Enhanced Kriging Models within a Bayesian Optimization Framework, to Handle both continuous and Categorical Inputs

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5 PUBLICATIONS 0 CITATIONS

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38 PUBLICATIONS 149 CITATIONS

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38 PUBLICATIONS 284 CITATIONS

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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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.

Context

New aircraft configurations = Unknown behaviors

➔ built as a **black box** (derivative-free & expensive-to-evaluate)

Bayesian optimization (efficient global optimization) can solve efficiently an expensive black box problem.

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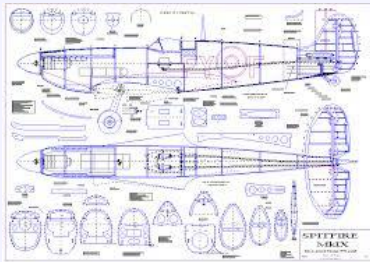

Aircraft design developments required:

- a large number of design variables

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- mixed integer variables

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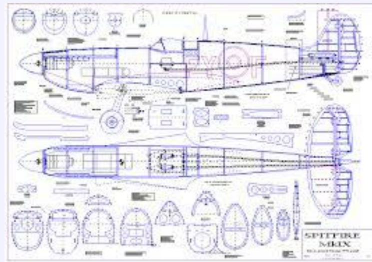
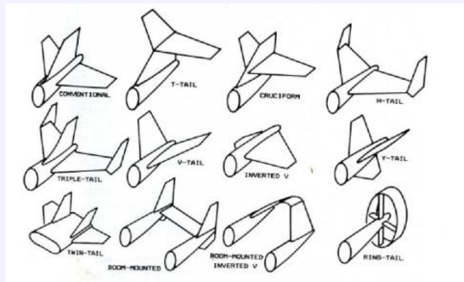


Discrete variables



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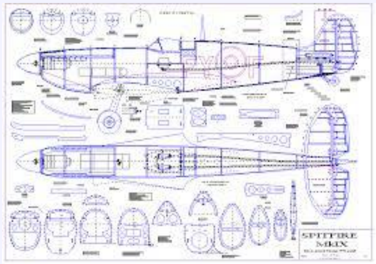

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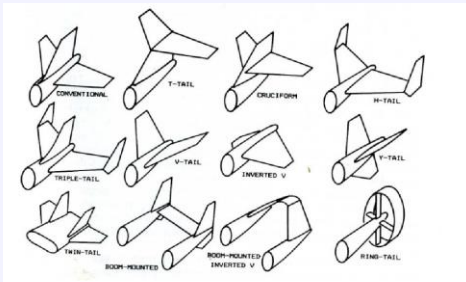
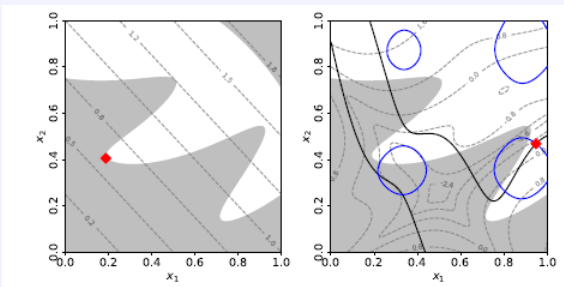


Multimodal constraints



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

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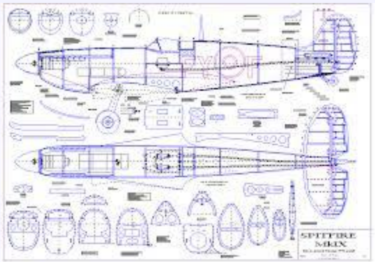

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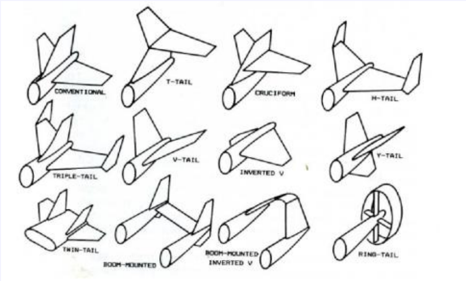

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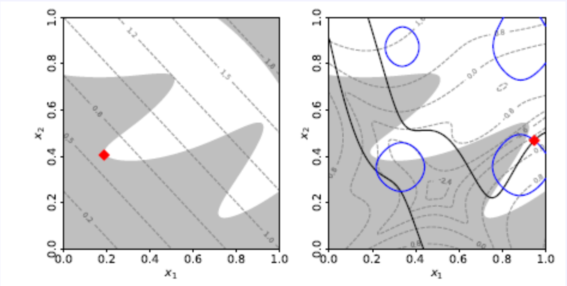

Bayesian optimization applied to aircraft design

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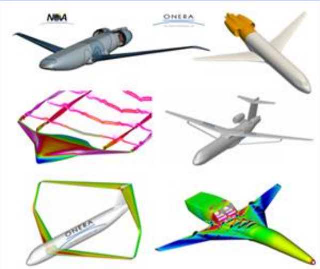
New concepts



Ω

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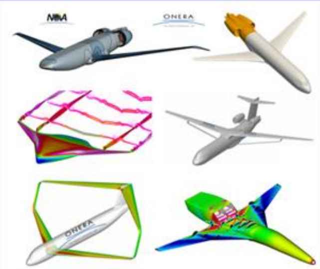

Ω

Analyze

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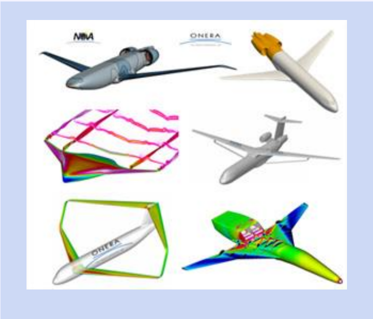
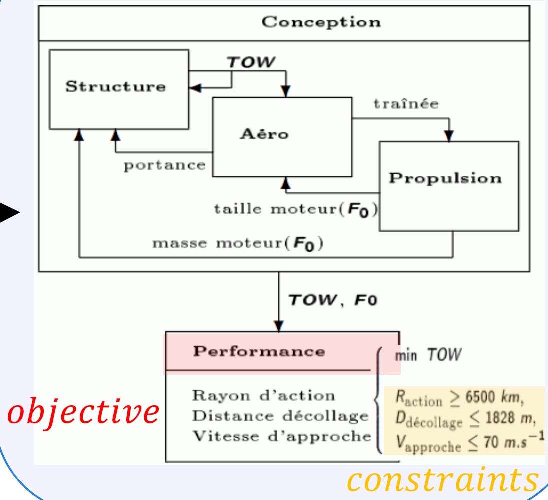


Ω

Analyze

Multidisciplinary Design Analysis



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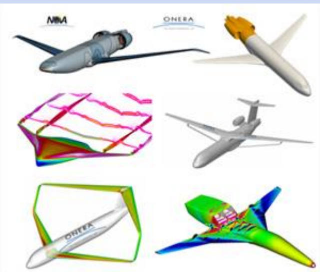

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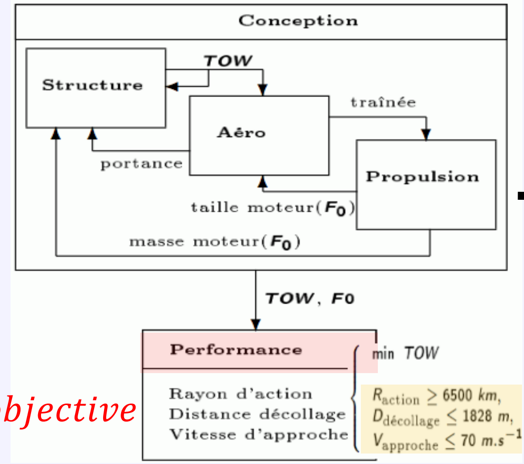

objective

constraints

Improvements

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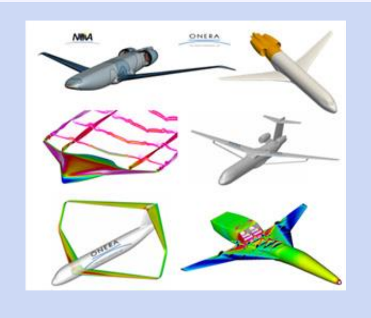
New concepts



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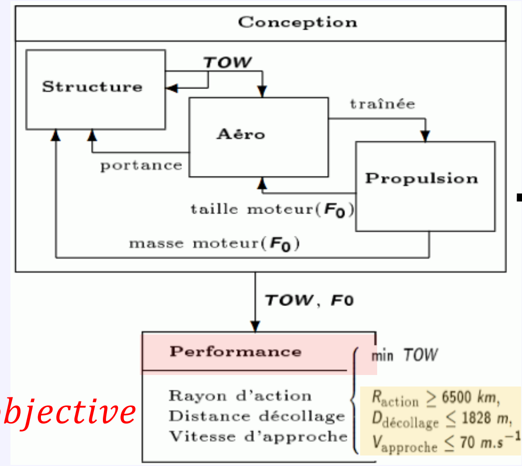

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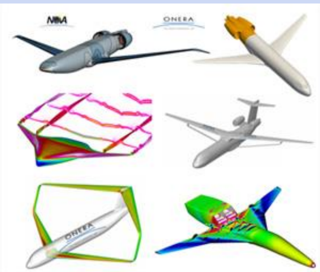
Global optimization

MDF Formulation

$$\min_{\text{inputs} \in \Omega} \ \text{objective}(\text{inputs})$$
$$s.t \quad \text{constraints}(\text{inputs})$$

Bayesian optimization applied to aircraft design

New concepts



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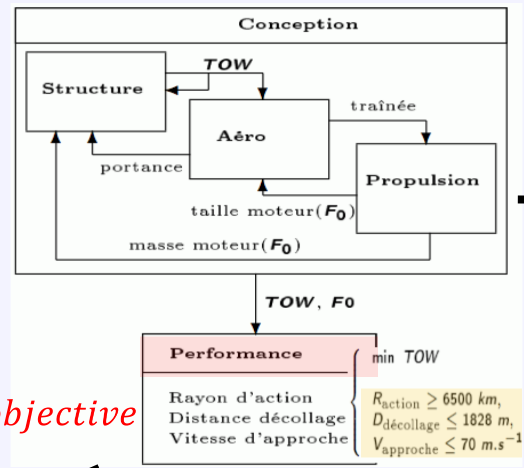

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Expensive computations

Bayesian optimization applied to aircraft design

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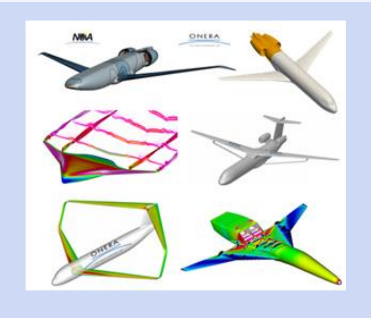

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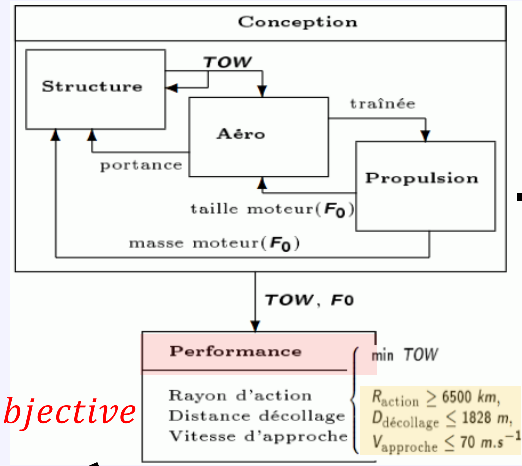

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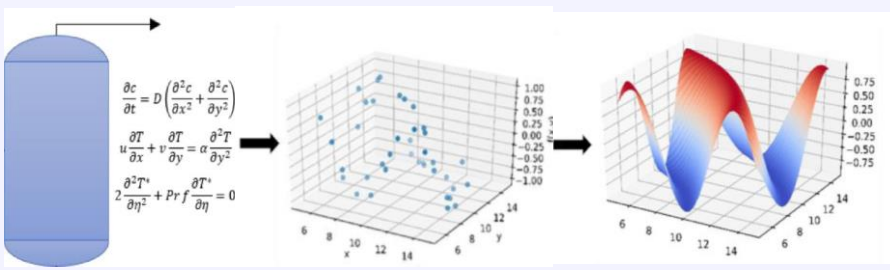
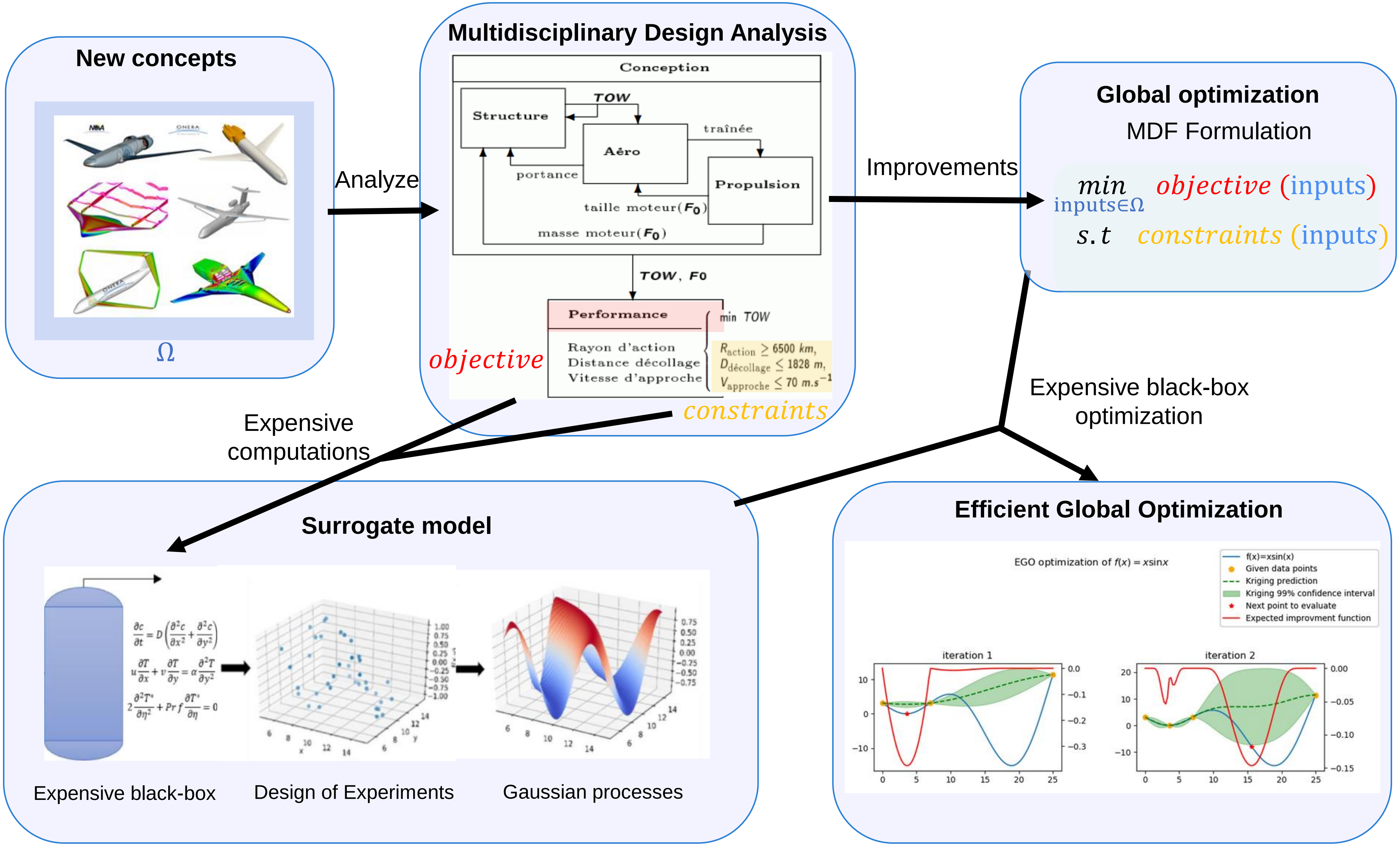
Surrogate model



Expensive black-box   Design of Experiments   Gaussian processes

Bayesian optimization applied to aircraft design



State-of-the-art

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Baseline method ⇨ Super Efficient Global Optimizer (SEGO)

M. J. Sasena, P. Papalambros, P. Goovaerts, “Exploration of Metamodeling Sampling Criteria for Constrained Global Optimization”, Engineering optimization 34 (2002), pages 263-278.

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Constraints ☺
High-Dimension ☺
Mixed integer ☹

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CAT-EGO

Mixed integer kernels coupled with adapted Mesh Adaptive Direct Search

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Bandit-BO

Multi-Armed Bandit for Bayesian Optimization

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Continuous relaxation

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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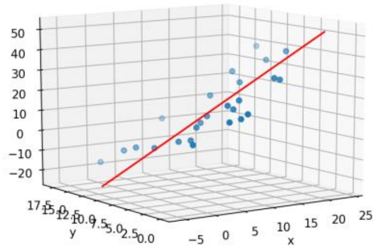
n_{var}

$\downarrow$

$n_{var,relaxed}$

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



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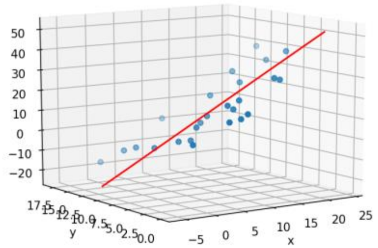

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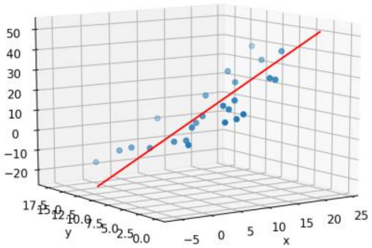

$$\begin{array}{c} n_{var,relaxed} \\ \downarrow \\ h \end{array}$$

iii. Fit the continuous Gaussian process metamodel on h dimensions

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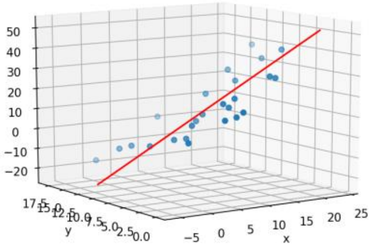

$n_{var,relaxed} \longrightarrow h$

iii. Fit the continuous Gaussian process metamodel on h dimensions

Initial DoE $\begin{cases} x_{DoE} = (x_{s,0}, .., x_{n,0}) \\ y_{DoE} = (y_{s,0}, .., y_{n,0}) \end{cases}$

$y_{pred}(x_{DoE}) = y_s$

$y_{pred}(x) = \hat{y} + \varepsilon(x)$

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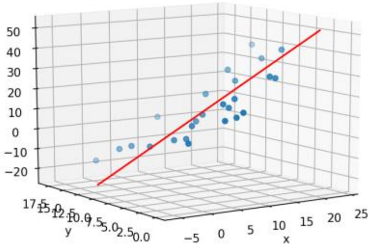


$n_{var,relaxed} \longrightarrow h$

iii. Fit the continuous Gaussian process metamodel on h dimensions

Initial DoE $\begin{cases} x_{DoE} = (x_{s,0}, .., x_{n,0}) \\ y_{DoE} = (y_{s,0}, .., y_{n,0}) \end{cases}$

$y_{pred}(x_{DoE}) = y_s$

$y_{pred}(x) = \hat{y} + \varepsilon(x)$ $\longrightarrow$ $\begin{cases} \varepsilon(x) \sim N(0, \sigma^2) \\ Corr(\varepsilon(x), \varepsilon(x')) = k(x^i - x^j, \Theta) \end{cases}$

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.

C. E. Rasmussen, and J. Quiñonero-Candela, "A Unifying View of Sparse Approximate Gaussian Process Regression". Journal of Machine Learning Research, vol. 6 (2005), pages 1939–1959.

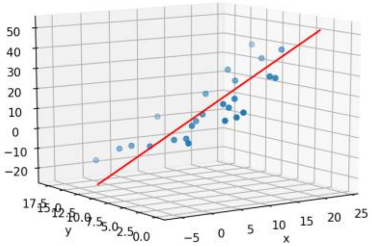
Proposed approach: the surrogate model (1/2)

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 $[0,1]$

$n_{var} \longrightarrow n_{var,relaxed}$

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



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$y_{pred}(x) = \hat{y} + \varepsilon(x) \longrightarrow \begin{cases} \varepsilon(x) \sim N(0, \sigma^2) \\ Corr(\varepsilon(x), \varepsilon(x')) = k(x^i - x^j, \Theta) \end{cases}$

The hyperparameters of the model are fit to data by maximum likelihood estimation.

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|relax continuously within the bounds

$\boldsymbol{if}$ $categorical$

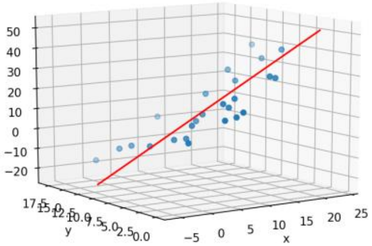
|Add a dimension by level with bounds $[0,1]$

n_{var}

$\downarrow$

$n_{var,relaxed}$

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



$n_{var,relaxed}$

$\downarrow$

h

iii. Fit the continuous Gaussian process metamodel on h dimensions

Initial DoE $\begin{cases} x_{DoE} = (x_{s,0}, .., x_{n,0}) \\ y_{DoE} = (y_{s,0}, .., y_{n,0}) \end{cases}$

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The hyperparameters of the model are fit to data by maximum likelihood estimation.

iv. Project back to respect the type of the variables

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C. E. Rasmussen, and J. Quiñonero-Candela, "A Unifying View of Sparse Approximate Gaussian Process Regression". Journal of Machine Learning Research, vol. 6 (2005), pages 1939–1959.

RÉPUBLIQUE FRANÇAISE

THE FRENCH AEROSPACE LAB

Proposed approach: the surrogate model (2/2)

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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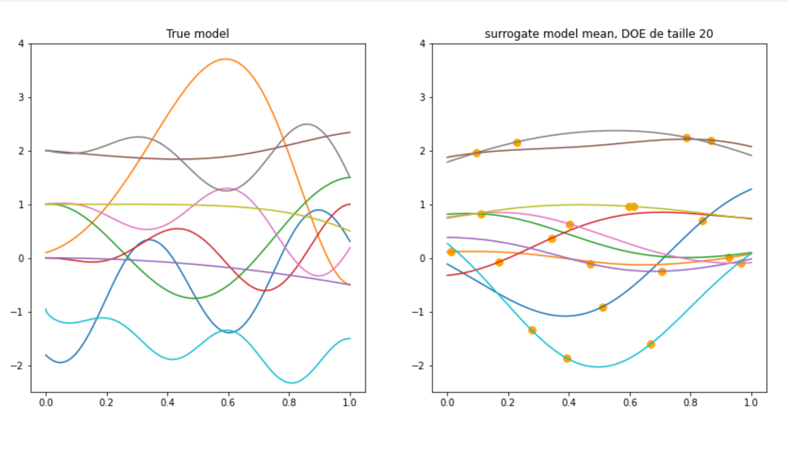
Proposed approach: the surrogate model (2/2)

Validation problem $n_{var} = 2$

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



Toy case

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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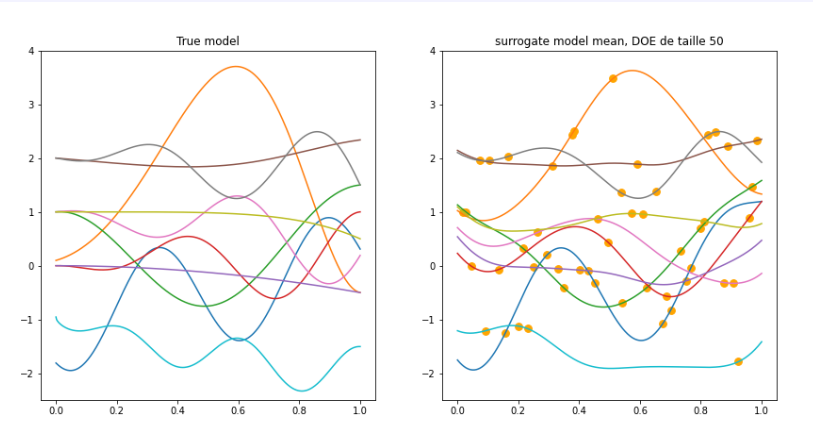

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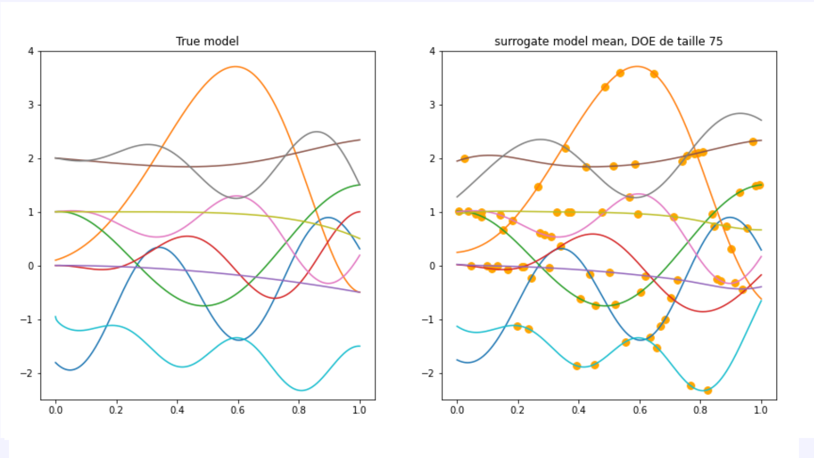

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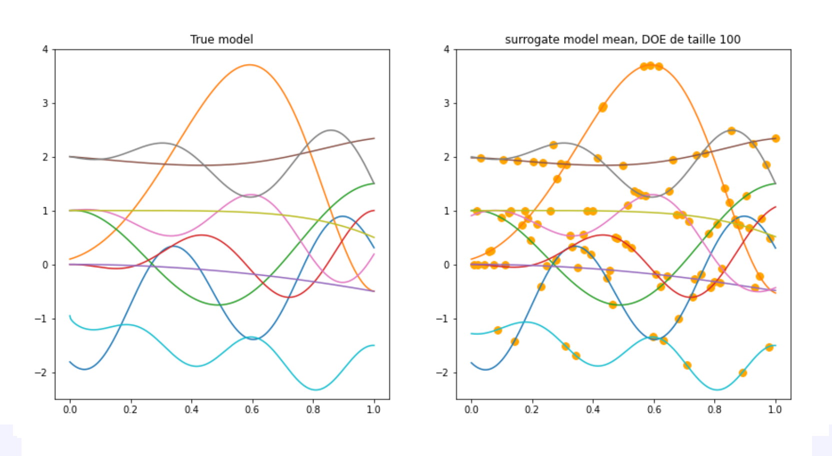

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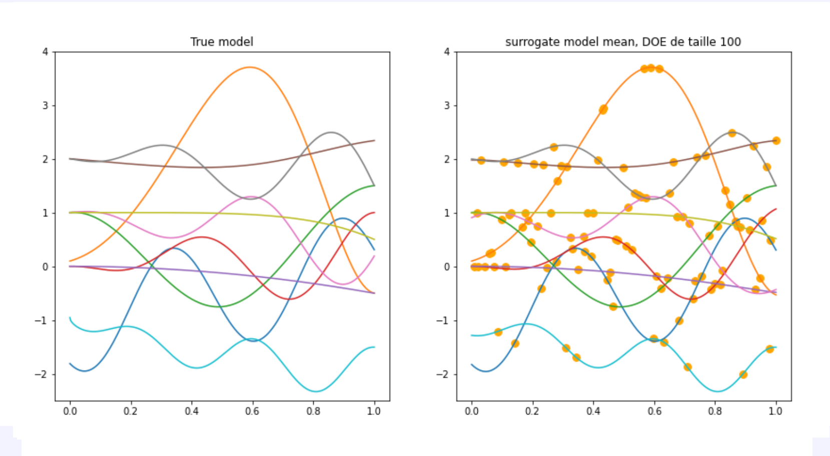
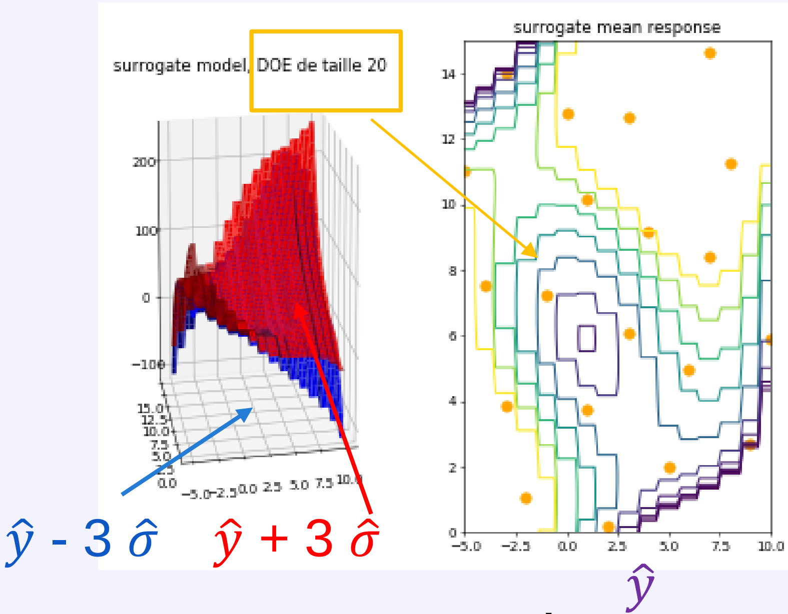


Toy case

Validation problem $n_{var} = 2$

- Variable types: continuous and integer



Integer Branin

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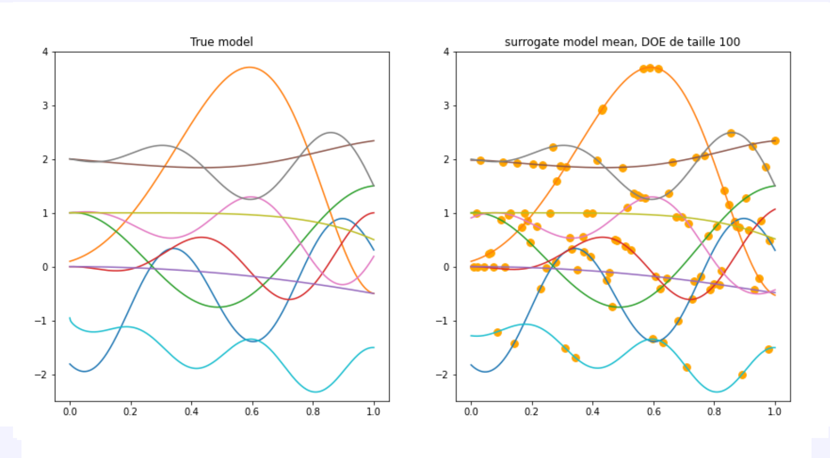

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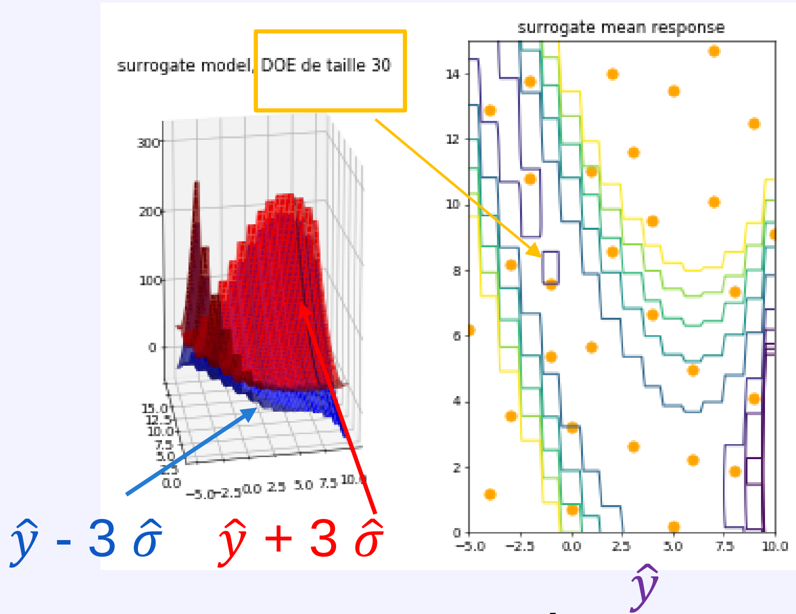

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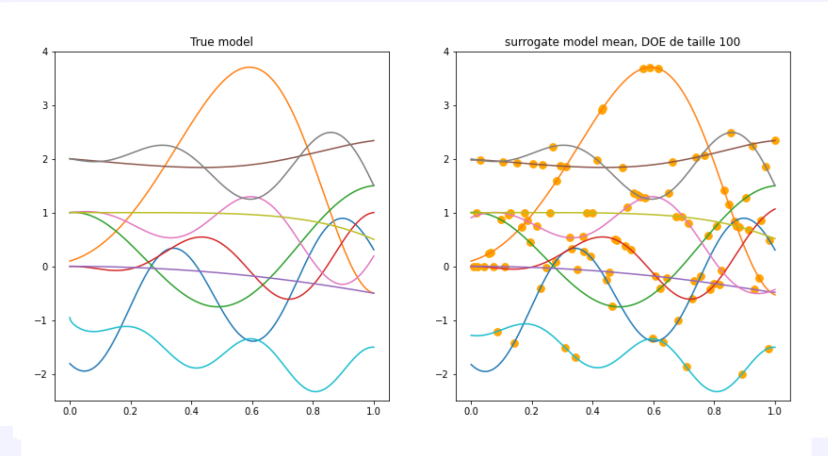

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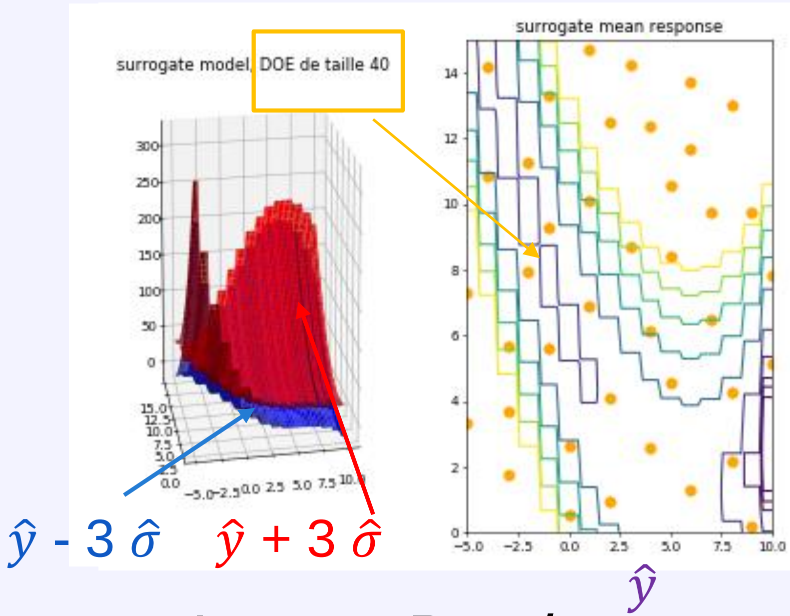

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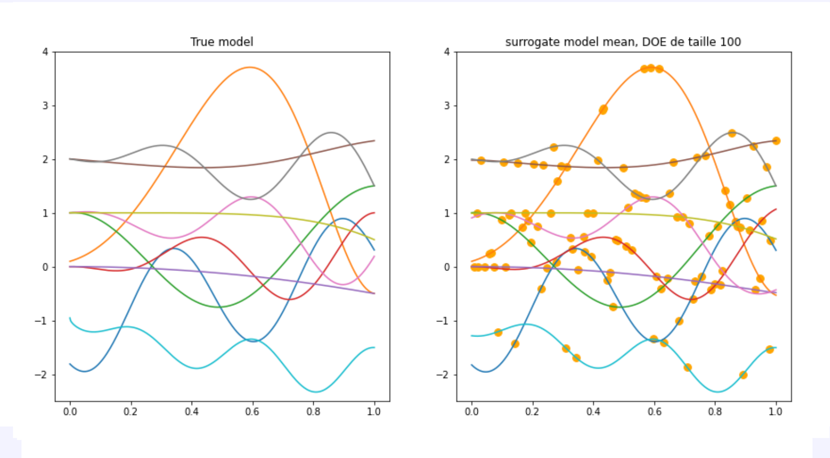

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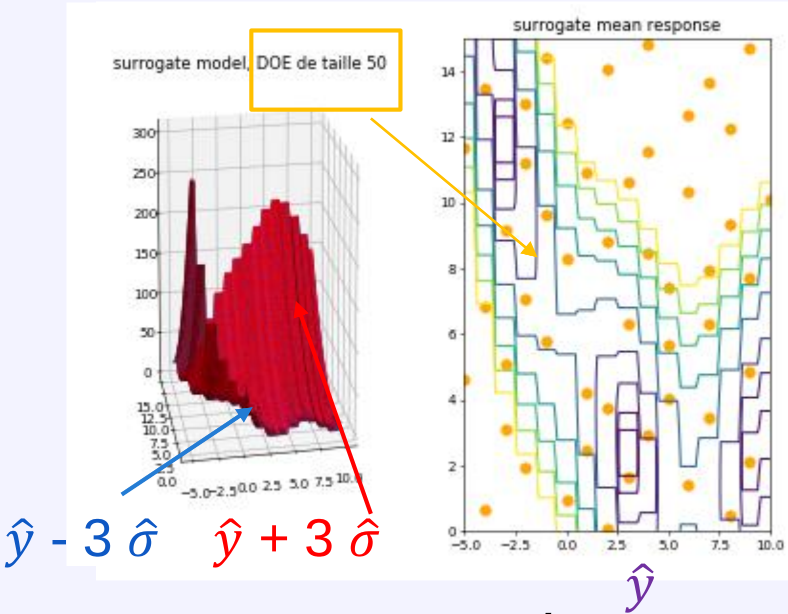

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Proposed approach: The optimization process

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

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

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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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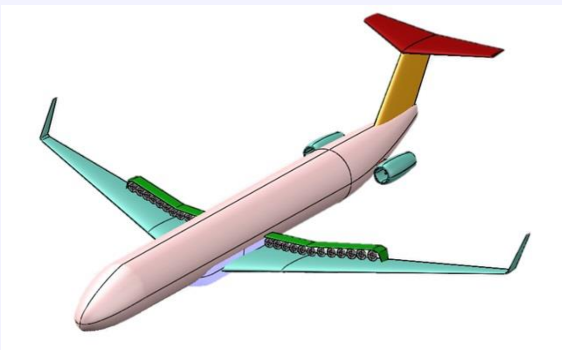
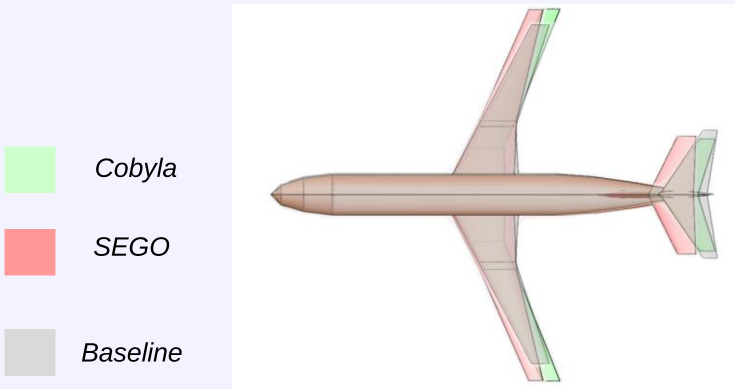
Hybrid aircraft concept with distributed propulsion



Validation problem *n_{var} = 12*

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



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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).
P. E. Gill, W. Murray, and M. A. Saunders. “SNOPT: An SQP Algorithm for Large-Scale Constrained Optimization”. SIAM Review 47.1 (2005), pages 99–131.

Optimization problems and options

Optimizers

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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

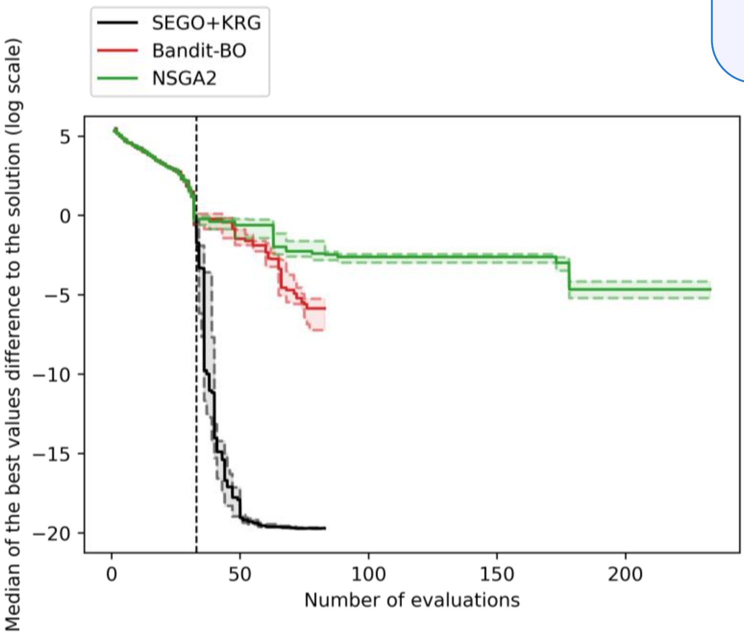
Unconstrained Bayesian optimization (1/2)

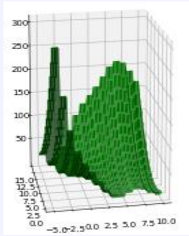
Validation problem $n_{var} = 2$

- Variable types: integer (1) and continuous (1).

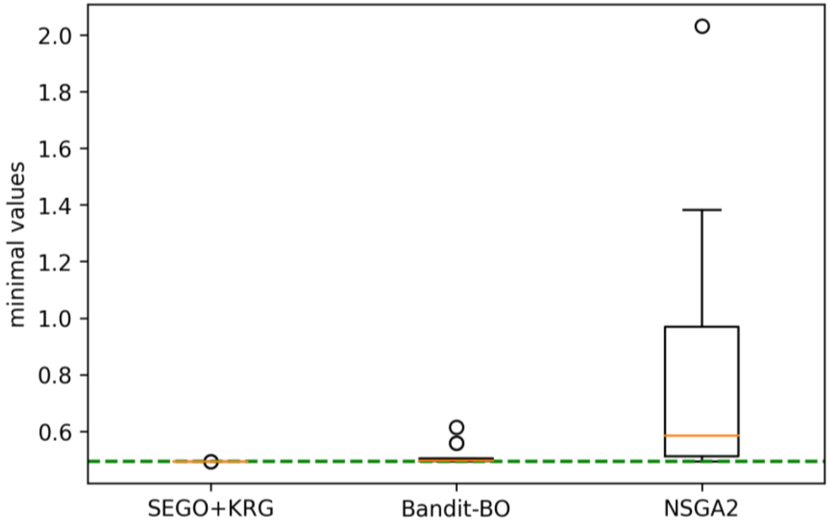
Options for Bandit-BO
16 arms, minimal DoE of 32 points

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.

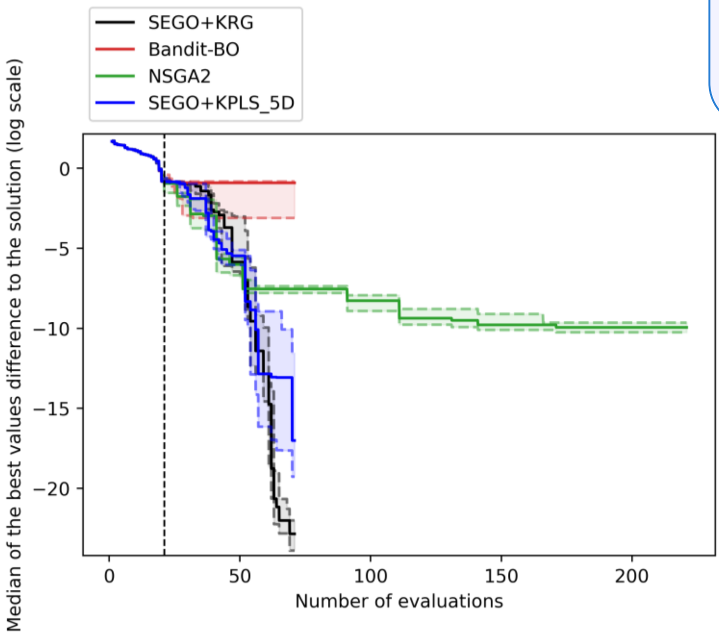
Unconstrained Bayesian optimization (2/2)

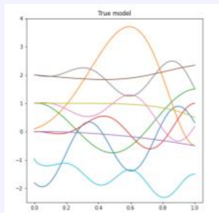
Validation problem $n_{var} = 2$

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

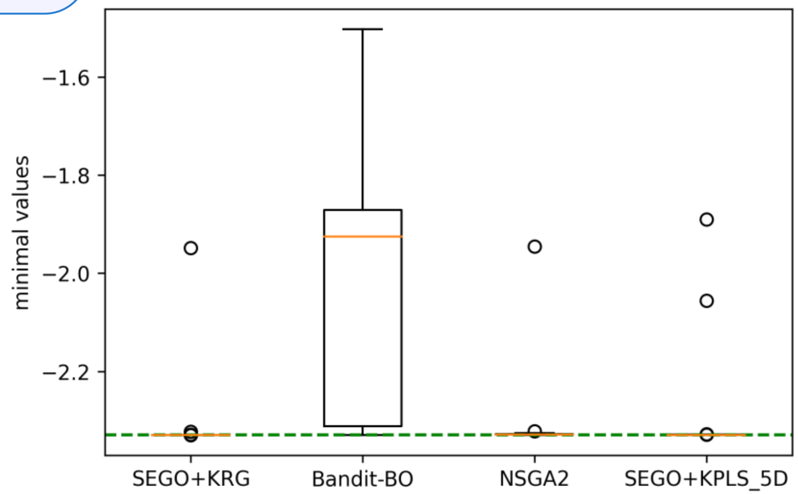
Options for Bandit-BO
10 arms, minimal DoE of 20 points
Options for NSGA2
Categorical variable treated as integer
Options for SEGO-KPLS
$n_{var,relaxed} = 11 \rightarrow h = 5$

Convergence plots for the Toy test case





Boxplots for the 20 optimization results after 50 iterations



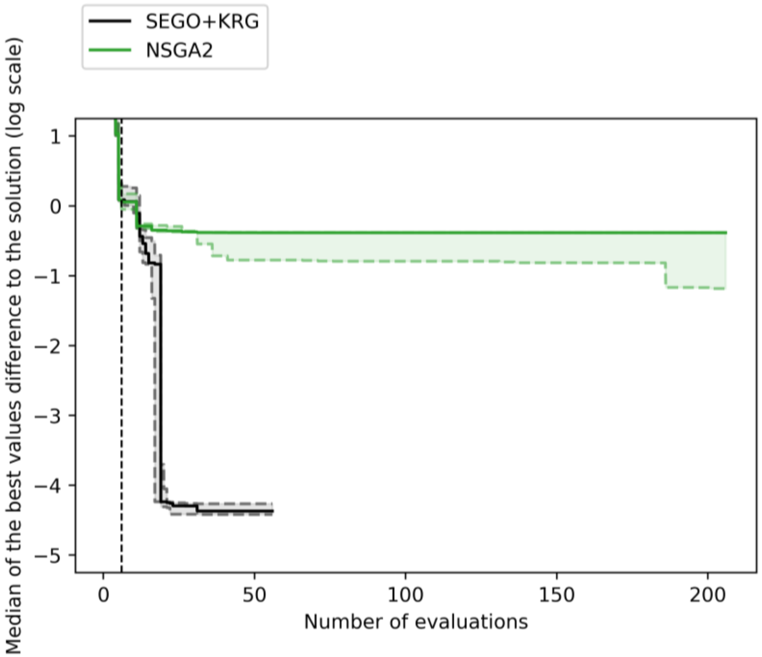
M. M. Zuniga, and D. Sinoquet. "Global optimization for mixed categorical-continuous variables based on Gaussian process models with a randomized categorical space exploration step". Information Systems and Operational Research, vol. 58 (2020), pages 1–32.

Constrained Bayesian optimization (1/2)

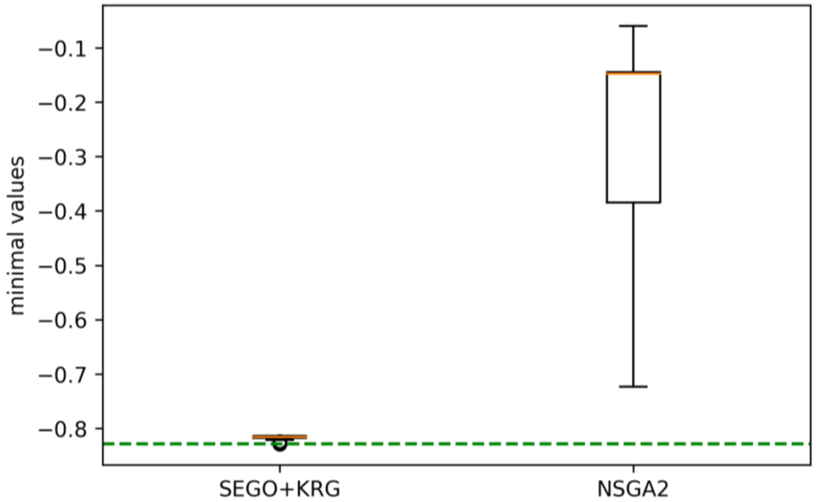
Validation problem $n_{var} = 4$
Variable types: continuous (2) and categorical (2 with 2 levels). $n_{var,relaxed} = 6$
- 1 constraint

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

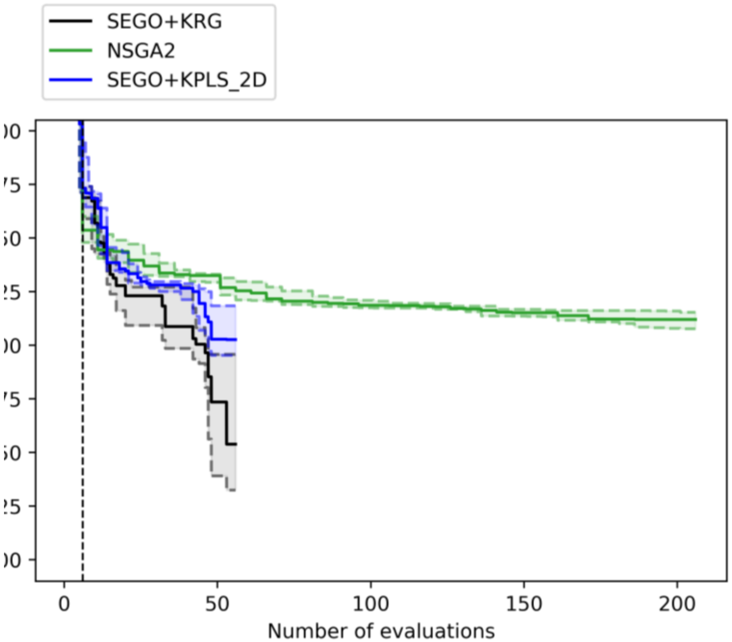
Constrained Bayesian optimization (2/2)

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

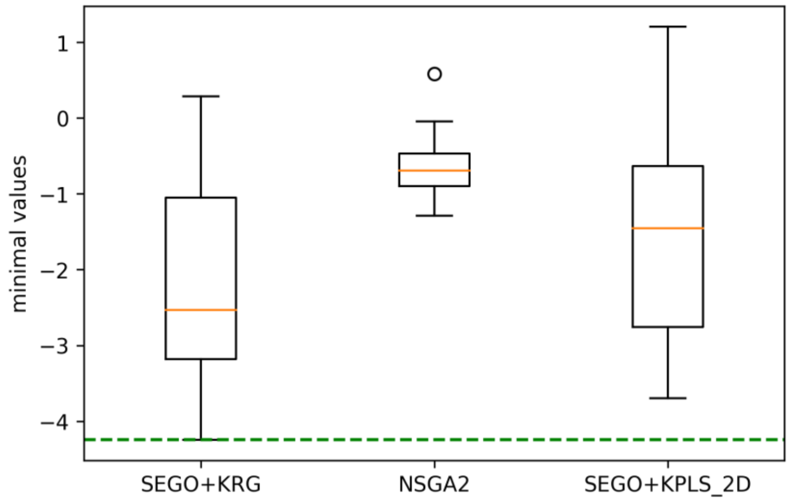
- 1 constraint

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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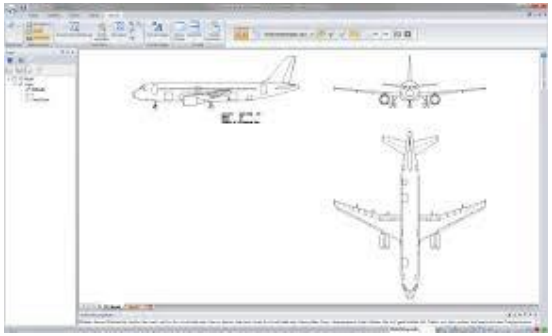
Optimization problem
Short range reference Aircraft CeRAS A320

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).

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.]
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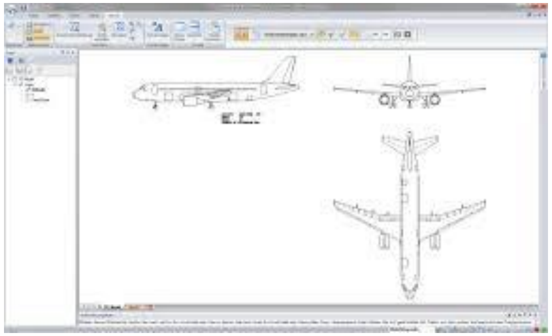

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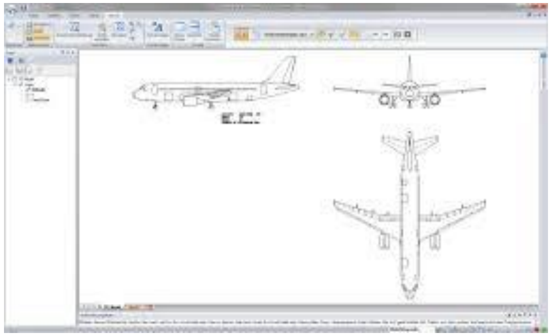

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Variable types: continuous (7), integer (1) and categorical (2 with 2 levels). each. $n_{var,relaxed} = 14$

	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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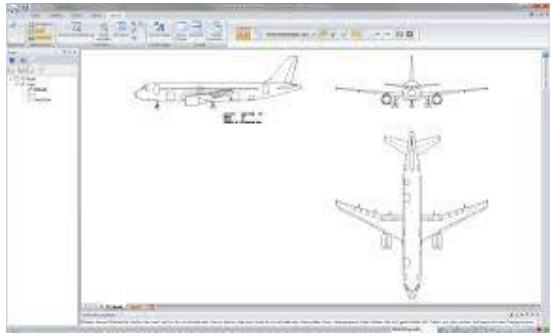

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- 2 inequality constraints
- Fuel-Mission

	Name	Lower	Value	Upper	Unit	Description
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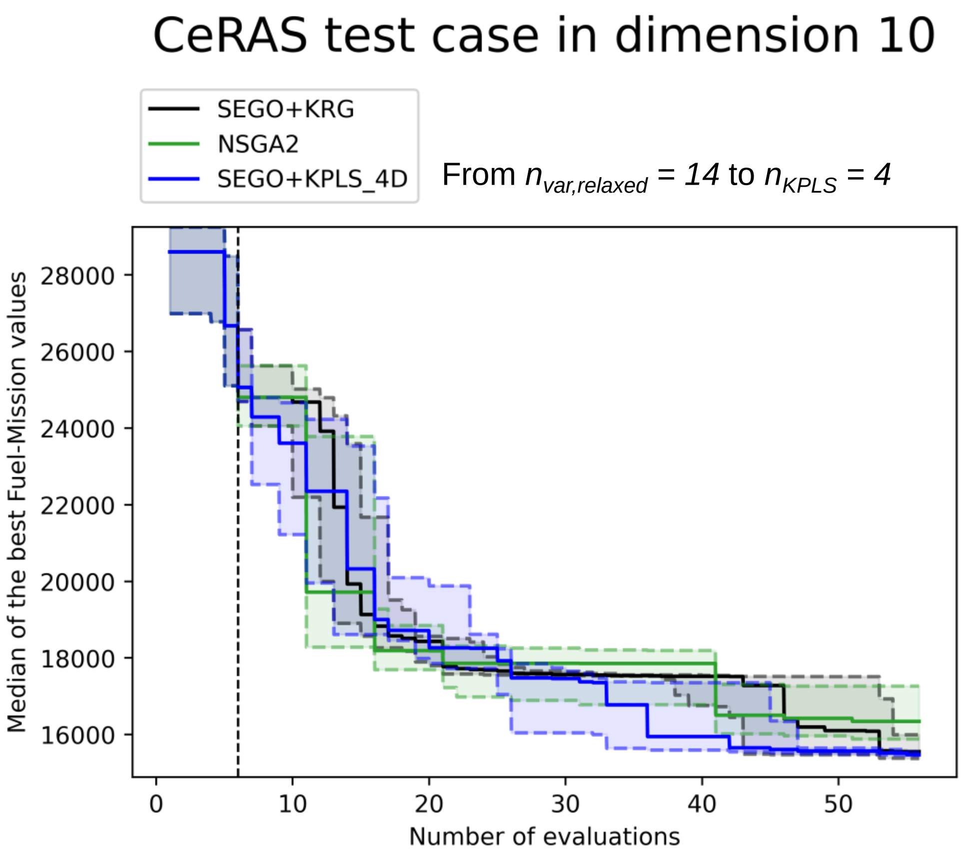
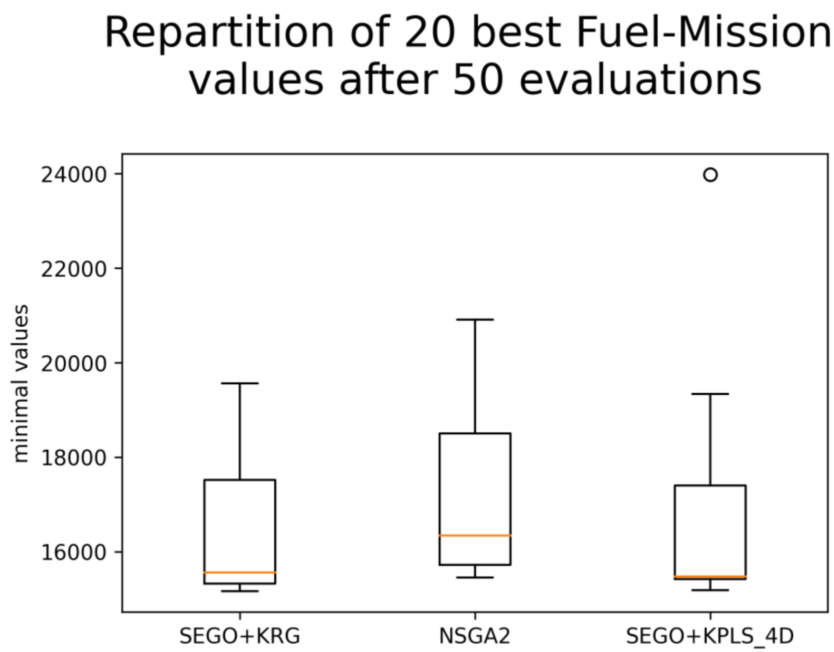
CeRAS A 320 Optimization results



From $n_{var,relaxed} = 14$ to $n_{KPLS} = 4$



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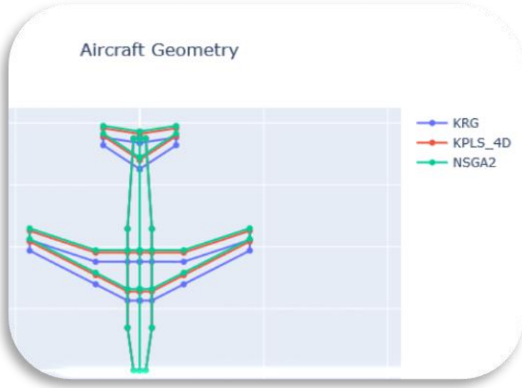

Perspectives

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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 !

Institut Supérieur de l'Aéronautique et de l'Espace
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