimization with Application to Aircraft Design”. Aerospace Science and Technology

Proposed approach: The optimization process

i. Build the surrogate model of the objective $(\hat{y}(x), \hat{\sigma}(x))$

ii. Build the surrogate model for each constraint $(\widehat{c_i}(x), \widehat{\sigma_i}(x))$ and compute $\Omega_f = \{x \in \Omega : \widehat{c_i}(x) - 3\widehat{\sigma_i}(x) \leq 0\}$

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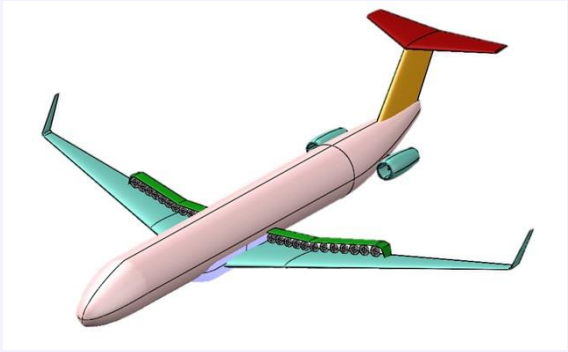
Hybrid aircraft concept with distributed propulsion



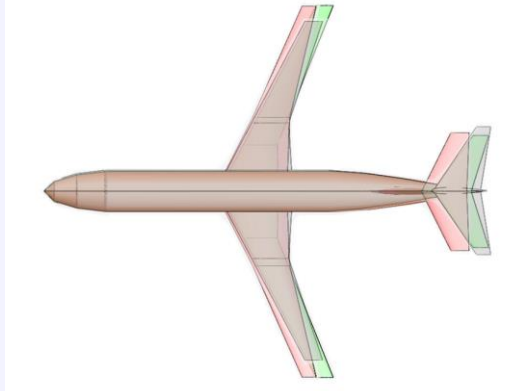
Validation problem $n_{var} = 12$

- 8 inequality constraints and 3 equality constraints.
- Total energy consumption.

Cobyla

SEGO

Baseline



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Optimization problems and options

Optimization problems and options

Optimizers

- Unconstrained cases: Bandit-BO

- No parallelization, batch = 1

D. Nguyen, S. Gupta, S. Rana, A. Shilto, and S. Venkatesh, “Bayesian Optimization for Categorical and Category-Specific Continuous Inputs”. In: AAAI Conference on Artificial Intelligence. 2020.

- Constrained cases: genetic algorithm NSGA2 (1 objective)

- Probability of crossover = 1, eta = 3 from the Open-Source Pymoo toolbox *https://pymoo.org/*

J. Blank and K. Deb, "Pymoo: Multi-Objective Optimization in Python," in IEEE Access, vol. 8, pp. 89497-89509, 2020.

- SEGO coupled with the Open-Source SMT toolbox *https://smt.readthedocs.io/*

- WB2s maximized with SNOPT *https://web.stanford.edu/group/SOL/snopt.htm*

- With and without Partial Least Squares.

M. A. Bouhlel, J. T. Hwang, N. Bartoli, R. Lafage, J. Morlier, and J. R. R. A. Martins. “A Python surrogate modeling framework with derivatives". Advances in Engineering Software 135 (2019).
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Test cases

- Validation on analytical test cases, with and without constraints (20 runs)

- For SEGO & Bandit-BO: 50 iterations

- For NSGA2: 200 iterations (5 individuals, 40 mutations)

- Validation on an expensive industrial case

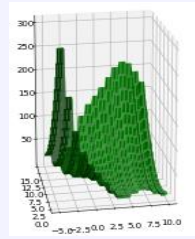
- For SEGO & NSGA2: 20 runs of 50 iterations

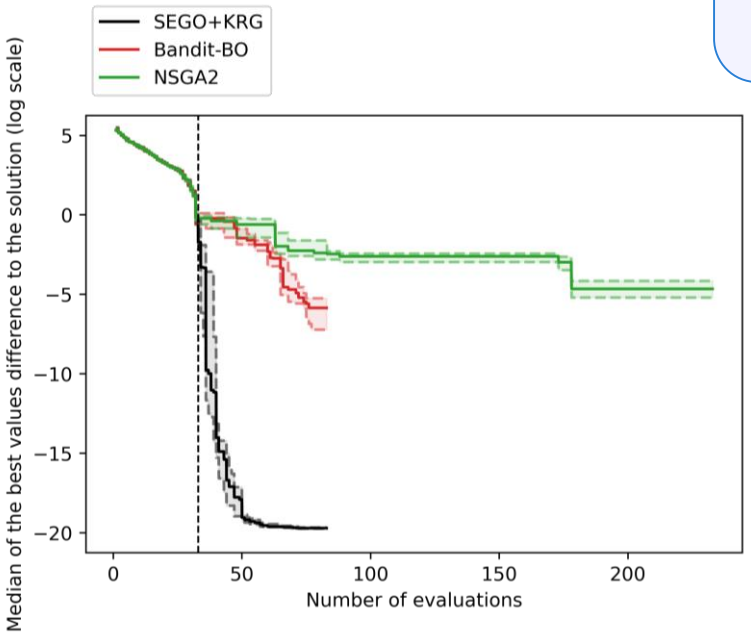
Unconstrained Bayesian optimization (1/2)

Validation problem $n_{var} = 2$
- Variable types: integer (1) and continuous (1).

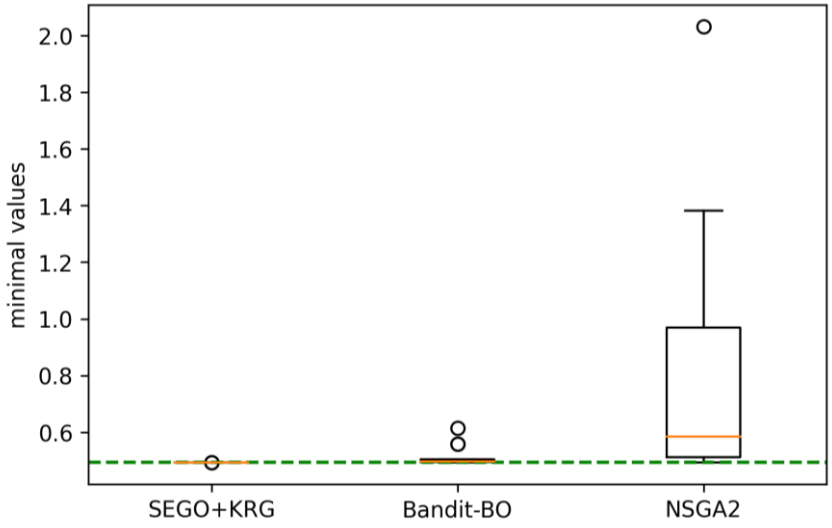
Options for Bandit-BO
16 arms, minimal DoE of 32 points

Convergence plots for the integer Branin test case





Boxplots for the 20 optimization results after 50 iterations



S. Roy, W. A. Crossley, B. Stanford, K. T. Moore, and J. S. Gray, “A Mixed Integer Efficient Global Optimization Algorithm with Multiple Infill Strategy - Applied to a Wing Topology Optimization Problem”. In: AIAA Scitech 2019 Forum.

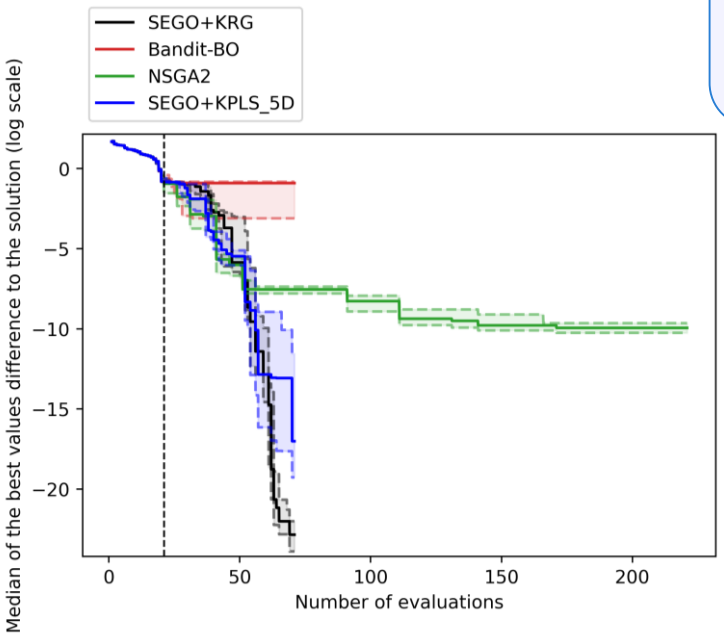
Unconstrained Bayesian optimization (2/2)

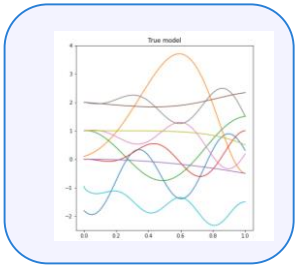
Validation problem $n_{var} = 2$

- Variable types: continuous (1) and categorical (1 with 10 levels). $n_{var,relaxed} = 11$

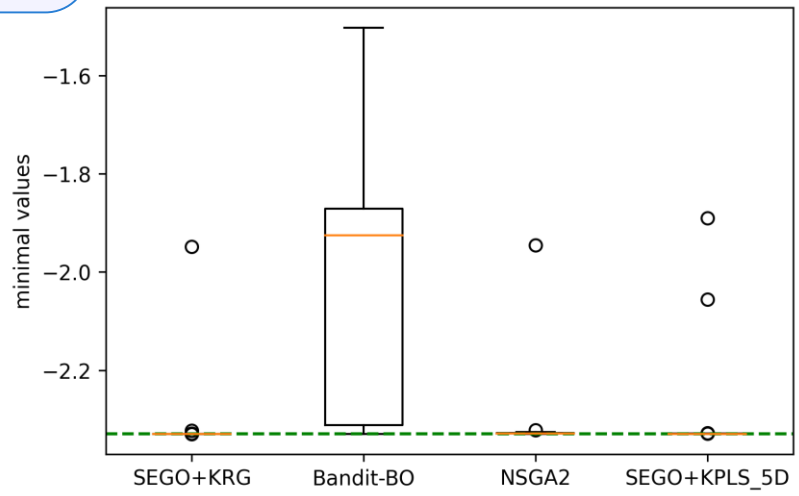
Options for Bandit-BO
10 arms, minimal DoE of 20 points
Options for NSGA2
Categorical variable treated as integer
Options for SEGO-KPLS
$n_{var,relaxed} = 11 \rightarrow h = 5$

Convergence plots for the Toy test case





Boxplots for the 20 optimization results after 50 iterations



M. M. Zuniga, and D. Sinoquet. "Global optimization for mixed categorical-continuous variables based on Gaussian process models with a randomized categorical space exploration step". Information Systems and Operational Research, vol. 58 (2020), pages 1–32.

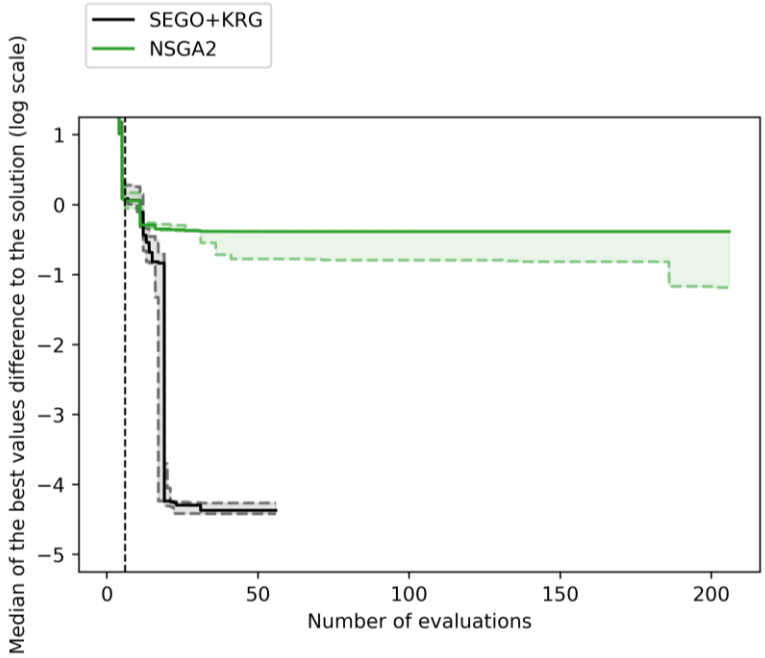
Constrained Bayesian optimization (1/2)

Validation problem $n_{var} = 4$
Variable types: continuous (2) and categorical (2 with 2 levels). $n_{var,relaxed} = 6$

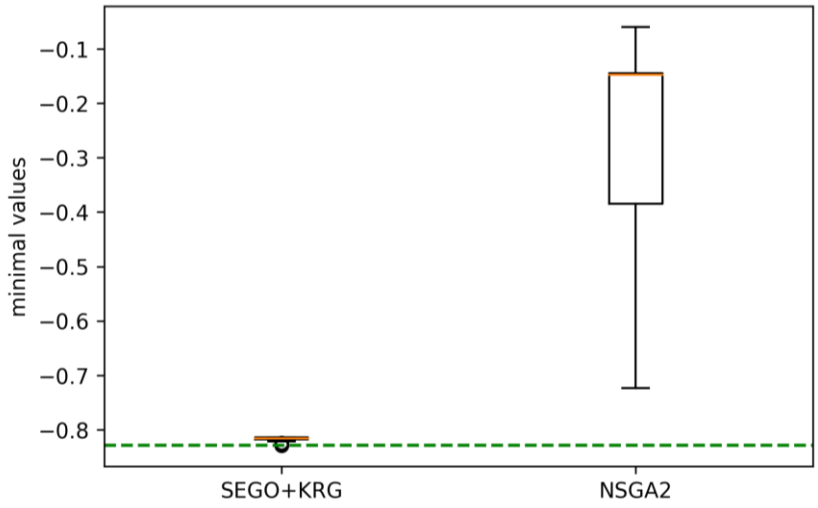
- 1 constraint

Options for NSGA2
Categorical variables treated as integer ones

Convergence plots for the categorical Branin test case



Boxplots for the 20 optimization results after 50 iterations



J. Pelamatti, L. Brevault, M. Balesdent, E.-G Talbi, and Y. Guerin. “Efficient global optimization of constrained mixed variable problems". Journal of Global Optimization 73 (2019), pages 583-613

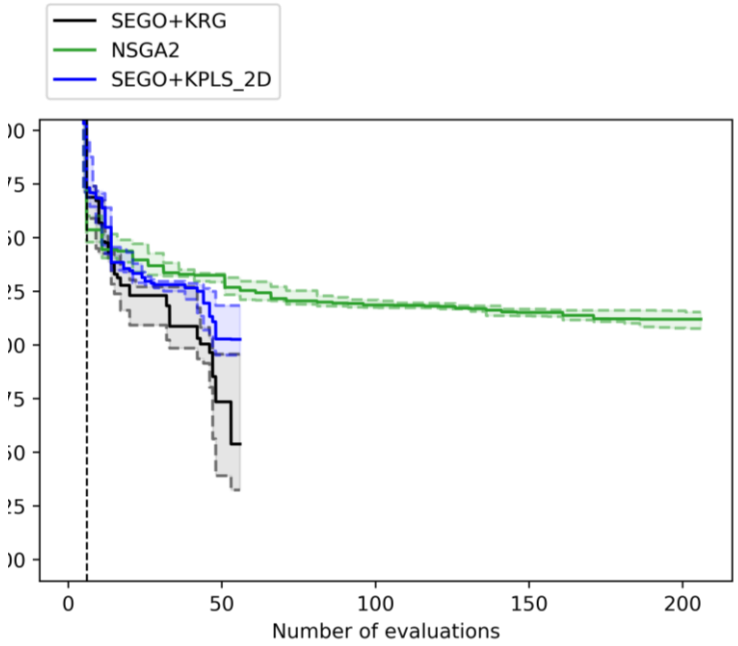
Constrained Bayesian optimization (2/2)

Validation problem $n_{var} = 12$
Variable types: continuous (10) and categorical (2 with 2 levels). $n_{var,relaxed} = 14$

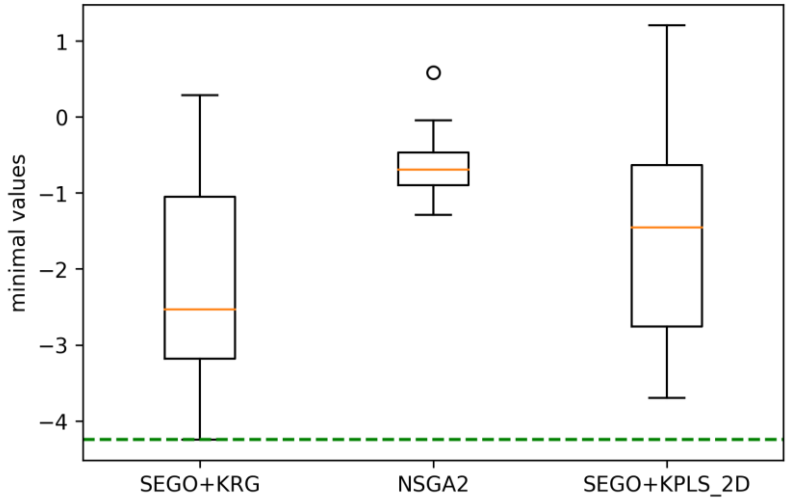
- 1 constraint

Options for NSGA2
Categorical variables treated as integer ones
Options for SEGO-KPLS
$n_{var,relaxed} = 14 \rightarrow h = 2$

Convergence plots for the augmented categorical Branin test case



Boxplots for the 20 optimization results after 50 iterations



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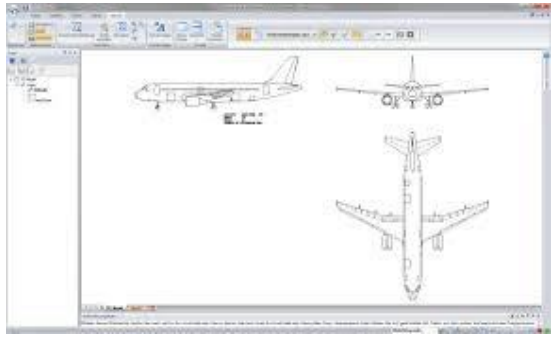
Optimization problem
Short range reference Aircraft CeRAS A320

Future Aircraft Sizing Tool-Overall Aircraft Design
https://github.com/fast-aircraft-design/FAST-OAD

Design variables	Nature	Range
Number of engines	discrete	{1,2,3,4}
Engine position	cat	Under wing/rear fuselage
Horizontal tail	cat	Attached fuselage / vertical tail
Mean average chord at 25%	cont	[16.,18.] (m)
Wing Aspect Ratio	cont	[3.,20.]
VT Aspect Ratio	cont	[3.,20.]
HT Aspect Ratio	cont	[1.5, 50.]
Wing taper ratio	cont	[0.,1.]
Angle for swept wing	cont	[20., 48] (°)
Cruise altitude	cont	[5000., 38000.] (feet)



$n_{var} = 10$

Variable types: continuous (7), integer (1) and categorical (2 with 2 levels). each. $n_{var,relaxed} = 14$

S. Delbecq, C. David, S. Defoort , P. Schmollgruber, and E. Benard, V. Pommier-Budinger. “ ”. In: 10th EASN Virtual International Conference on Innovation in Aviation & Space to the Satisfaction of the European Citizens (2020).

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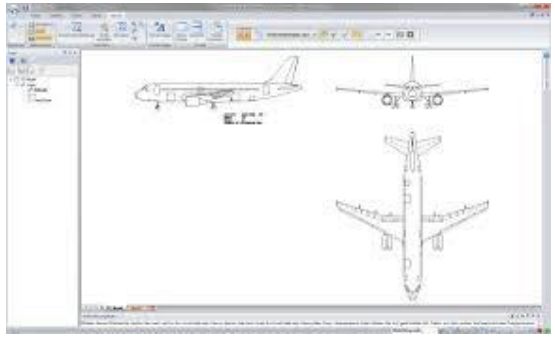

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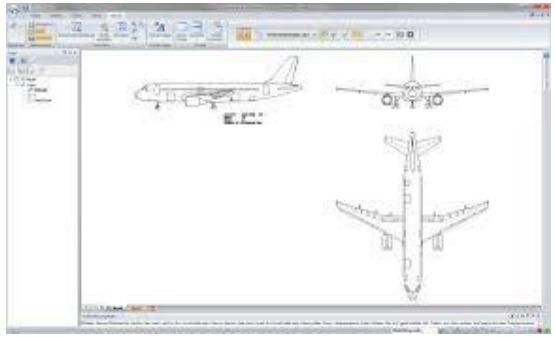

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Variable types: continuous (7), integer (1) and categorical (2 with 2 levels). each. $n_{var,relaxed} = 14$

	Name	Lower	Value	Upper	Unit	Description
1	data:handling_qualities:static_margin	0.05	0.04999981508569307	0.1		(X-position of neutral point - X-position of center of gravity) / (mean aerodynamic chord)

	Name	Value	Unit	Description
2	data:mission:sizing:fuel	20564.57070885031	kg	consumed fuel mass during whole mission

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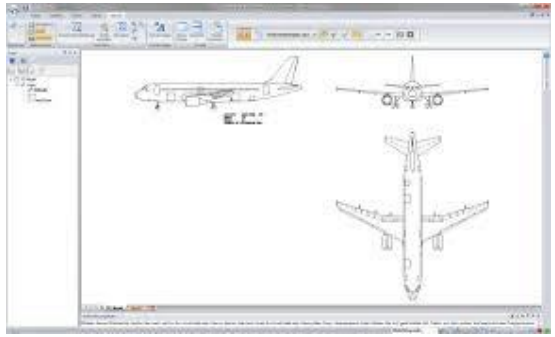

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- 2 inequality constraints
- Fuel-Mission

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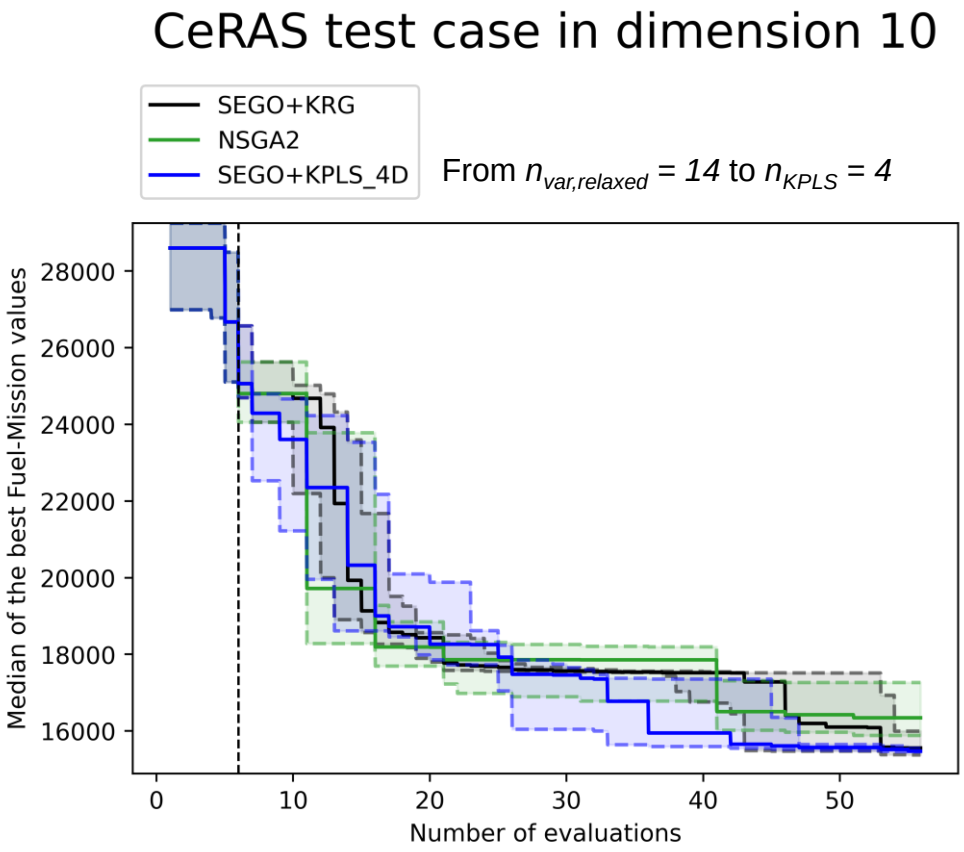
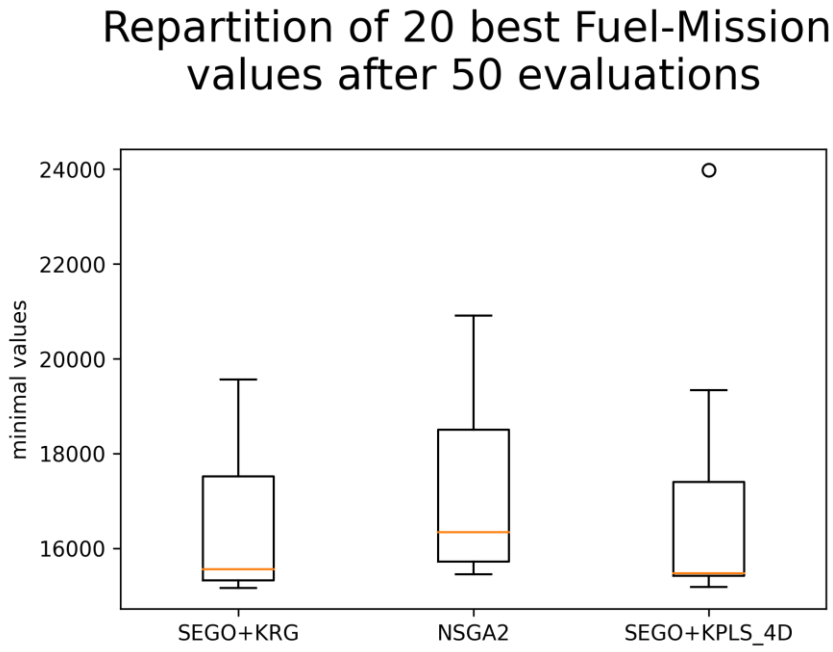
CeRAS A 320 Optimization results





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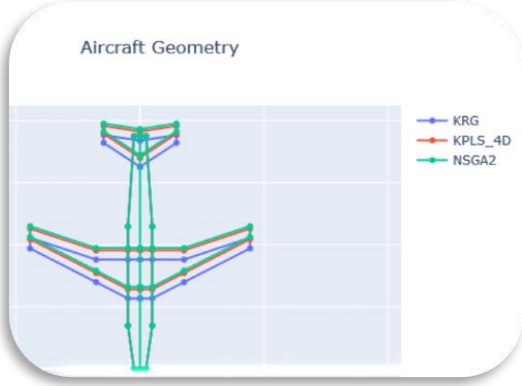

Perspectives

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➔ Confirm the potential of continuous relaxation over mixed integer Gaussian kernels for high-dimensional black-box problems.

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➔ Investigate other mixed optimization heuristics (SO-MI, Bi-level, CAT-EGO,…) for high-dimensional optimization.

J. Mueller, C. Shoemaker, and R. Piché. “SO-MI: A surrogate model algorithm for computationally expensive nonlinear mixed-integer black-box global optimization problems". Computers and Operations Research 40 (2013), pages 1383-1400.

PJ. Barjhoux, Y. Diouane, S. Grihon, D. Bettebghor, J. Morlier. “A bi-level methodology for solving large-scale mixed categorical structural optimization”. Struct Multidisc Optim 62 (2020), pages 337–351 .

M. Muniga, and D. Sinoquet. “Global optimization for mixed categorical-continuous variables based on Gaussian process models with a randomized categorical space exploration step”. Information Systems and Operational Research, vol. 58 (2020), pages 1–32.

The End

Thank you for your attention !

ISAE Institut Supérieur de l'Aéronautique et de l'Espace SUPAERO

RÉPUBLIQUE FRANÇAISE
Liberté
Égalité
Fraternité

ONERA
THE FRENCH AEROSPACE LAB