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Bayesian optimization applied to constrained black-box problems for different aeronautical applications

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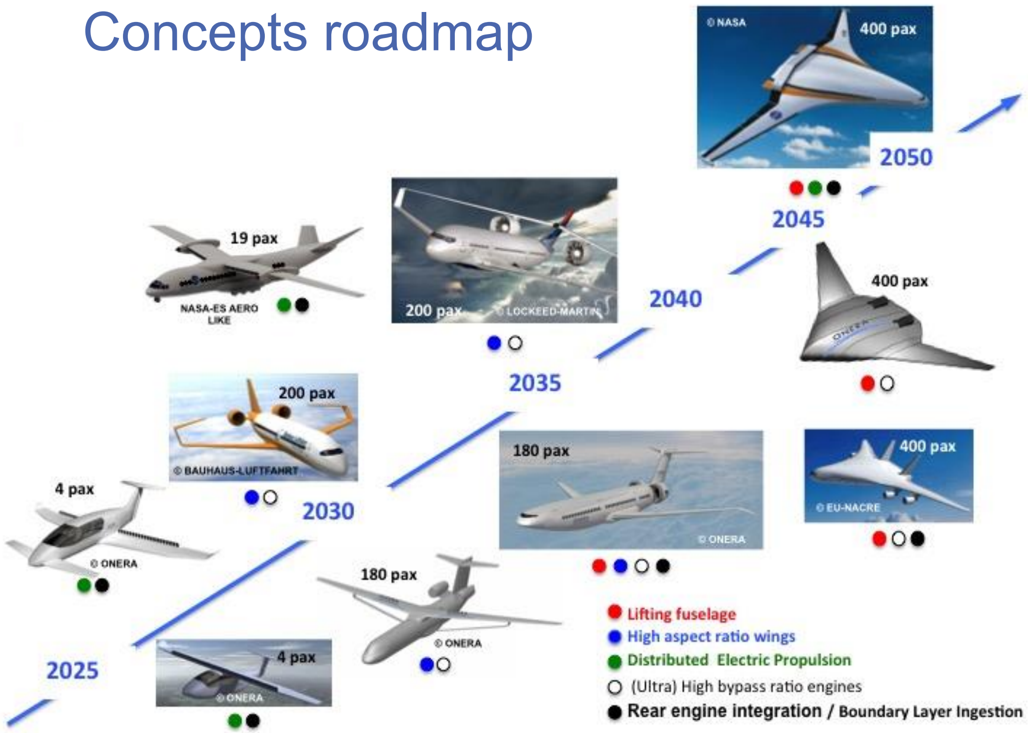
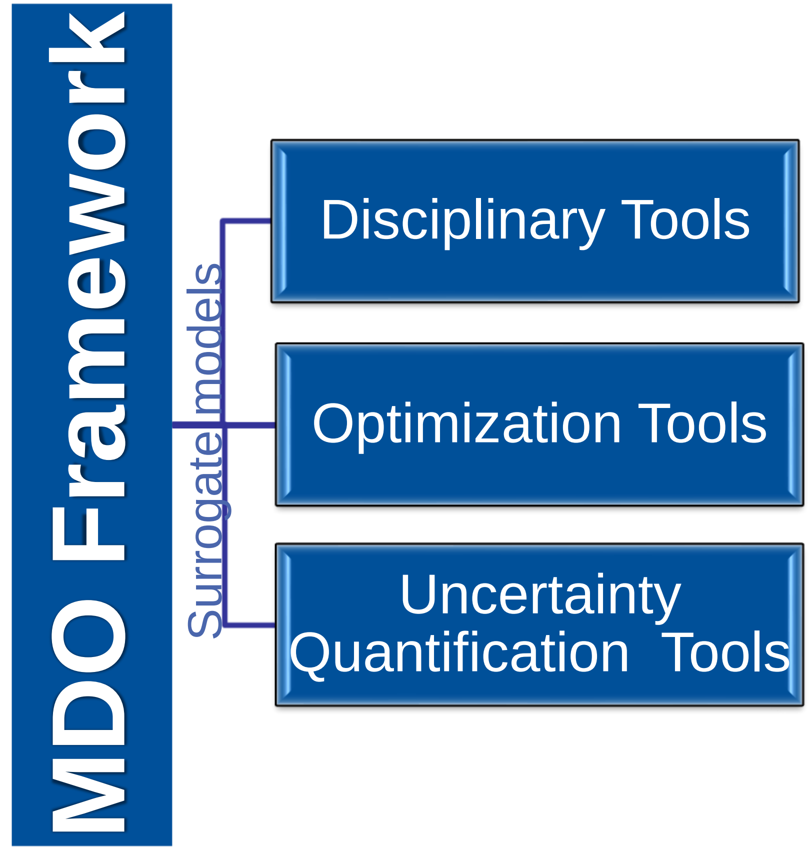
Isae
Institut Supérieur de l'Aéronautique et de l'Espace
SUPAERO
ICA

ANR GAP 2025

Tools to design the new aircraft configurations

Concepts roadmap

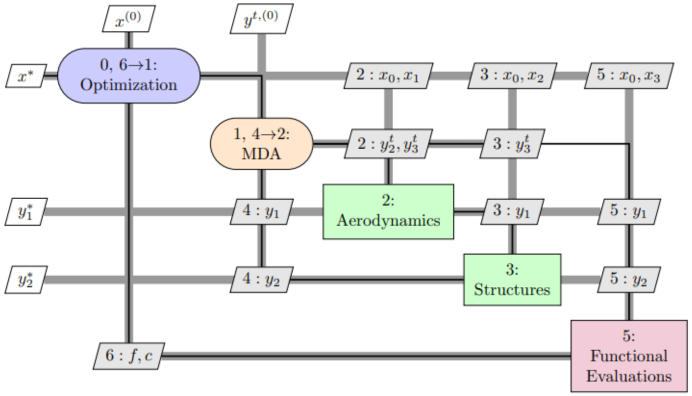




➔ Take into account more information earlier in the design process

➔ Keep a design space as large as possible

Different strategies to solve Multidisciplinary Design Analysis and Optimization

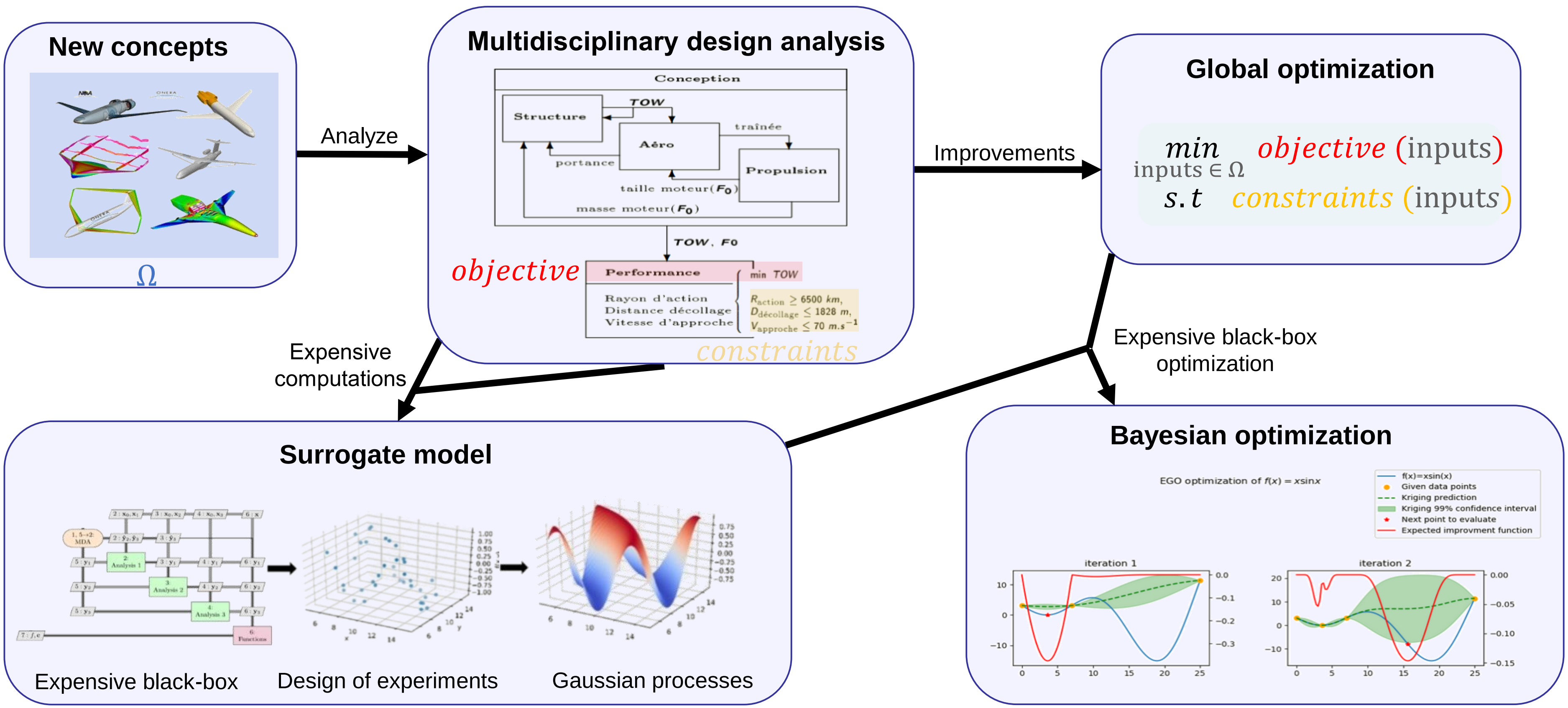


- **Coupled disciplines** (Multidisciplinary Design Analysis)
  ➔Overall Aircraft Design process for new configurations

- **Multiple quantities of interest** (Objectives and Constraints)

- **Mixed Integer variables** (number of batteries, choice of materials, choice of architectures…)

Overview



New concepts
Ω
Analyze
Multidisciplinary design analysis
Conception
Structure
TOW
Aéro
traînée
Propulsion
portance
taille moteur(F_0)
masse moteur(F_0)
TOW, F0
objective
Performance
min TOW
Rayon d'action
Distance décollage
Vitesse d'approche
$R_{action} \geq 6500$ km,
$D_{décollage} \leq 1828$ m,
$V_{approche} \leq 70$ m.s^{-1}
constraints
Improvements
Global optimization
$\min_{\text{inputs} \in \Omega}$ objective (inputs)
s.t constraints (inputs)
Expensive computations
Expensive black-box optimization
Surrogate model
Expensive black-box
Design of experiments
Gaussian processes
Bayesian optimization
EGO optimization of f(x) = xsinx
f(x)=xsin(x)
Given data points
Kriging prediction
Kriging 99% confidence interval
Next point to evaluate
Expected improvment function
iteration 1
iteration 2

Outline

- Kriging based surrogate models
- Bayesian optimization
  - mono & multiobjective
  - extension to multifidelity
- Applications
  - DRAGON: ONERA hybrid electric aircraft
  - AGILE4.0 application: family concept design
  - Drone design

Methodology developments: Surrogate Models

Definition of a metamodel library dedicated to Aircraft design

- Models to handle a large number of design variables
  - ⟶ New Kriging models: KPLS & KPLS-K
- Models to handle heterogeneous function
  - ⟶ Mixture of experts (MOE)
- Models to handle heterogeneous variables
  - ⟶ Kriging based on continuous relaxation
  - ⟶ Dedicated categorical kernels
- Models to handle multi-fidelity data
  - ⟶ Co-Kriging (MFKPLS, MFKPLS-K)
  - ⟶ Co-Kriging with heteroscedastic Noise

open source python toolbox for surrogate models

SMT: Surrogate Modeling Toolbox

github.com/SMTorg/smt

➔ **Surrogate models with some focus on derivatives**

➔ **Included some Jupyter notebooks**

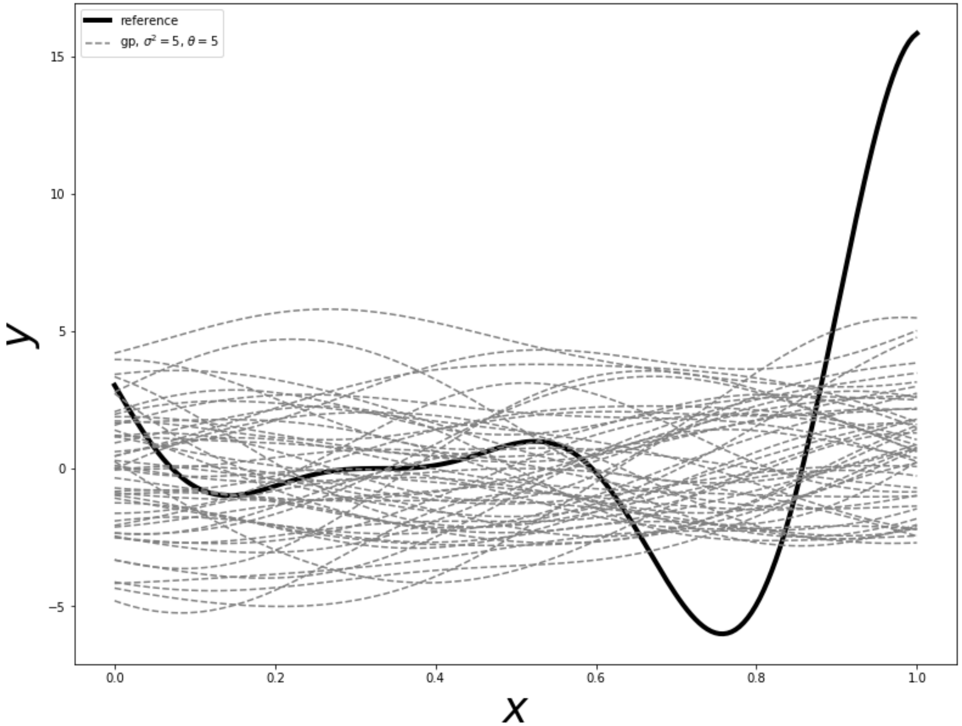
SMT 2.9.3 features (July 2025):

- Models to handle a large number of design variables (KPLS – KPLSK – MGP)
- **Mixture of experts** to handle heterogeneous functions (MOE)
- Different covariance kernels added
- **Multi-fidelity models** (MFK – MFKPLS – MFKPLSK)
- Noisy kriging to handle uncertainties on data
- Kriging models for **mixed variables** (continuous, discrete, categorical) & associated kernels
- Kriging models for hierarchical variables (meta, neutral, decreed) & associated kernels
- Sparse GP models to handle large database & multi-fidelity
- **Bayesian optimization** (EGO without constraint) for continuous and mixed variables

Bouhlel, M. A., Hwang, J. T., Bartoli, N., Lafage, R., Morlier, J., & Martins, J. R. (2019). A Python surrogate modeling framework with derivatives. Advances in Engineering Software, 135, 102662.
Saves, P., Lafage, R., Bartoli, N., Diouane, Y., Bussemaker, J., Lefebvre, T., Hwang J. & Martins, J. R. (2024). SMT 2.0: A Surrogate Modeling Toolbox with a focus on hierarchical and mixed variables Gaussian processes. Advances in Engineering Software, 188, 103571.

Gaussian process or Kriging model

$x \in \mathbb{R}^d$
$y(x) \in \mathbb{R}$



Gaussian process characterized by:

- its mean (or trend)
  $\mu(x) \in \mathbb{R}$
- its covariance Kernel
  $\mathrm{k}(x, x') \in \mathbb{R}$

$$k(x,x') = \sigma^2 \exp\left(-\sum_{i=1}^{d} \theta_i |x_i - x_i'|^2\right)$$

Krige D. G. A statistical approach to some basic mine valuation problems on the witwatersrand. Journal of the Southern African Institute of Mining and Metallurgy, 52(6):119–139, 1951
Rasmussen C. E. and Williams C. K. . Gaussian processes for machine learning. volume 1. MIT press Cambridge. 2006.

Gaussian process or Kriging model

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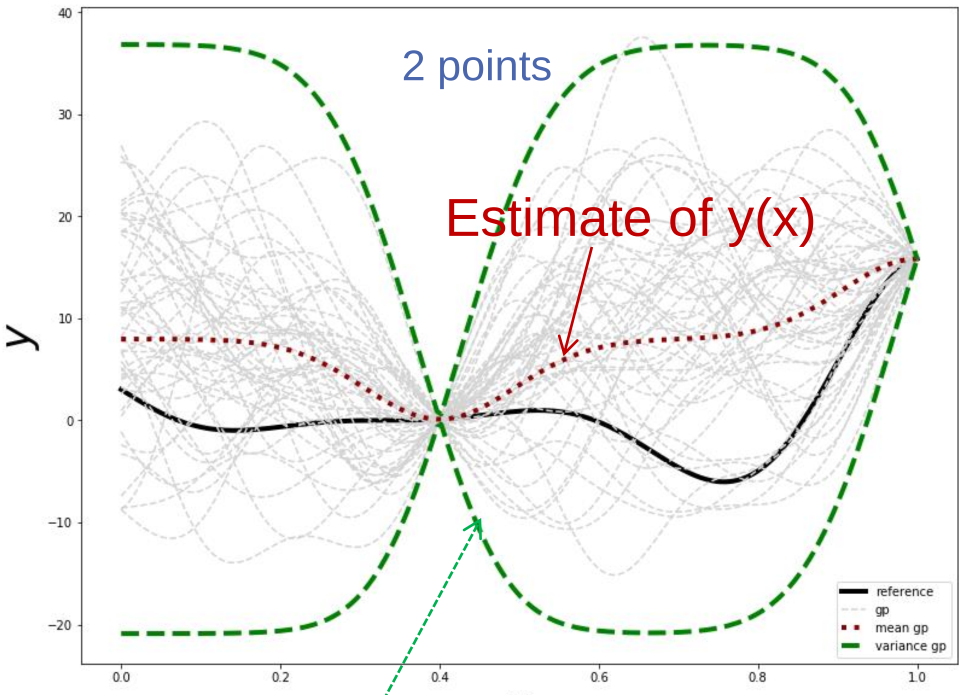

Quantification of the uncertainties in these estimates

Gaussian process characterized by:

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- its covariance Kernel

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+ information provided by data

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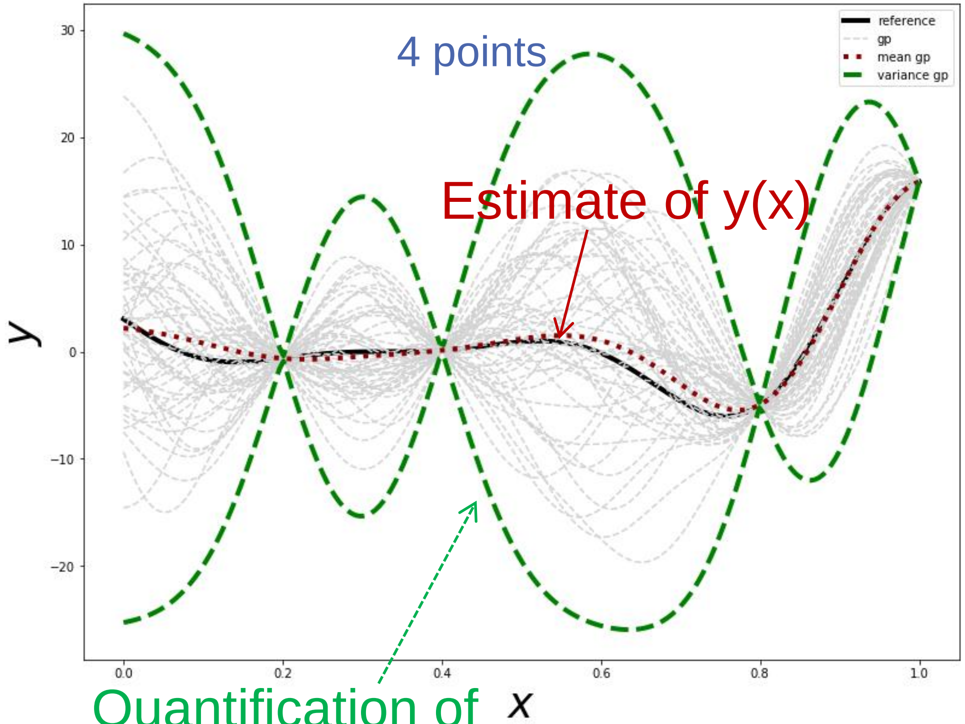

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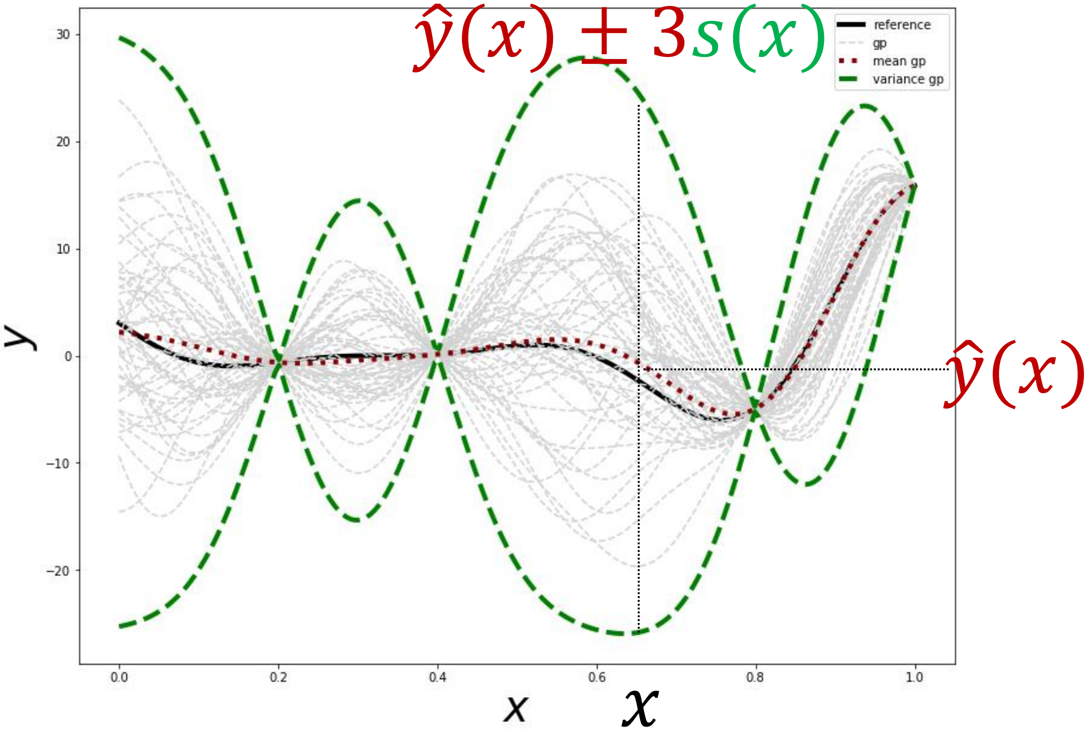

99% confidence interval

$$f(x) \Rightarrow Y(x) = N(\hat{y}(x), s^2(x))$$

DOE (LHS)

↓

Estimation of hyperparameters θ_i (i=1,…,*d*) by MLE

d parameters θ_i to evaluate

$$k(x, x') = \sigma^2 \exp\left(-\sum_{i=1}^{d} \theta_i |x_i - x_i'|^2\right)$$

↓

Covariance matrix

↓

Prediction $\hat{y}$ and variance s^2 estimations at a new point

Krige D. G. A statistical approach to some basic mine valuation problems on the witwatersrand. Journal of the Southern African Institute of Mining and Metallurgy, 52(6):119–139, 1951
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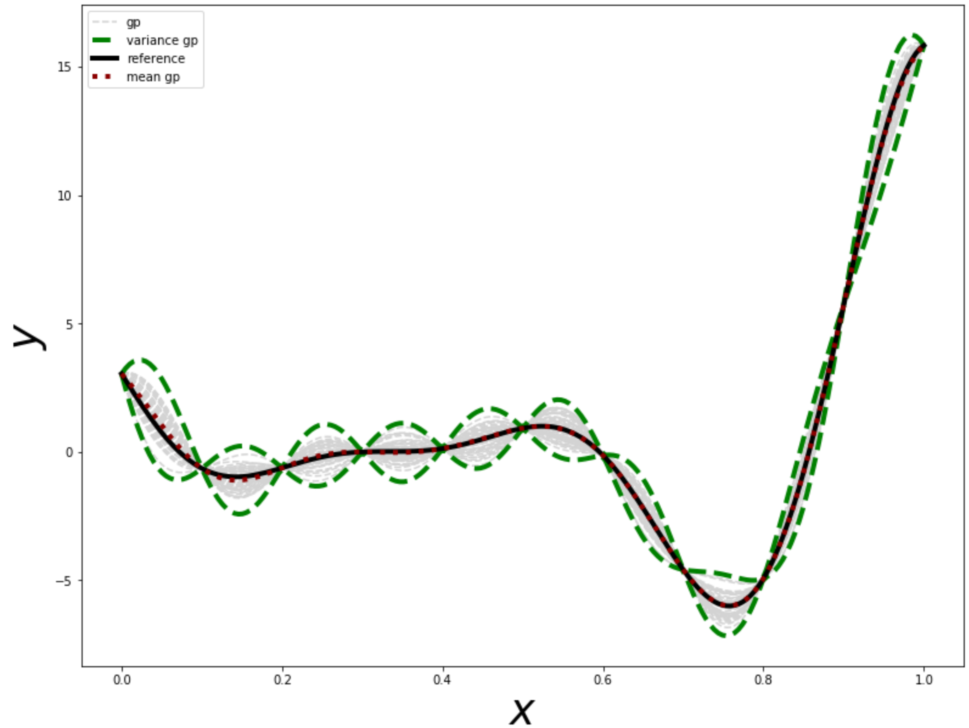
Gaussian process or Kriging model



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$y(x) \in \mathbb{R}$

DOE (LHS)

↓

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↓

Covariance matrix

↓

Prediction $\hat{y}$ and variance s^2 estimations at a new point

- ➔ Hyperparameters tuning
- ➔ Number of hyperparameters increases with the dimension *d* (number of design variables)
- ➔ Curse of dimensionality

Krige D. G. A statistical approach to some basic mine valuation problems on the witwatersrand. Journal of the Southern African Institute of Mining and Metallurgy, 52(6):119–139, 1951
Rasmussen C. E. and Williams C. K. . Gaussian processes for machine learning. volume 1. MIT press Cambridge. 2006.

Models to handle a large number of design variables

Kriging models: KPLS & KPLS-K

➔ Exploitation of information provided by PLS (Partial Least Squares) in the construction of the Kriging model to reduce the dimension: KPLS and KPLS-K models

Ordinary Kriging

$$k(x, x') = \sigma^2 \exp\left(-\sum_{i=1}^{d} \theta_i |x_i - x_i'|^{p_i}\right)$$

with

d parameters θ_i to evaluate

$h \ll d$

Covariance kernel

KPLS

$$k_{PLS}(x, x') = \sigma^2 \exp\left(-\sum_{i=1}^{d} \eta_i |x_i - x_i'|^{p_i}\right)$$

with

$$\eta_i = \sum_{j=1}^{h} \theta_j \left|w_{i,j}\right|^{p_i}$$

h parameters θ_j to evaluate

- $\left|w_{i,j}\right|_{i=1,\cdots,d}$ describes how sensitive the *j*-th principal component is to each design variable *i* ➔ **PLS**
- θ_j describes how sensitive the function is to each principal component (max *h*≈ 4) ➔ **MLE**
- If $h = d$ ➔ classical Kriging (exponential kernels)

Wold H (1966) Estimation of Principal Components and Related Models by Iterative Least squares, Academic Press, New York, pp 391–420

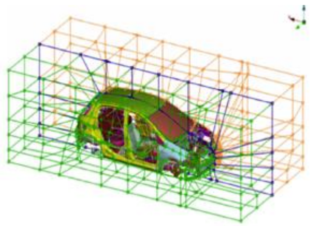
Bouhlel, M. A., Bartoli, N., Otsmane, A., and Morlier, J., “Improving kriging surrogates of high-dimensional design models by Partial Least Squares dimension reduction,” Structural and Multidisciplinary Optimization, Vol. 53, No. 5, 2016, pp. 935–952.

Bouhlel, M. A., Bartoli, N., Otsmane, A., and Morlier, J., “An Improved Approach for Estimating the hyperparameters of the Kriging Model for high-dimensional problems through The Partial Least Squares Method”, Mathematical Problems in Engineering, Vol. 2016(4), May 2016

Models to handle a large number of design variables

Kriging models: KPLS & KPLS-K

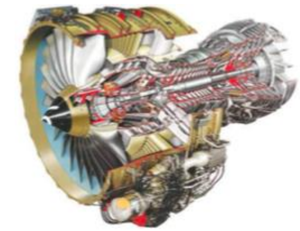
MOPTA test case function from automotive industry



d=124 inputs 1 output
training: 500 points LHS,
validation: 100 points

$$RE = \frac{\|y-\hat{y}\|_2}{\|y\|_2}100$$

SNECMA test case (turbomachinery)



d=98 inputs 1 output
training: 340 points LHS,
validation: 24 points LHS

Surrogate	RE (%)	CPU time
Ordinary Kriging (Scikit-Learn)	3.28e-7	17 min 23 s
KPLS *h*=4	4.52e-7	37 s

Time / 28

Intel(R) Core(TM) i7-4500U CPU@1.80GHz, 6.00 Go RAM

Surrogate	RE (%)	CPU time
Ordinary Kriging (Snecma ref)	2.24	1min 33s
KPLS *h*=1	1.62	0.90 s
KPLS *h*=2	1.62	1.56 s

Time / 60

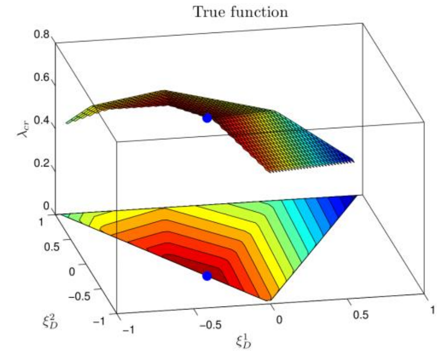
Intel(R) Xeron(R) CPU W3565@3.20GHz, 7.98 Go RAM Quad core

➔ CPU time drastically reduced: interest for adaptive enrichment optimization method

➔ Automatic choice for the number of PLS components

Jones, D., "Large-scale multi-disciplinary mass optimization in the auto industry," MOPTA 2008 Conference (20 August 2008)
Bouhlel, M.-A., Ph.D. thesis, ISAE-SUPAERO, 2016, https://hal.archives-ouvertes.fr/tel-01293319

Models to handle heterogeneous functions



Mixture of Experts (MOE)

→ **Mixture of experts technique**

- Divide the database into K clusters (Expectation-Maximization)
- Build a local surrogate model on each cluster (RBF, Polynomial functions, Kriging,…)
- Recombine the K local models into a global model

$$\hat{f}(x) = \sum_{i=1}^{K} P(k = i/X = x)\hat{f}_i$$

K number of clusters (Gaussian components)

$P(k = i/X = x)$ probability to be in the cluster *i*

(posterior probability given by the Expectation-Maximization algorithm)

$\hat{f}_i$ local expert build using the points in cluster *i* (RBF, Polynomial functions, Kriging,…)

Jordan, M. I., Jacobs, R. A, “Hierarchical mixtures of experts and the EM algorithm“, Neural Comput. 6 (1994) 181–214.
Bettebghor, D., Bartoli, N., Grihon, S., Morlier, J., and Samuelides, M., “Surrogate modeling approximation using a mixture of experts based on EM joint estimation,” Structural and Multidisciplinary Optimization, Vol. 43, No. 2, 2011, pp. 243–259
Liem, R. P., Mader, C. A., and Martins, J. R. R. A., “Surrogate Models and Mixtures of Experts in Aerodynamic Performance Prediction for Mission Analysis,” Aerospace Science and Technology, Vol. 43, 2015, pp. 126–151

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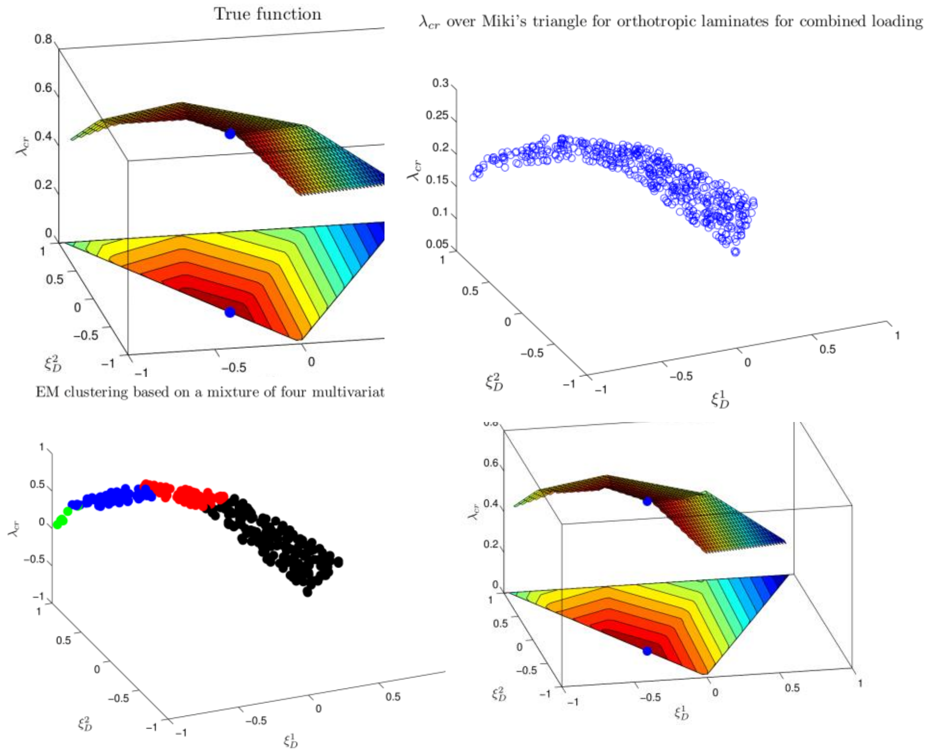

Comparison on Buckling critical loads PhD D. Bettebghor 2011

Jordan, M. I., Jacobs, R. A, "Hierarchical mixtures of experts and the EM algorithm", Neural Comput. 6 (1994) 181–214.
Bettebghor, D., Bartoli, N., Grihon, S., Morlier, J., and Samuelides, M., "Surrogate modeling approximation using a mixture of experts based on EM joint estimation," Structural and Multidisciplinary Optimization, Vol. 43, No. 2, 2011, pp. 243–259
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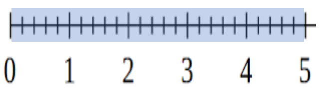
Models to handle mixed variables (continuous, discrete, categorical)

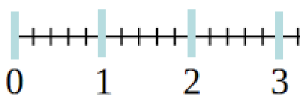
Hybrid variables

Variables types:

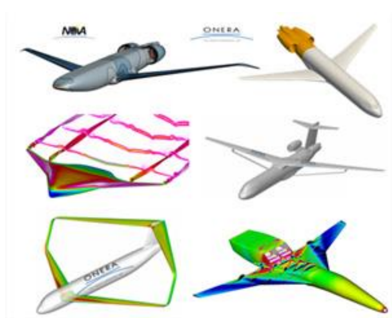
- **Continuous (x) Ex:** wing length



- **Integer (z) Ex:** winglet number



- **Categorical (u) Ex:** Plane shape / material properties



Categorical variables: n variables,
n=2
u1= shape
u2= color

Levels: L_i levels for I in 1,..n,
L_1=3, L_2=2
Levels(u1)= square, circle, rhombus
Levels(u2)= blue, red

Categories: $\prod_{i=1}^{n} L_i$, **2*3=6**
- **Blue square**
- **Blue circle**
- **Blue rhombus**
- **Red square**
- **Red circle**
- **Red rhombus**

6 possibilities

➔ **Different possible kernels:** Gower distance, Continuous Relaxation, Homoscedastic hypersphere, **Exponential Homoscedastic hypersphere**

Pelamatti, J., Brevault, L., Balesdent, M., Talbi, E.-G., and Guerin, Y., Overview and Comparison of Gaussian Process-Based Surrogate Models for Mixed Continuous and Discrete Variables: Application on Aerospace Design Problems, Springer International Publishing, 2020, pp. 189–224
Saves, P., Diouane, Y., Bartoli, N., Lefebvre, T., & Morlier, J. (2023). A mixed-categorical correlation kernel for Gaussian process. *Neurocomputing*, *550*, 126472.

State of the Art approach: Continuous Relaxation

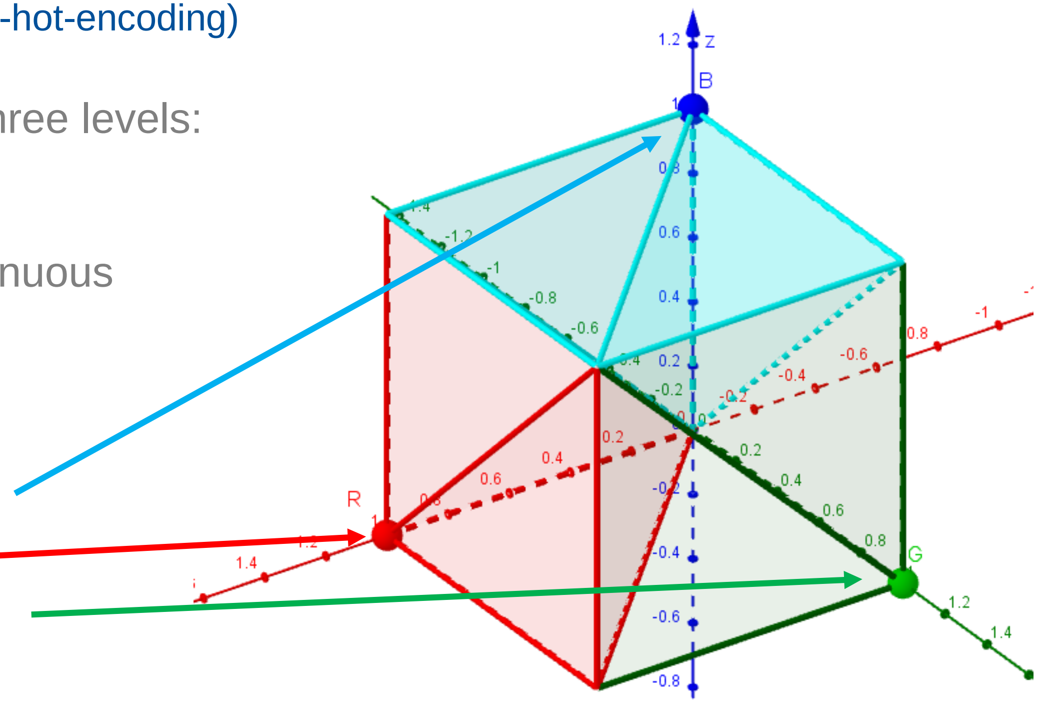
➔ Model as a **Continuous Relaxation** (one-hot-encoding)

Example with 1 categorical variable X and three levels:
Red color, Blue color, Green color

➔ 1 Categorical variable replaced by 3 continuous variables denoted by X_1, X_2 and $X_3 \in [0,1]$

➔ Rounding operator:

- If $X_1 > X_2, X_3 \Rightarrow e_{c_1^b} = (1., 0., 0.) \Rightarrow$ Blue color
- If $X_2 > X_1, X_3 \Rightarrow e_{c_1^r} = (0., 1., 0.) \Rightarrow$ Red color
- If $X_3 > X_1, X_2 \Rightarrow e_{c_1^g} = (0., 0., 1.) \Rightarrow$ Green color



A continuous kernel
(in the relaxed dimension)

$$k(x^r, x^s, \theta^{cont}) = \prod_{j=1}^{d'} \exp\left(-(x_j^r - x_j^s)\theta_j^{cont}(x_j^r - x_j^s)\right)$$

E. C. Garrido-Merchán, and D. Hernández-Lobato. "Dealing with categorical and integer-valued variables in Bayesian Optimization with Gaussian processes". Neurocomputing, vol. 380 (2020), pages 20-35
Saves, P., Bartoli, N., Diouane, Y., Morlier, J., & Lefebvre, T. (2021, March). Enhanced Kriging models within a Bayesian optimization framework to handle both continuous and categorical inputs. In SIAM CSE21

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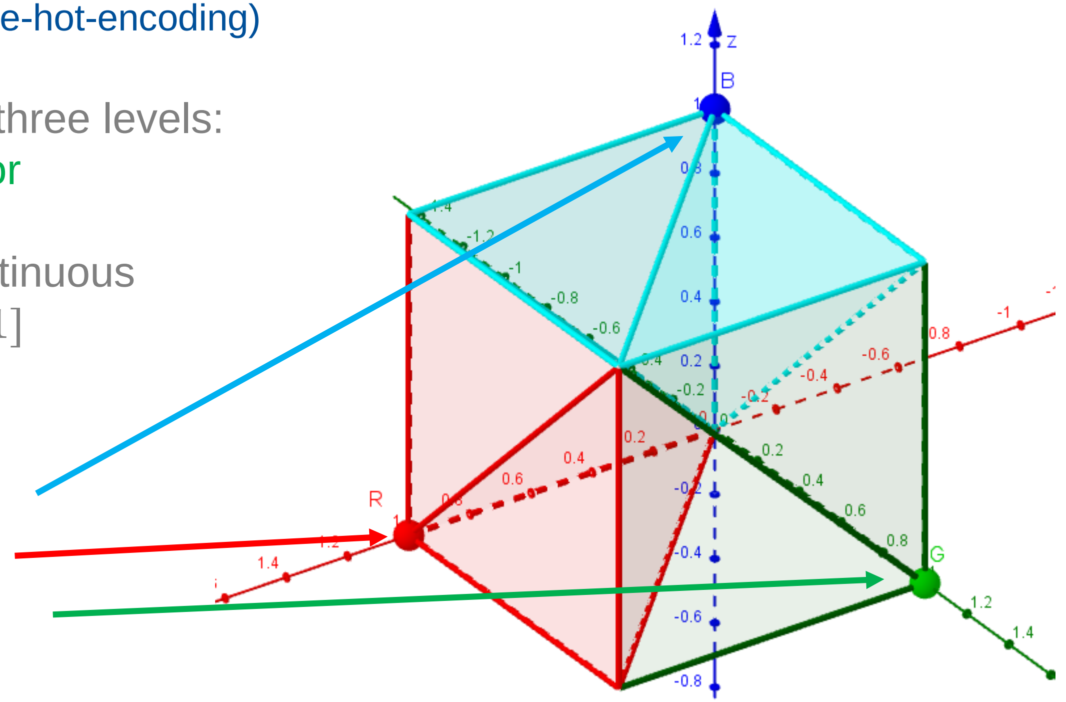

A continuous kernel
(in the relaxed dimension)

➔ **Increase the dimension**

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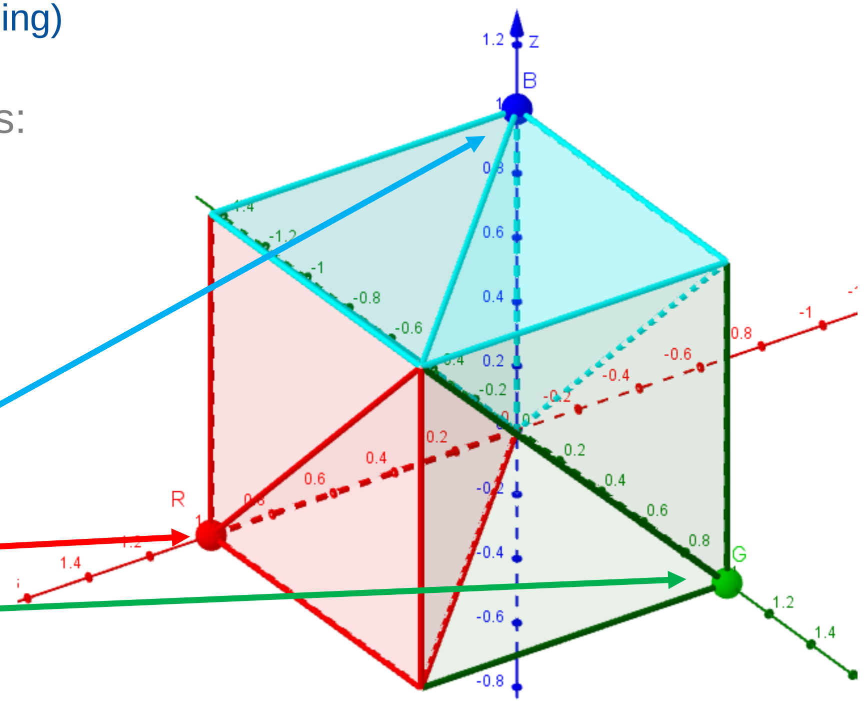

➔ Use of KPLS models to decrease the dimension

E. C. Garrido-Merchán, and D. Hernández-Lobato. "Dealing with categorical and integer-valued variables in Bayesian Optimization with Gaussian processes". Neurocomputing, vol. 380 (2020), pages 20-35
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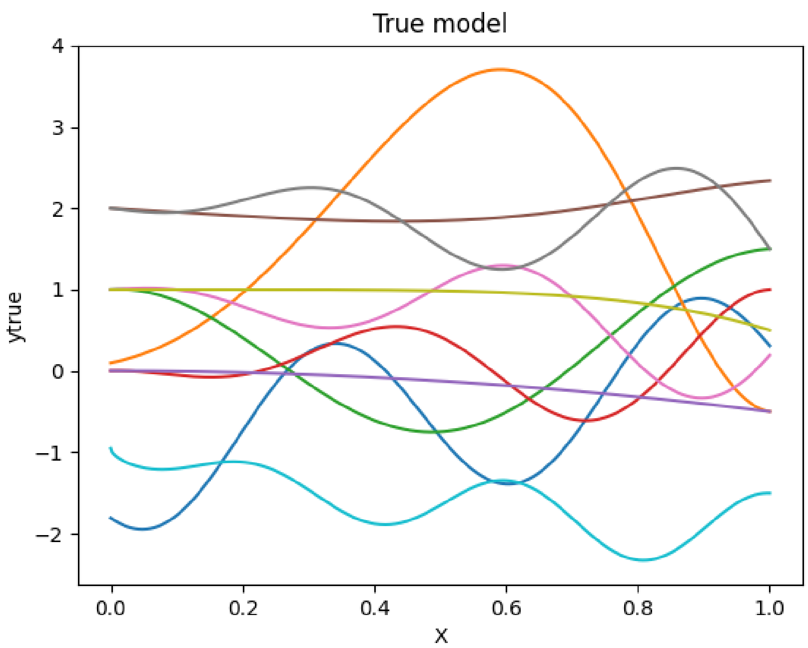
Models to handle mixed variables (continuous, discrete, categorical)

Toy function with a categorical variable (10 levels)

$$f(x,z) = \begin{cases} \cos(3.6\pi(x-2)) + x - 1 & \text{if} \quad z = 1, \\ 2\cos(1.1\pi\exp(x)) - \frac{x}{2} + 2 & \text{if} \quad z = 2, \\ \cos(2\pi x) + \frac{1}{2}x & \text{if} \quad z = 3, \\ x\left(\cos(3.4\pi(x-1)) - \frac{x-1}{2}\right) & \text{if} \quad z = 4, \\ -\frac{x^2}{2} & \text{if} \quad z = 5, \\ 2\cos(\frac{\pi}{4}\exp(-x^4))^2 - \frac{x}{2} + 1 & \text{if} \quad z = 6, \\ x\cos(3.4\pi x) - \frac{x}{2} + 1 & \text{if} \quad z = 7, \\ x(-\cos\left(7\frac{\pi}{2}x\right) - \frac{x}{2}) + 2 & \text{if} \quad z = 8, \\ -\frac{x^5}{2} + 1 & \text{if} \quad z = 9, \\ -\cos(5\frac{\pi}{2}x)^2\sqrt{x} - \frac{\ln(x+0.5)}{2} - 1.3 & \text{if} \quad z = 10. \end{cases}$$

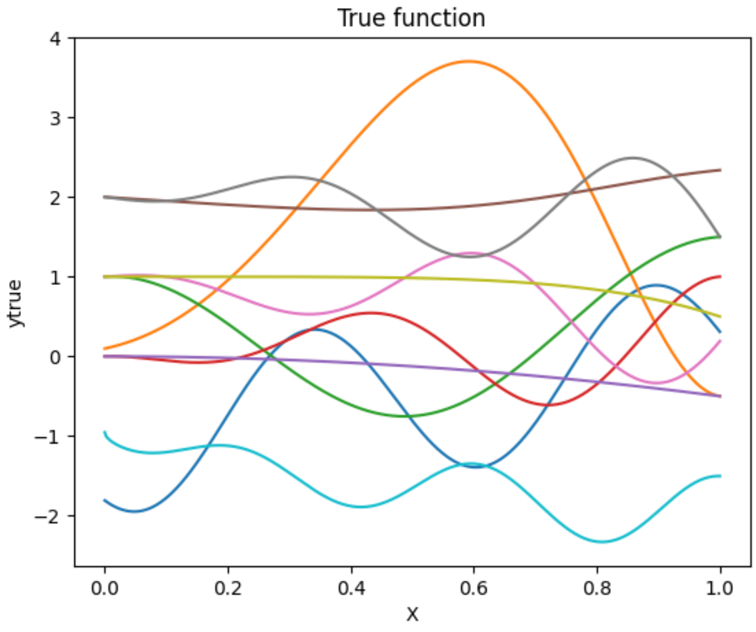


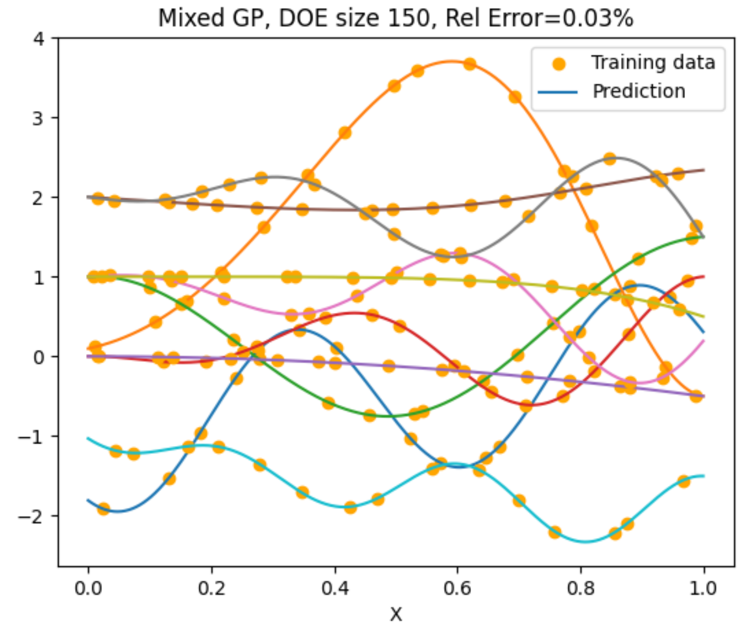
1 continuous + 1 categorical variable (10 levels) ➔ 11 continuous variables

Models to handle mixed variables (continuous, discrete, categorical)

Toy function with a categorical variable (10 levels)

$$f(x,z) = \begin{cases} \cos(3.6\pi(x-2)) + x - 1 & \text{if} \quad z = 1, \\ 2\cos(1.1\pi \exp(x)) - \frac{x}{2} + 2 & \text{if} \quad z = 2, \\ \cos(2\pi x) + \frac{1}{2}x & \text{if} \quad z = 3, \\ x\left(\cos(3.4\pi(x-1)) - \frac{x-1}{2}\right) & \text{if} \quad z = 4, \\ -\frac{x^2}{2} & \text{if} \quad z = 5, \\ 2\cos(\frac{\pi}{4}\exp(-x^4))^2 - \frac{x}{2} + 1 & \text{if} \quad z = 6, \\ x\cos(3.4\pi x) - \frac{x}{2} + 1 & \text{if} \quad z = 7, \\ x(-\cos\left(7\frac{\pi}{2}x\right) - \frac{x}{2}) + 2 & \text{if} \quad z = 8, \\ -\frac{x^5}{2} + 1 & \text{if} \quad z = 9, \\ -\cos(5\frac{\pi}{2}x)^2\sqrt{x} - \frac{\ln(x+0.5)}{2} - 1.3 & \text{if} \quad z = 10. \end{cases}$$





➔ Smaller errors compared to independant GPs

Models to handle multi-information sources

Multi-fidelity Kriging (MFK) or co-kriging

- **Access to different information sources that approximate $y(x)$ with varying accuracy and cost**

Hierarchical relationships among information sources: low-fidelity / high-fidelity

→ Use low-fidelity information to enhance the high-fidelity model:
MFK models $Y^{HF}(\mathbf{x}) = \rho(\mathbf{x})Y^{LF}(\mathbf{x}) + \gamma(\mathbf{x})$

- **Recursive co-Kriging formulation:** ℓ levels of fidelity

$$\mu_{HF} = \rho\, \mu_{LF} + \mu_\delta \qquad \longrightarrow \qquad \mu_k = \rho_{k-1}\, \mu_{k-1} + \mu_{\delta_k}$$

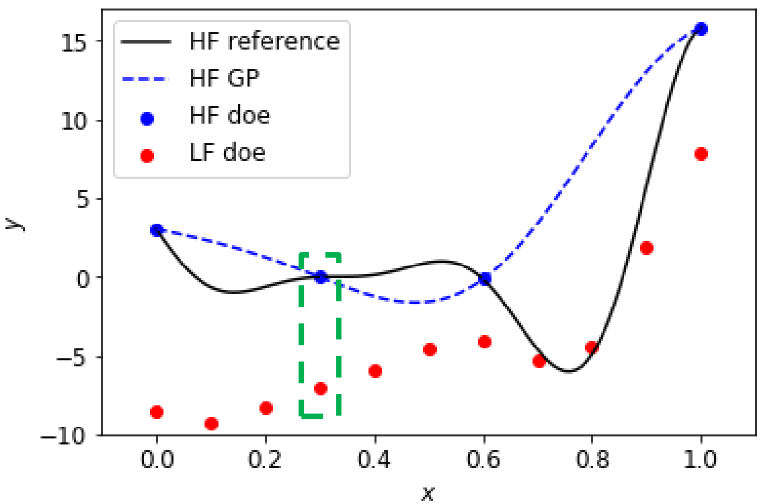
$$\sigma^2_{HF} = \rho^2\, \sigma^2_{LF} + \sigma^2_\delta \qquad \longrightarrow \qquad \sigma^2_k = \rho^2_{k-1}\, \sigma^2_{k-1} + \sigma^2_{\delta_k}$$

- Different scaling factors $\rho(x)$, extension to KPLS & KPLS-K
- Design of experiments adapted to multi-fidelity (nested DOE)

$$X_{HF} \subset X_{LF}$$

Kennedy, Marc C., and Anthony O'Hagan. "Bayesian calibration of computer models." Journal of the Royal Statistical Society: Series B (Statistical Methodology) 63.3 (2001): 425-464.
Le Gratiet, Loic, and Josselin Garnier. "Recursive co-kriging model for design of computer experiments with multiple levels of fidelity." International Journal for Uncertainty Quantification 4.5 (2014).

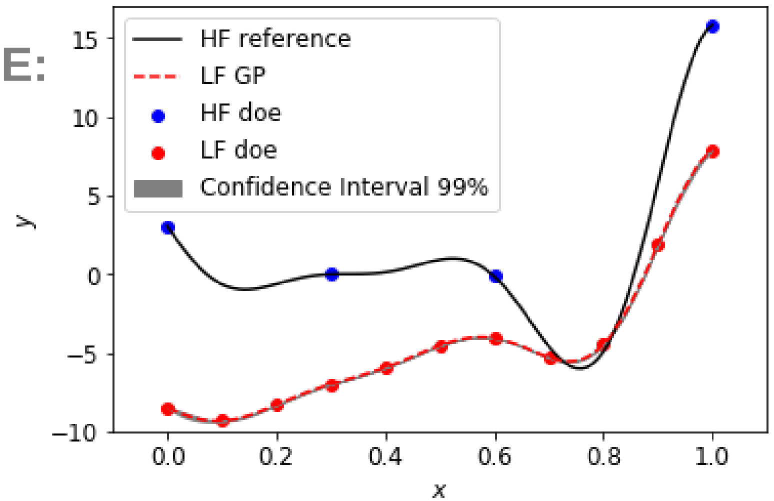
Multi-fidelity Kriging example with 2 levels

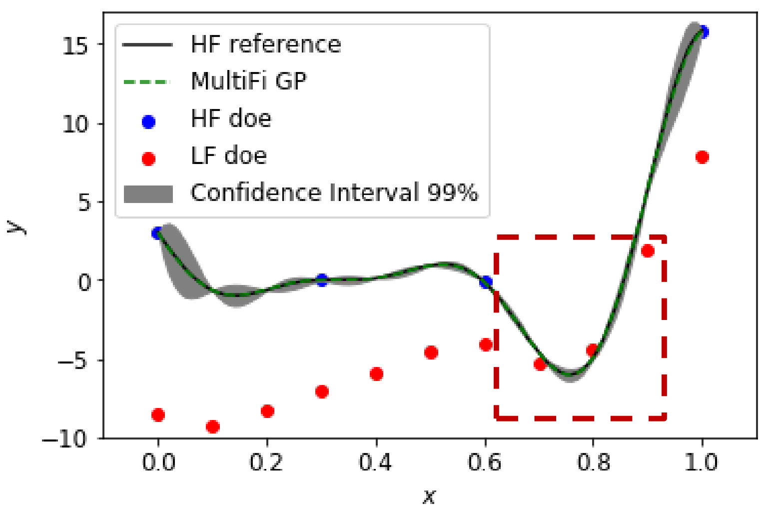


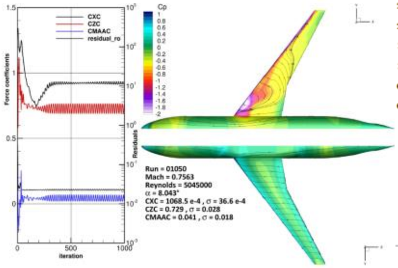
Nested DOE:

4 pts HF

11 pts LF

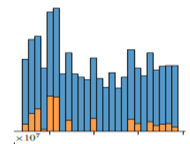


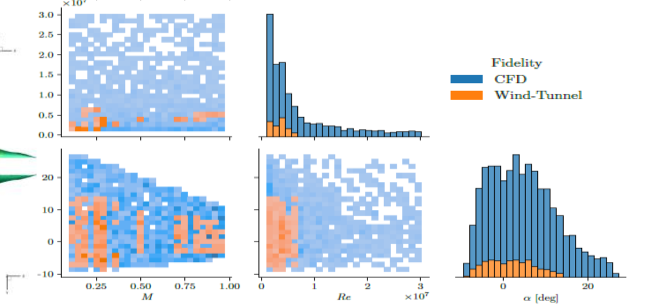




CFD & WIND TUNNEL database

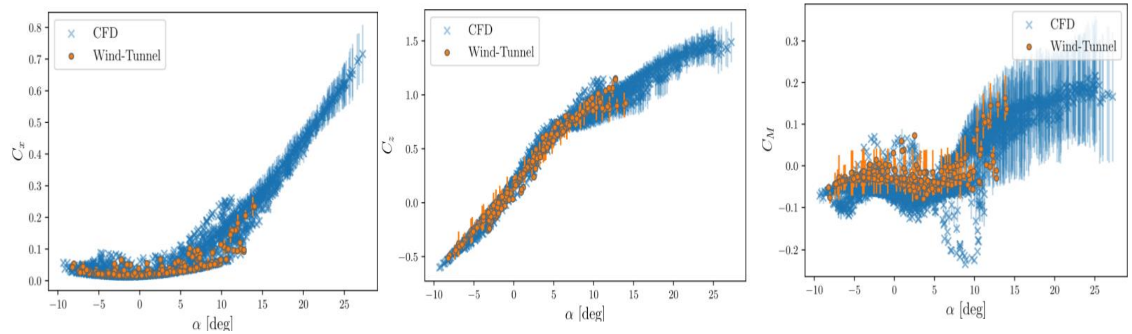
	High fidelity	Low fidelity
	Wind Tunnel	elsA CFD
Mach Number (M)	[0.01, 0.95]	[0.01, 0.97]
Reynolds Number (Re) [1×10^6]	[0.77, 6.60]	[0.1, 30.0]
Angle of Attack (α) [deg]	[-9.3, 20.5]	[-10.0, 30.0]
Number of samples	250	2000





Raudin, R., "Développement de modèles réduits multi-fidélité en vue de l'optimisation de structures aéronautiques", Master Thesis rep., ISAE-SUPAERO / École des Mines de St Etienne, July 2021
Conde Arenzana, R., Lopez-Lopez, A., Mouton, S., Bartoli, N. and Lefebvre, T., "Multi-fidelity Gaussian Process Model for CFD and Wind Tunnel …", Portugal, 2024-23
Meliani, M. "High Dimensional Efficient Global Optimization via Multi-Fidelity Surrogate Modeling", Master Thesis rep., ISAE-SUAPERO, 2018

Multi-fidelity Kriging: CFD & Wind Tunnel database



	High fidelity	Low fidelity
	Wind Tunnel	elsA CFD
Mach Number (M)	[0.01, 0.95]	[0.01, 0.97]
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Angle of Attack (α) [deg]	[-9.3, 20.5]	[-10.0, 30.0]
Number of samples	250	2000

Outputs	Symbol
Drag Coefficient	C_x
Lift coefficient	C_z
Pitch Moment Coefficient	C_M

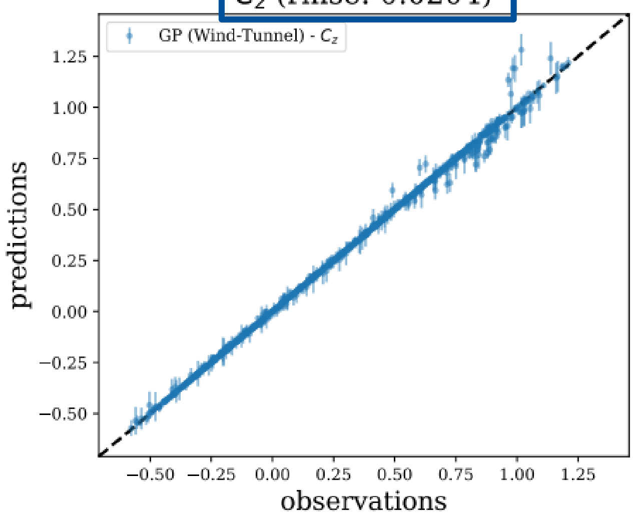
Test: 1000 points from the database

$$RMSE = \sqrt{\frac{1}{n_{test}}\sum_{i-1}^{n_{test}}(y_i - \mu_i)^2}$$

Single-Fidelity approach

Training: 100 % HF (250 points)

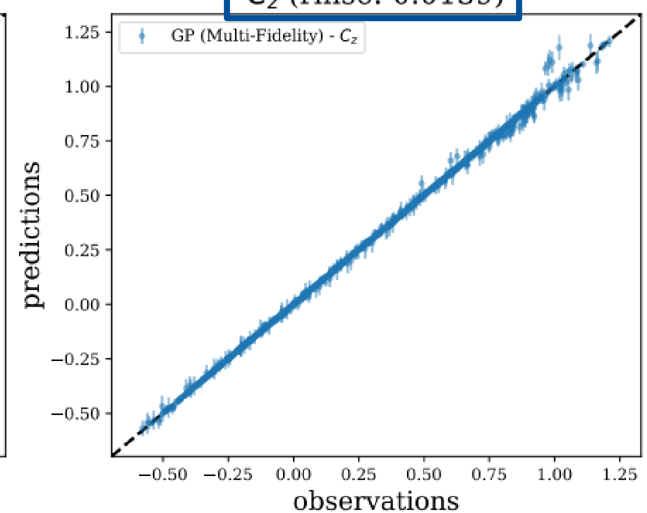
C_z (rmse: 0.0204)



Multi-Fidelity approach

Training: 100% HF (250 points) + 100% LF (1949 points)

C_z (rmse: 0.0139)



R. Conde Arenzana, A.F. Lopez-Lopera, S. Mouton, N. Bartoli and T. Lefebvre, "Multi-fidelity Gaussian Process Model for CFD and Wind Tunnel Data Fusion", *AeroBest 2021*, Lisboa, Portugal, 21-23 July 2021

Multi-fidelity Kriging: CFD & Wind Tunnel database

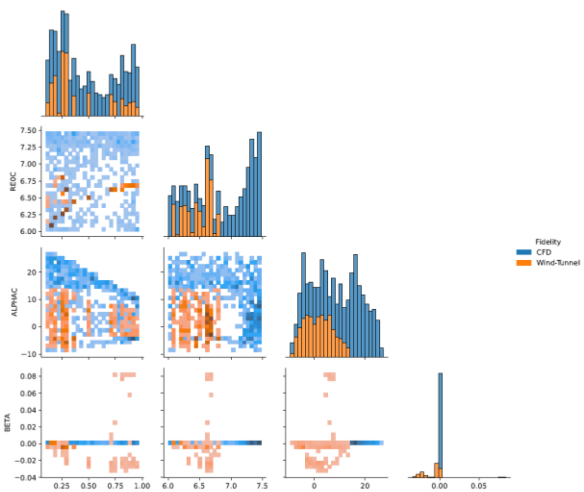
Extension for non nested DOE

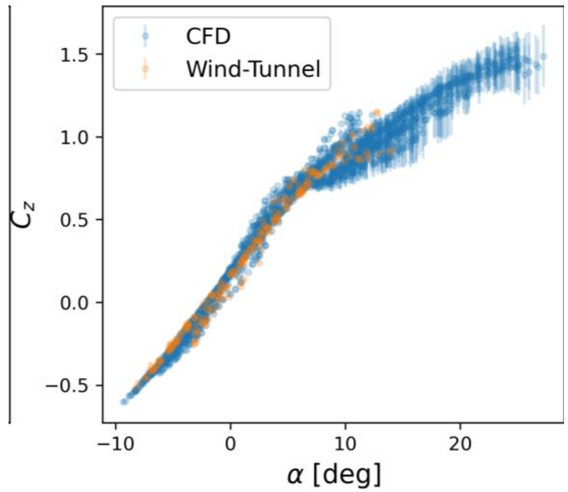
PhD Mauricio Castano Aguirre (UPHF, ONERA)

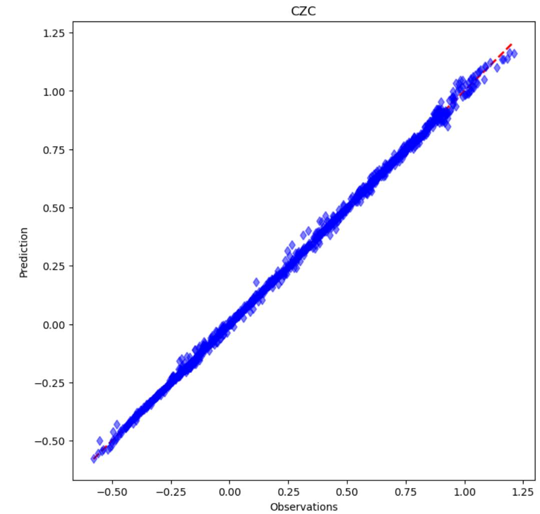
Non-nested DoE

- 250 Wind-Tunnel data observations
- 1345 CFD data observations

By filtering LF observations
to guarantee a non-nested DoE.







$$RMSE = \sqrt{\frac{1}{n_{test}} \sum_{i-1}^{n_{test}} (y_i - \mu_i)^2}$$

1000 WT validation points

RMSE = 0.0158

Extension to large & multi-fidelity dataset
➔ see Poster

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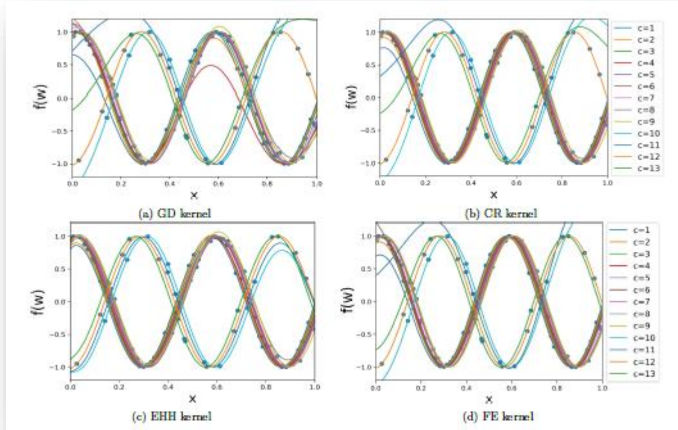
Recent activities

github.com/SMTorg/smt

- Mixed kernels integration (Phd P. Saves 2024)
  + KPLS for dimension reduction with automatic choice for number of PLS components



- Extension to hierarchical variables (variable-size problems)
  Consider conditionally active distances
  New proposed kernels (Phd P. Saves & Collab. E. Hallé-Hannan Polytechnique Montréal)
  New application cases (Collab. J. H Bussemaker DLR)

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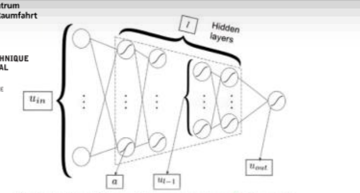
POLYTECHNIQUE MONTRÉAL

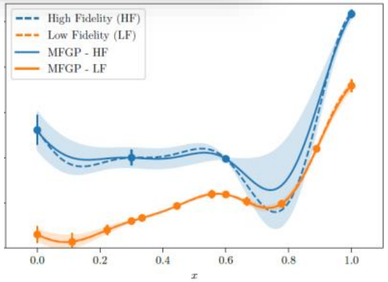


(a) Illustration of the multi-layer perceptron [2, Figure 1]

Hyperparameter of the MLP	Variable	Domain	Type	Role
Learning rate	r	$[10^{-5}, 10^{-2}]$	FLOAT	NEUTRAL
Activation function	a	{ReLU, Sigmoid}	ENUM	NEUTRAL
Batch-size	b	$\{8, 16, \ldots, 128, 256\}$	ORD	NEUTRAL
# of hidden layers	l	$\{1, 2, 3\}$	ORD	META
# of units hidden layer i	u_i	$\{50, 51, \ldots, 55\}$	ORD	DECREED

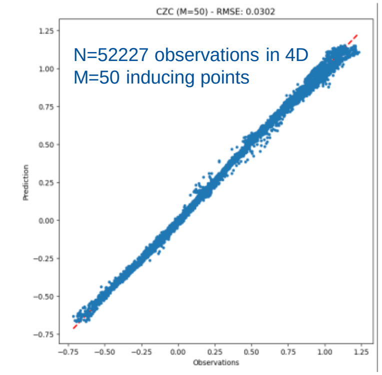
(b) Description of the variables for the problem

Figure 4: The hierarchical multi-layer perceptron problem [2].

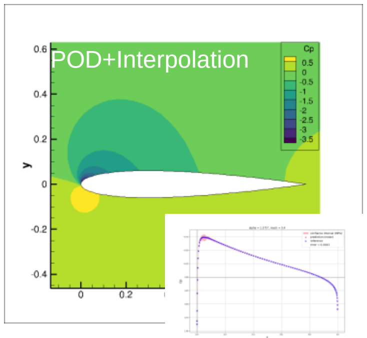


- Multi-fidelity surrogates with heterogenous uncertainties on data
  (Phd R. Charayron 2023 – PhD M. Castano Aguirre 2024-2027)

- Gaussian models for large database (N points)
  Low-rank representation with $M < N$ inducing points
  Training cost $O(N^3)$ ➔ $O(NM^2)$ (Intern. H Valayer)



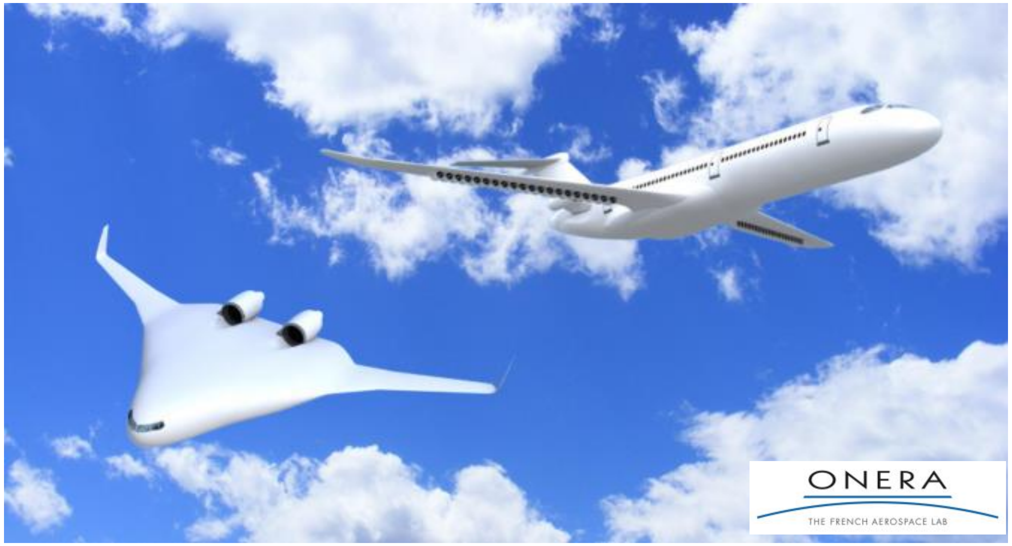
- Proper Orthogonal Decomposition + GP interpolation
  Prediction of vectorial outputs (Intern. H. Reimeringer)

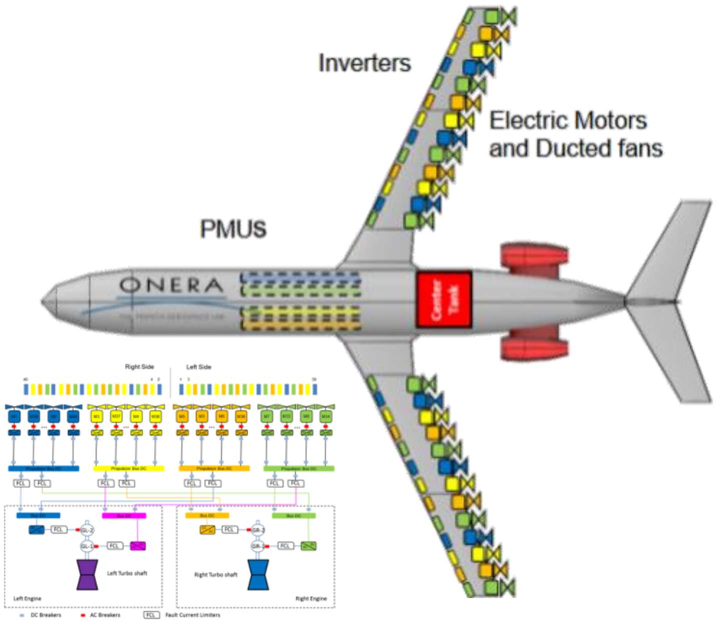


Saves, P., Diouane, Y., Bartoli, N., Lefebvre, T., & Morlier, J. (2023). A mixed-categorical correlation kernel for Gaussian process. Neurocomputing, 550, 126472.
Bussemaker, J. H., Bartoli, N., Lefebvre, T., Ciampa, P. D., & Nagel, B. (2021). Effectiveness of Surrogate-Based Optimization Algorithms for System Architecture Optimization. In AIAA AVIATION 2021 FORUM (p. 3095).
Valayer, H., Bartoli, N., Castaño-Aguirre, M., Lafage, R., Lefebvre, T., López-Lopera, A. F., & Mouton, S. (2024). A Python Toolbox for Data-Driven Aerodynamic Modeling Using Sparse Gaussian Processes. Aerospace, 11(4), 260.

Multidisciplinary Design Analysis and Optimization for new configurations

Goal: Aircraft/drone design optimization





min objective function f(x,y(x))
with respect to design variables x (continuous, discrete, categorical, hierarchical)
subject to constraints g(x,y(x))

➔ y(x) are solution of a non linear system (MDA)

➔ Objective and constraint functions could be costly

Optimization problem in the field of aircraft design

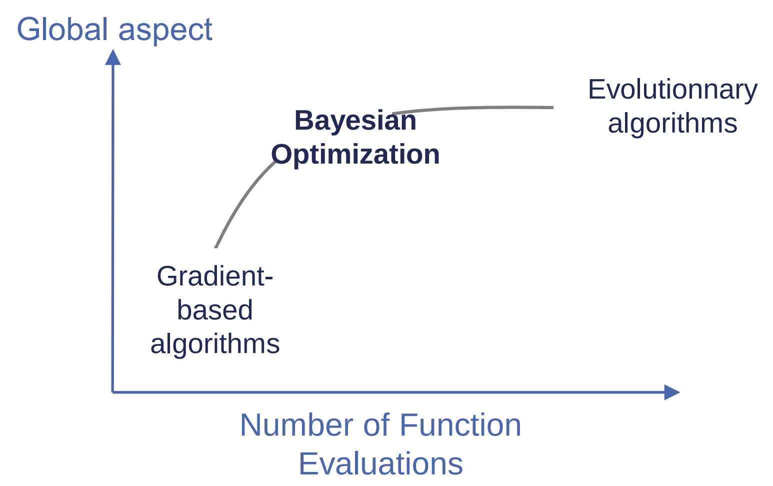
$$\begin{cases} \min\limits_{\boldsymbol{x}\in\mathbb{R}^d} \quad \boldsymbol{f}(\boldsymbol{x}) = [f_1(\boldsymbol{x}), f_2(\boldsymbol{x}), \cdots, f_n(\boldsymbol{x})] \\ \text{s.t.} \\ c_1(\boldsymbol{x}) \leq 0 \ldots c_j(\boldsymbol{x}) = 0 \ldots c_m(\boldsymbol{x}) \leq 0 \end{cases}$$

1 to n objectives
d design variables
m mixed constraints (eq. & ineq)

- Main characteristics for aircraft design problem
  - **Mono & Multi** objective, multi-constraints (1 ~ 100 constraints)
  - Intermediate dimension problem (1 ~ 100 variables), **mixed variables**
  - Costly evaluation (CFD, FEM, objective and/or constraints)
  - Handling non linear constraints (black box, no derivative available)
  - Handling hidden constraints
- Applications
  - Disciplinary solvers (aerodynamic, structure, propulsion, …)
  - Overall aircraft design process (MDA)

How to build an efficient iterative process?

- Find the global minimum with a limited budget of function evaluations
- Use Bayesian information to detect interesting and promising areas (exploitation/exploration trade-off)

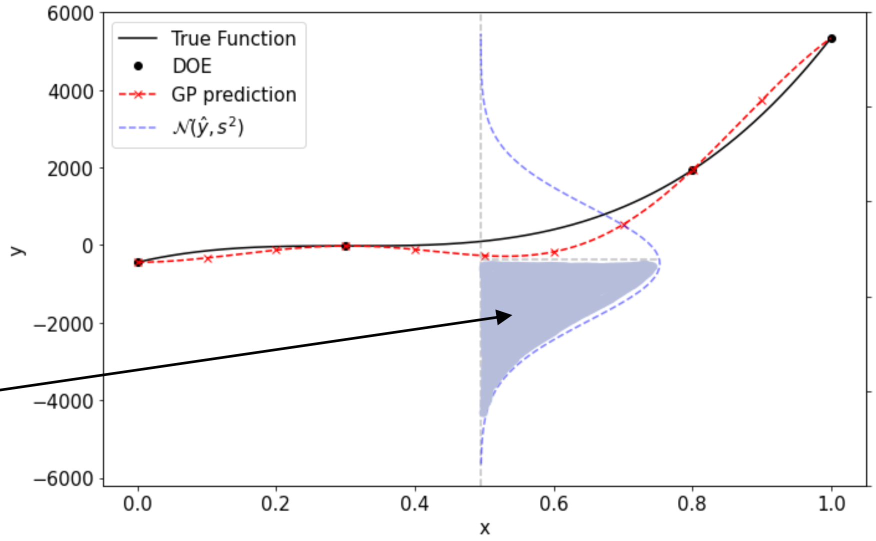


Enrichment infill sampling criterion

$f(x) \Rightarrow Y(x) = \mathcal{N}(\hat{y}(\boldsymbol{x}), s^2(\boldsymbol{x}))$

Measure of progress defined by the Improvement

$$I(x) = \max(0, \underbrace{y_{min} - Y(x)}_{>0 \text{ if } Y(x) < y_{min}})$$



y_{min}= current min of the database

Expected Improvement

$$EI(x) = \mathbb{E}[I(x)] = \mathbb{E}[\max\{0, y_{min} - Y(x)\}]$$

EGO for Efficient Global Optimization

Jones, D. R., Schonlau, M., and Welch, W. J., “Efficient global optimization of expensive black-box functions,” Journal of Global optimization, Vol. 13, No. 4, 1998, pp. 455–492.

Enrichment infill sampling criterion

$f(x) \Rightarrow Y(x) = N(\hat{y}(\boldsymbol{x}), s^2(\boldsymbol{x}))$ **Expected Improvement criterion (EI)**

Kriging or Gaussian process of the objective function

$$\mathrm{EI}(\mathbf{x}) = \mathbb{E}[\max(y_{\min} - Y(\mathbf{x}), 0)]$$

Φ cumulative distribution function
ϕ probability density function of $\mathcal{N}(0,1)$

$$\mathrm{EI}(x) = (y_{min} - \hat{y}(\boldsymbol{x}))\Phi\left(\frac{y_{min} - \hat{y}(\boldsymbol{x})}{s(\boldsymbol{x})}\right) + s(\boldsymbol{x})\phi\left(\frac{y_{min} - \hat{y}(\boldsymbol{x})}{s(\boldsymbol{x})}\right)$$

Exploitation **Exploration**

Jones, D. R., Schonlau, M., and Welch, W. J., "Efficient global optimization of expensive black-box functions," Journal of Global optimization, Vol. 13, No. 4, 1998, pp. 455–492.
Bartoli, N., Lefebvre, T., Dubreuil, S., Olivanti, R., Priem, R., Bons, N., Martins, J. R. A. A., Morlier, J. Adaptive modeling strategy for constrained global optimization with application to aerodynamic wing design. Aerospace Science and Technology, 90:85–102, 2019.

Enrichment infill sampling criterion

$f(x) \Rightarrow Y(x) = N(\hat{y}(x), s^2(x))$ **Expected Improvement criterion (EI)**

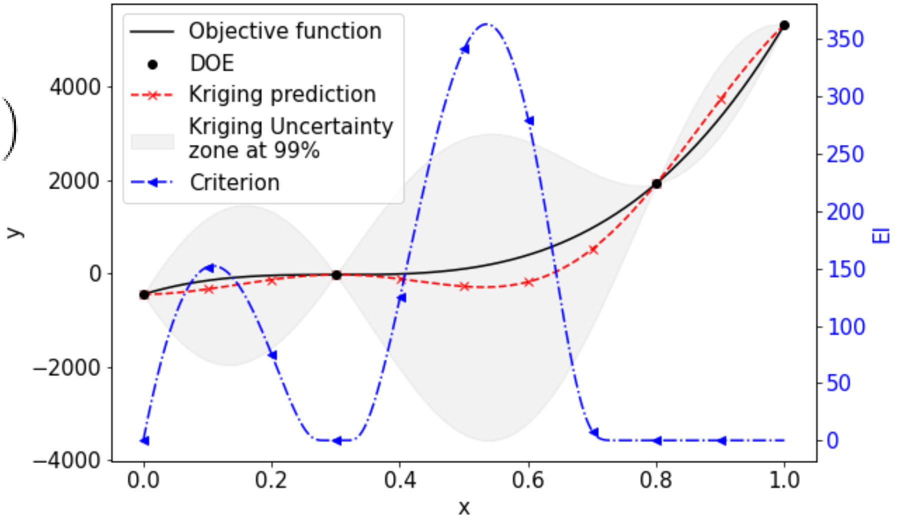
$$\mathrm{EI}(\mathbf{x}) = \mathbb{E}[\max(y_{\min} - Y(\mathbf{x}), 0)]$$

Kriging or Gaussian process of the objective function

$$\begin{cases} \min_{\mathbf{x}\in\mathbb{R}^d} f(\mathbf{x}) \\ \text{s.t.} \\ c_1(\mathbf{x}) \leq 0 \\ \vdots \\ c_m(\mathbf{x}) \leq 0 \end{cases}$$

Surrogate models
(objective & constraints)

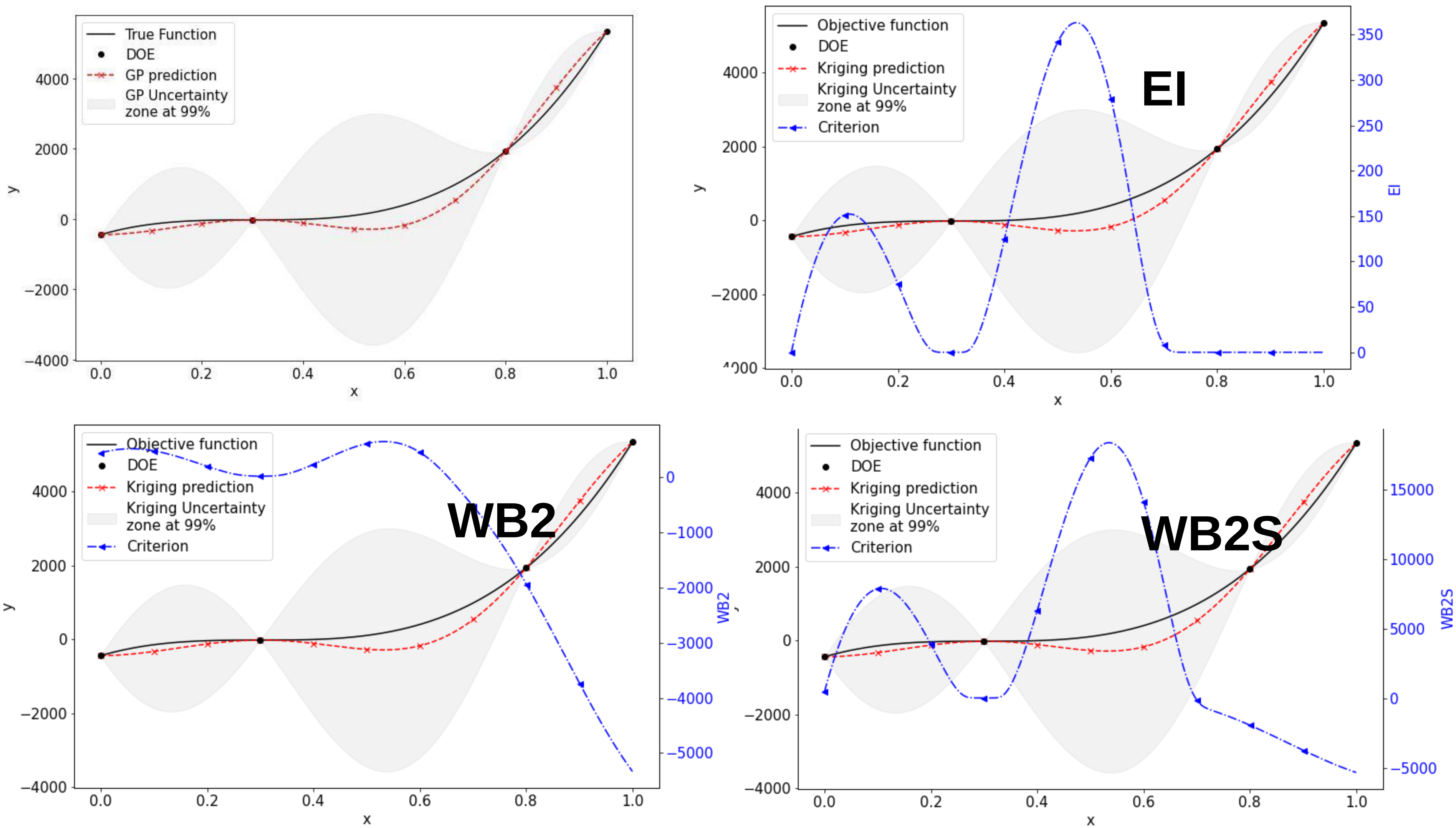
$$\begin{cases} \max_{\mathbf{x}\in\mathbb{R}^d} \mathrm{EI}(\mathbf{x}) \\ \text{s.t.} \\ \hat{c}_1(\mathbf{x}) \leq 0 \\ \vdots \\ \hat{c}_m(\mathbf{x}) \leq 0 \end{cases}$$



➔ **Different criteria available for the acquisition function (EI, WB2, WB2S)**

Jones, D. R., Schonlau, M., and Welch, W. J., "Efficient global optimization of expensive black-box functions," Journal of Global optimization, Vol. 13, No. 4, 1998, pp. 455–492.
Bartoli, N., Lefebvre, T., Dubreuil, S., Olivanti, R., Priem, R., Bons, N., Martins, J. R. A. A., Morlier, J. Adaptive modeling strategy for constrained global optimization with application to aerodynamic wing design. Aerospace Science and Technology, 90:85–102, 2019.

Mono objective: different criteria available



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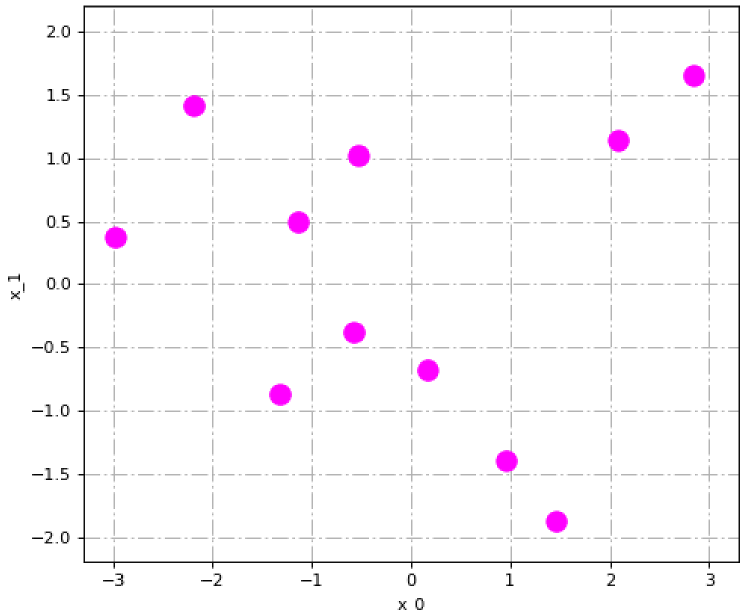
Bartoli, N., Lefebvre, T., Dubreuil, S., Olivanti, R., Priem, R., Bons, N., Martins, J. R. A. A., Morlier, J. Adaptive modeling strategy for constrained global optimization with application to aerodynamic wing design. Aerospace Science and Technology, 90:85–102, 2019.

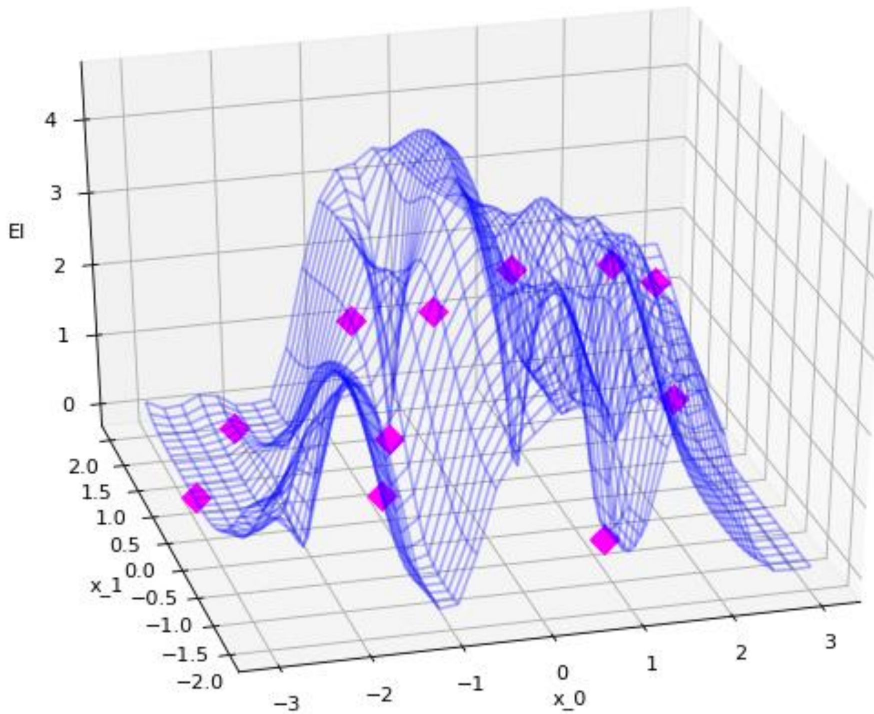
Enrichment for global optimization

$$\begin{cases} \max\limits_{x \in \mathbb{R}^d} \quad \alpha_f(\boldsymbol{x}) \\ \text{s.t.} \\ \hat{c_1}(\boldsymbol{x}) \leq 0 \\ \vdots \\ \hat{c_m}(\boldsymbol{x}) \leq 0 \end{cases}$$

max Acquisition function

Local optimizer (Cobyla, Slsqp, Snopt) with ‘multi-start’ approach





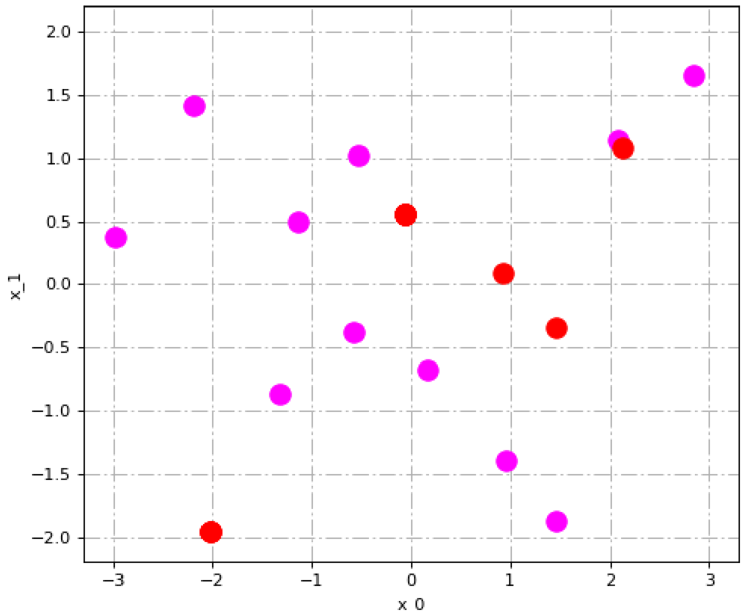
● Initial DOE (LHS)

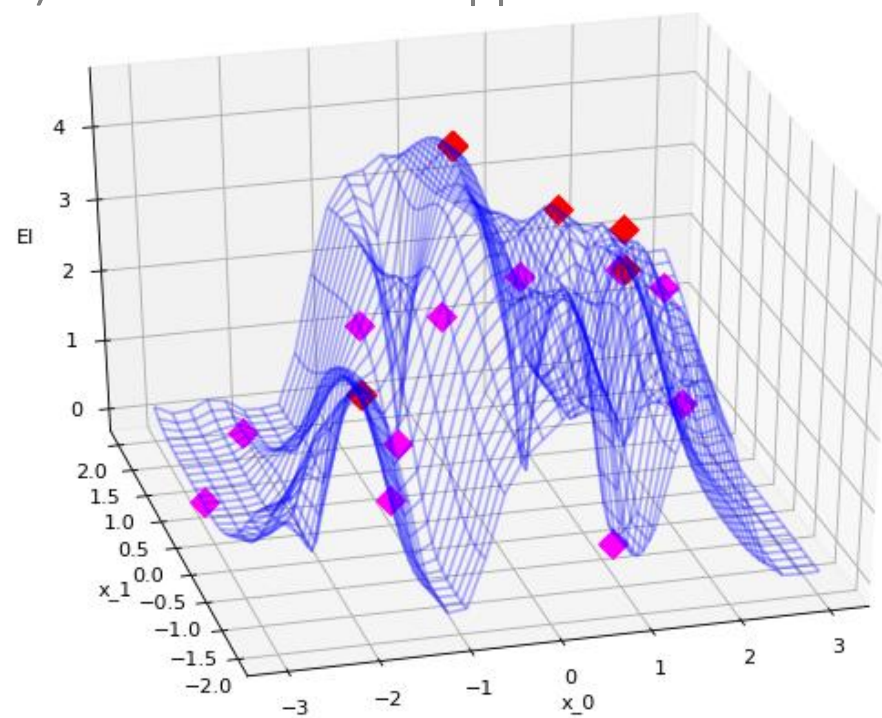
SNOPT: Sparse Nonlinear OPTimizer, Philip Gill , Walter Murray and Michael Saunders, Standford Business Software Inc.

Enrichment for global optimization

$$\begin{cases} \max_{x \in \mathbb{R}^d} & \alpha_f(\boldsymbol{x}) \\ \text{s.t.} & \\ \hat{c_1}(\boldsymbol{x}) \leq 0 & \\ \vdots & \\ \hat{c_m}(\boldsymbol{x}) \leq 0 & \end{cases}$$

Local optimizer (Cobyla, Slsqp, Snopt) with 'multi-start' approach





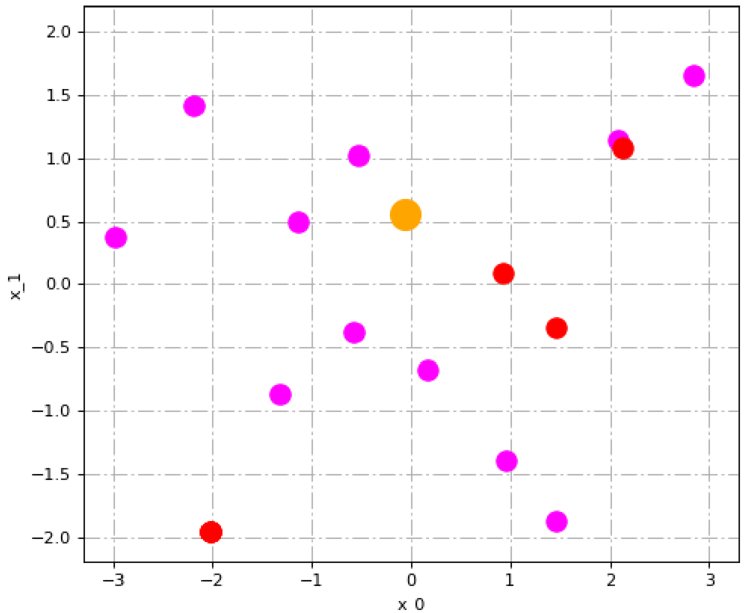
- **Initial DOE(LHS)**
- **Optimization results**

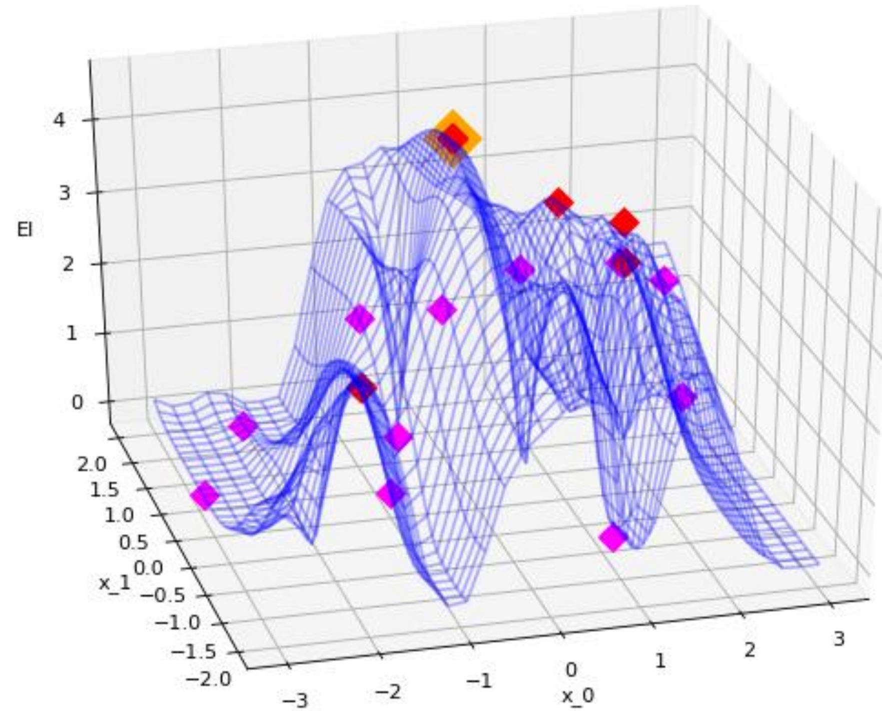
➡ Sensitivity to starting points
Drives the global behaviour

Enrichment for global optimization

$$\begin{cases} \max\limits_{x \in \mathbb{R}^d} & \alpha_f(\boldsymbol{x}) \\ \text{s.t.} & \\ \hat{c_1}(\boldsymbol{x}) \leq 0 & \\ \vdots & \\ \hat{c_m}(\boldsymbol{x}) \leq 0 & \end{cases}$$

Local optimizer (Cobyla, Slsqp, Snopt) with ‘multi-start’ approach





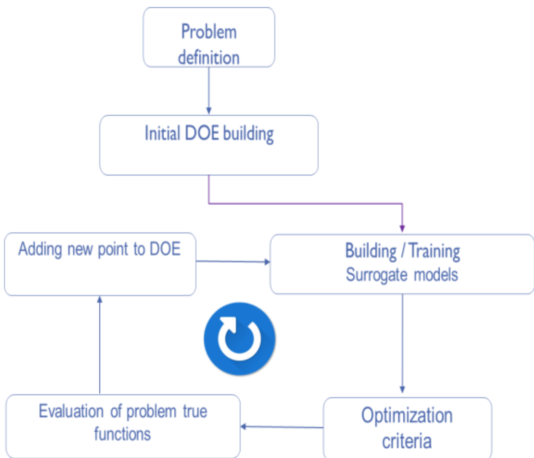
- **Initial DOE(LHS)**
- **Optimization results**
- **Retained point**

➡ Sensitivity to starting points
Drives the global behaviour

SEGOMOE

SEGO

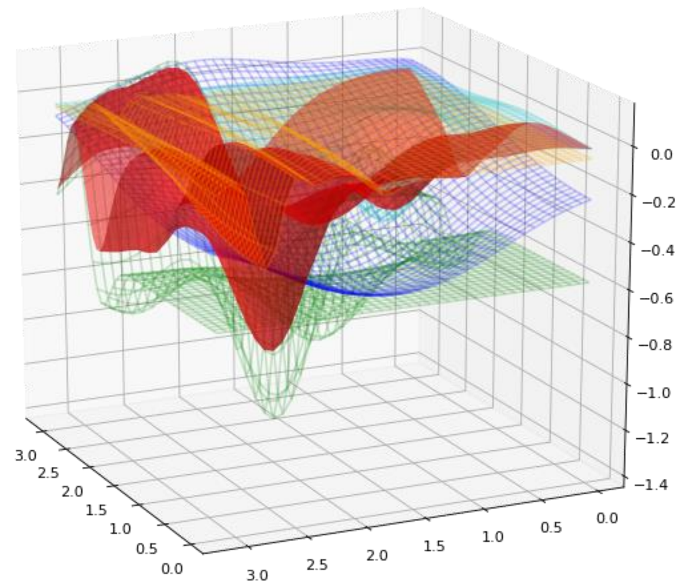
Super Efficient Global Optimization



Global optimization with limited number of function evaluations

MOE

Mixture Of Experts



Combination of surrogate models

Jones, D. R., Schonlau, M., and Welch, W. J., "Efficient global optimization of expensive black-box functions," Journal of Global optimization, Vol. 13, No. 4, 1998, pp. 455–492.
Sasena, M., Flexibility and efficiency enhancements for constrained global design optimization with Kriging approximations, Ph.D. thesis, niversity of Michigan, 2002

Jordan, M. I., Jacobs, R. A, "Hierarchical mixtures of experts and the EM algorithm", Neural Comput. 6 (1994) 181–214.
Bettebghor, D., Bartoli, N., Grihon, S., Morlier, J., and Samuelides, M., "Surrogate modeling approximation using a mixture of experts based on EM joint estimation," Structural and Multidisciplinary Optimization, Vol. 43, No. 2, 2011, pp. 243–259
Liem, R. P., Mader, C. A., and Martins, J. R. R. A., "Surrogate Models and Mixtures of Experts in Aerodynamic Performance Prediction for Mission Analysis," Aerospace Science and Technology, Vol. 43, 2015, pp. 126–151

SEGOMOE main characteristics

$$\begin{cases} \min\limits_{x \in \mathbb{R}^d} & f(x) = [f_1(x), f_2(x), \cdots, f_n(x)] \\ \text{s.t.} & \\ c_1(x) \leq 0 \ldots c_j(x) = 0 \ldots c_m(x) \leq 0 & \end{cases}$$

1 to n objectives

d design variables

m mixed constraints

- **Mono & multi objective** Bayesian optimizer
- **Mono & Multi fidelity** sources
- Equality & inequality constraints (1 ~ 100 constraints)
- Intermediate dimension problem (1 ~ 100 variables)
- **Heterogenous variables** (continuous, discrete, categorical, hierarchical)
- Costly evaluation (CFD, FEM, objective and/or constraints)
- Handling non linear objectives & constraints (black box, no derivative available) and **hidden constraints**
- Based on **SMT** toolbox for surrogate models

- Remote access via a web interface ONERA WhatsOpt
- Opensource version in EgoBox (Mono Obj & Mono Fidelity)

The Journal of Open Source Software

egobox, a Rust toolbox for efficient global optimization

Bartoli, N., Lefebvre, T., Dubreuil, S., Olivanti, R., Priem, R., Bons, N., Martins, J.R.R.A., Bouhlel, M.-A. Bouhlel & Morlier, J. (2019). Adaptive modeling strategy for constrained global optimization with application to aerodynamic wing design. Aerospace Science and technology, 90, 85-102.

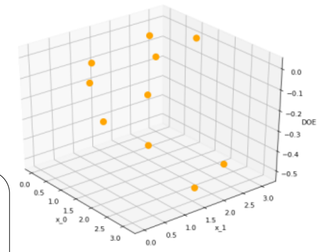
Lafage, R. (2022). egobox, a Rust toolbox for efficient global optimization. Journal of Open Source Software, 7(78), 4737

SEGOMOE algorithm – Mono objective

$$\begin{cases} \min_{\mathbf{x}\in\mathbb{R}^d} f(\mathbf{x}) \\ \text{s.t.} \\ c_1(\mathbf{x}) \leq 0 \\ \vdots \\ c_m(\mathbf{x}) \leq 0 \end{cases}$$

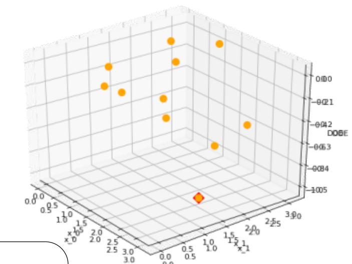
Problem definition

Initial DOE building

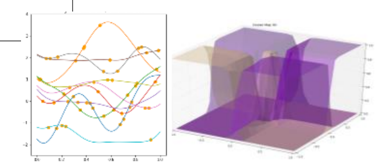


Building / Training Surrogate models

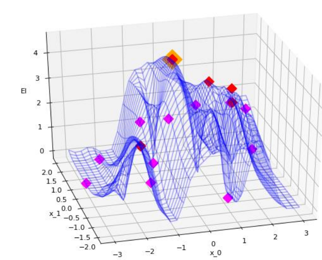
MOE SMT



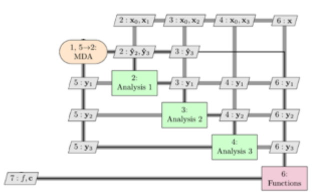
$(\hat{y}(\boldsymbol{x}), s^2(\boldsymbol{x}))$



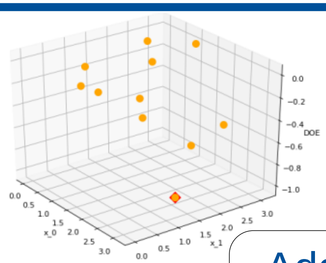
Optimization criteria



Evaluation of problem true functions



Adding new point to DOE



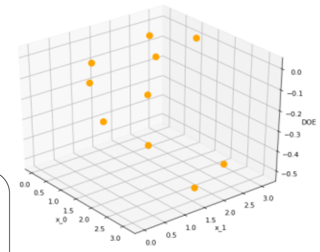
Bartoli, N., Lefebvre, T., Dubreuil, S., Olivanti, R., Priem, R., Bons, N., Martins, J.R.R.A., Bouhlel, M.-A. Bouhlel & Morlier, J. (2019). Adaptive modeling strategy for constrained global optimization with application to aerodynamic wing design. Aerospace Science and technology, 90, 85-102.

SEGOMOE algorithm – Mono objective

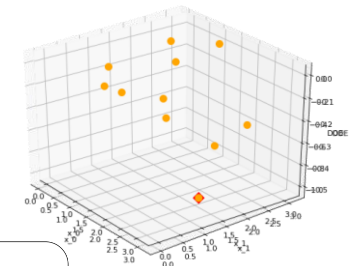
$$\begin{cases} \max_{\mathbf{x}\in\mathbb{R}^d} \mathrm{EI}(\mathbf{x})/\mathrm{WB2}(\mathbf{x})/\mathrm{WB2S}(\mathbf{x}) \\ \text{s.t.} \\ \hat{c_1}(\mathbf{x}) \leq 0 \\ \vdots \\ \hat{c_m}(\mathbf{x}) \leq 0 \end{cases}$$

Problem definition

Initial DOE building

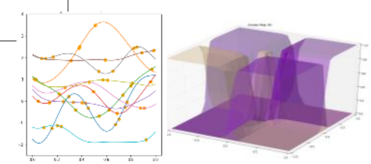


Building / Training Surrogate models

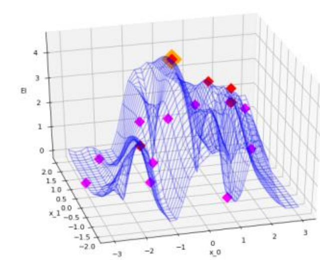


MOE SMT

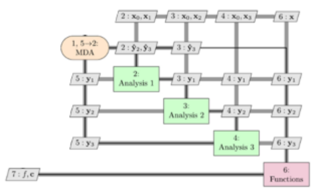
$(\hat{y}(\boldsymbol{x}), s^2(\boldsymbol{x}))$



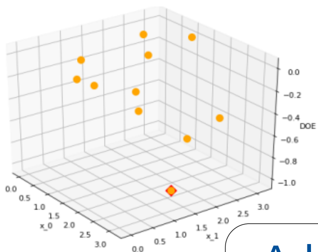
Optimization criteria



Evaluation of problem true functions



Adding new point to DOE



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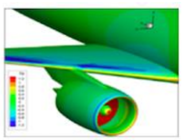
Some SEGOMOE application examples

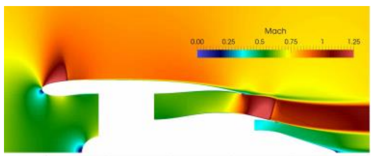
Phd M-A Bouhlel 2016, R. Priem 2020, R. Charayron 2023, P. Saves 2024, J. Bussemaker 2025

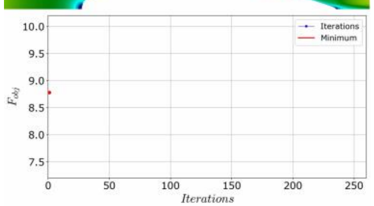
Nacelle aerodynamic

Mono, Continuous
d = 18, c = 2



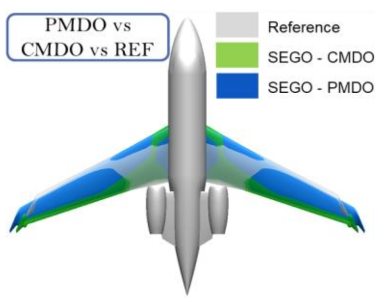
Mach number distribution





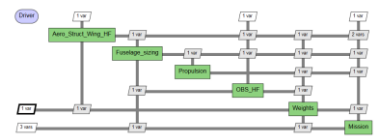
Bombardier Research Aircraft Configuration

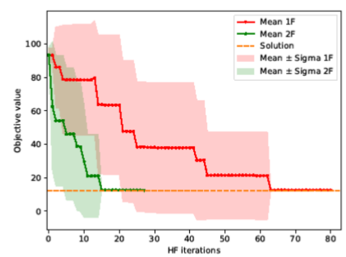
Mono, Continuous
d = 18, c = 8



Drone design electric aircraft

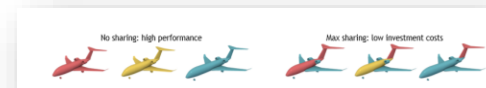
Mono, 2 fidelity levels
d = 15, c = 8

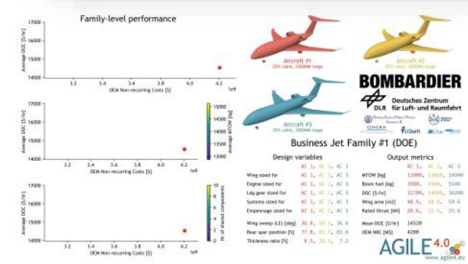




Business jet family

Multi, Mixed
d = 19, c = 2





Bartoli N, Lefebvre T, Dubreuil S, Panzeri M, d'Ippolito R, Anisimov K, Savelyev A. *Robust Nacelle Optimization design investigated in the AGILE European Project,* 19th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, AIAA AVIATION Forum, (AIAA 2018-3250)

Priem, R., Gagnon, H., Chittick, I., Dufresne, S., Diouane, Y., & Bartoli, N. (2020). An efficient application of Bayesian optimization to an industrial MDO framework for aircraft design. In AIAA aviation 2020 forum (p. 3152).

Charayron, R., Lefebvre, T., Bartoli, N., & Morlier, J. (2023). Towards a multi-fidelity & multi-objective Bayesian optimization efficient algorithm. Aerospace Science and technology, 142, 108673.

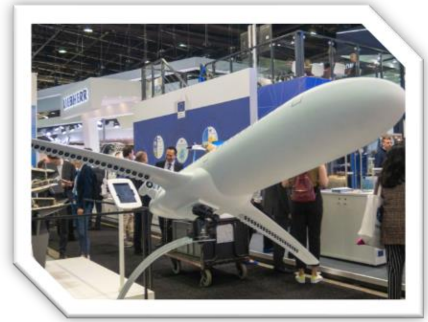
Bussemaker, J. H., Ciampa, P. D., Singh, J., Fioriti, M., Cabaleiro De La Hoz, C., Wang, Z., ... & Mandorino, M. (2022). Collaborative Design of a Business Jet Family Using the AGILE 4.0 MBSE Environment. In AIAA Aviation 2022 Forum (p. 3934).

Recent methodological developments

SEGOMOE capabilities

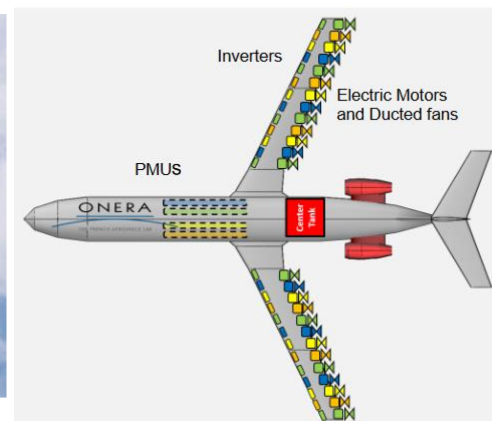
- To handle a large number of design variables
  → KPLS based models & Cooperative approach
- To handle heterogeneous functions
  → Mixture of experts models
- To handle highly non-convex constraints
  → Adapted acquisition function
- To handle mixed integer variables
  → Continuous relaxation & KPLS models
- To handle multifidelity models
  → 2-step approach based on multifidelity Kriging
- To handle multiple objectives
  → Predicted Pareto Front approach
- To handle hidden constraints
  → Comparisons of different strategies

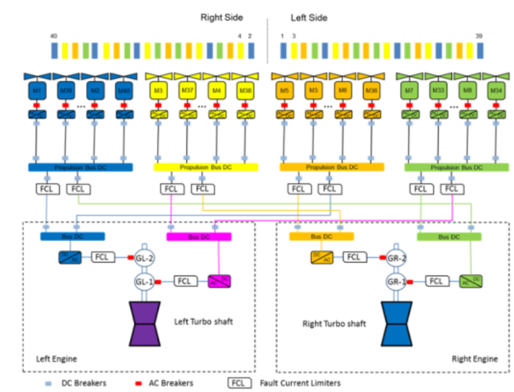
Application to mixed categorical optimization problem



DRAGON green aircraft concept

- ✓ **30% reduction of CO_2 emissions by 2035**
- ✓ **Distributed electric propulsion aircraft: propulsive efficiency**
- ✓ **150 passengers over 2750nm**
- ✓ **Transonic cruise speed (M0.78)**





Phd P. Saves in collaboration with E. Nguyen Van, C. David, S. Defoort

P. Schmollgruber, C. Doll, J. Hermetz, R. Liaboeuf, M. Ridel, I. Cafarelli, O. Atinault, C. Francois, and B. Paluch. “Multidisciplinary Exploration of DRAGON: an ONERA Hybrid Electric Distributed Propulsion Concept”. In: AIAA Scitech 2019, 2019

DRAGON green aircraft concept

FAST OAD

Future Aircraft Sizing Tool - Overall Aircraft Design

https://github.com/fast-aircraft-design/FAST-OAD

	Function/variable	Nature	Quantity	Range
Minimize	Fuel mass	cont	1	
	Total objectives		**1**	
with respect to	Fan operating pressure ratio	cont	1	[1.05, 1.3]
	Wing aspect ratio	cont	1	[8, 12]
	Angle for swept wing	cont	1	[15, 40] (°)
	Wing taper ratio	cont	1	[0.2, 0.5]
	HT aspect ratio	cont	1	[3, 6]
	Angle for swept HT	cont	1	[20, 40] (°)
	HT taper ratio	cont	1	[0.3, 0.5]
	TOFL for sizing	cont	1	[1800., 2500.] (m)
	Top of climb vertical speed for sizing	cont	1	[300., 800.](ft/min)
	Start of climb slope angle	cont	1	[0.075., 0.15.](rad)
	Total continuous variables		10	
	Turboshaft layout	cat	2 levels	{1,2}
2 possibilities	Architecture_cat	cat	17 levels	{1,2,3, . . . ,15,16,17}
	Number of cores	int	1	{2,4,6}
	Number of motors*	int	1	{8,12,16,20,. . . ,40}
	*graph-structure dependence to the core value			
subject to	Wing span < 36 (m)	cont	1	
	TOFL < 2200 (m)	cont	1	
	Wing trailing edge occupied by fans < 14.4 (m)	cont	1	
	Climb duration < 1740 (s)	cont	1	
	Top of climb slope > 0.0108 (rad)	cont	1	
	Total constraints		**5**	

Categorical
or
Hierarchical

- *10 continuous design variables*
- *2 categorical design variables*
  - *Electric propulsion Architecture: 17 choices*
  - *Turboshaft layout: 2 choices*

➔ 29 variables in relaxed dimension
➔ 14 variables in relaxed dimension

- 5 inequality constraints (MC)
- Fuel mass to minimize

17x2 possibilities ➔ 34 associated optimization problems to solve ☹
or use dedicated kernels in your GP models ➔ 1 optimization problem to solve ☺

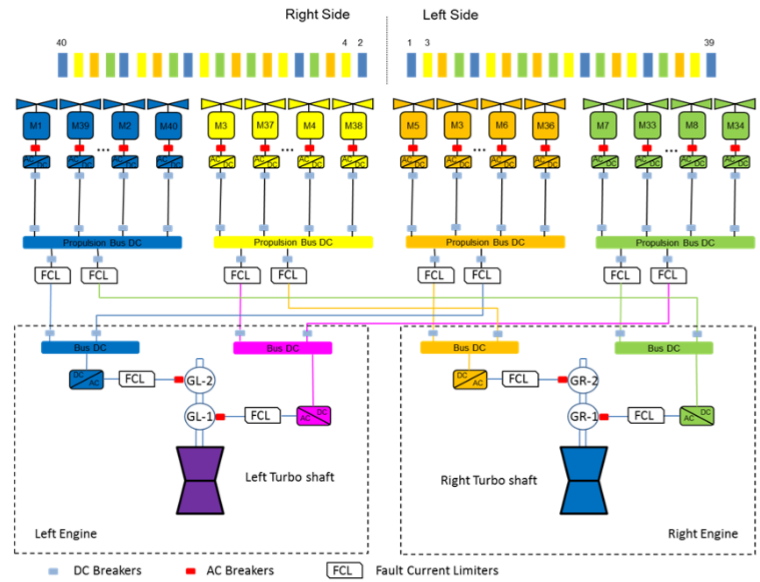
Saves, P., Bartoli, N., Diouane, Y., Lefebvre, T., Morlier, J., David, C., ... & Defoort, S. (2022). Bayesian optimization for mixed variables using an adaptive dimension reduction process: applications to aircraft design. In *AIAA SCITECH 2022 Forum* (p. 0082).

DRAGON optimization test case

Architecture	cat	17 levels	{1,2,3, . . . ,15,16,17}
Turboshaft layout	cat	2 levels	{1,2}
Total categorical variables		2	
Total relaxed variables		**29**	

Architecture number	number of generators	number of motors
1	2	8
2	2	12
3	2	16
4	2	20
5	2	24
6	2	28
7	2	32
8	2	36
9	2	40
10	4	8
11	4	16
12	4	24
13	4	32
14	4	40
15	6	12
16	6	24
17	6	36

Neutral Meta Decreed



layout	position	y ratio	tail	VT aspect ratio	VT taper ratio
1	under wing	0.25	without T-tail	1.8	0.3
2	behind	0.34	with T-tail	1.2	0.85

- 2 possibilities for dealing with categorical variables:

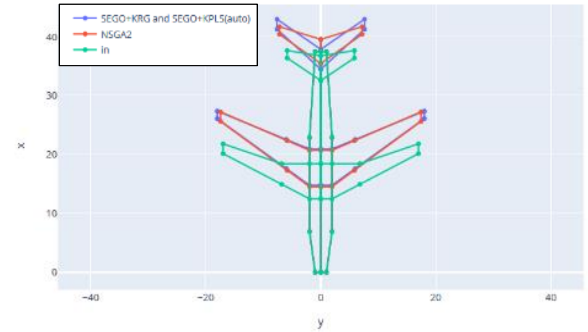
➔ **Categorical choice:**
29 variables in relaxed dimension (10+17+2)

➔ **Hierarchical choice:**
14 variables in relaxed dimension (10+2+2)

- Need dedicated kernels (with adapted distance)

Saves, P., Bartoli, N., Diouane, Y., Lefebvre, T., Morlier, J., David, C., ... & Defoort, S. (2022). Bayesian optimization for mixed variables using an adaptive dimension reduction process: applications to aircraft design. In *AIAA SCITECH 2022 Forum* (p. 0082).

DRAGON optimization results



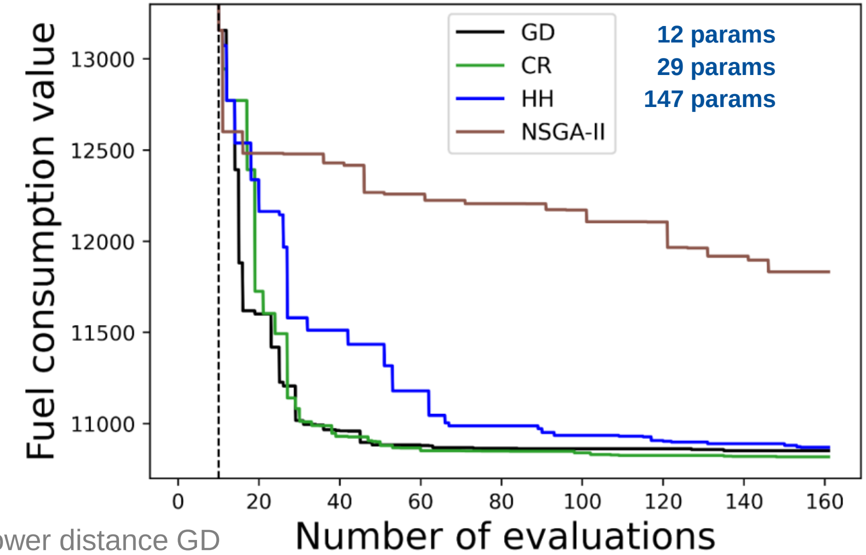
Comparison of BO with different kernels & NSGAII

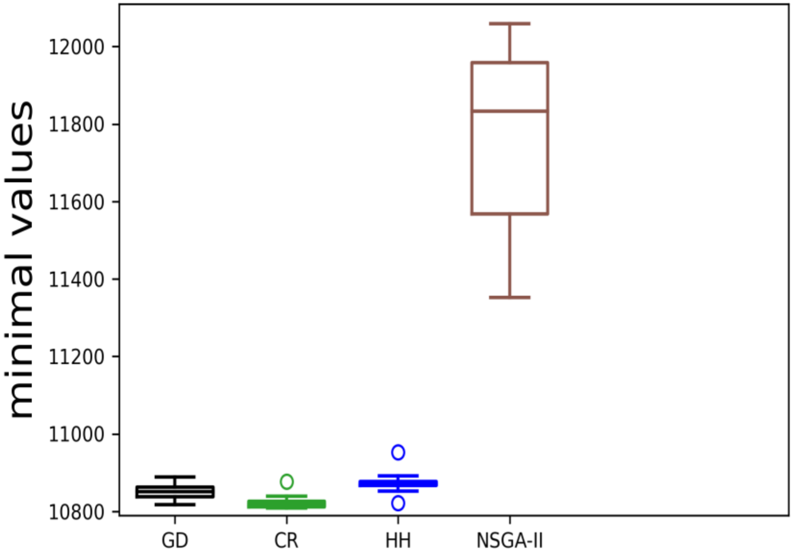
10 runs of (10 + 150) iterations

Convergence plots

Categorical variants without PLS

Boxplots
after 160 evaluations

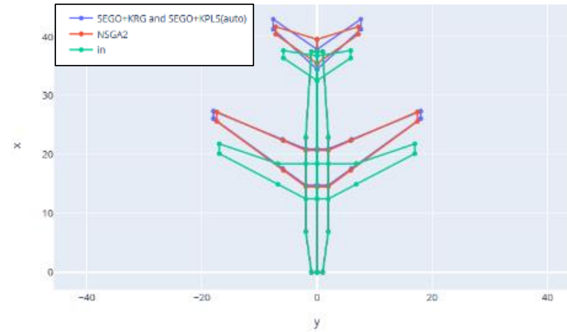




Gower distance GD
Continuous Relaxation CR
Homoscedastic hypersphere HH

Saves, P., Bartoli, N., Diouane, Y., Lefebvre, T., Morlier, J., David, C., ... & Defoort, S. (2022). Bayesian optimization for mixed variables using an adaptive dimension reduction process: applications to aircraft design. In *AIAA SCITECH 2022 Forum* (p. 0082)
Blank J. and Deb K., pymoo: Multi-Objective Optimization in Python, in IEEE Access, vol. 8, pp. 89497-89509, 2020, doi: 10.1109/ACCESS.2020.2990567

DRADRAGON optimization results

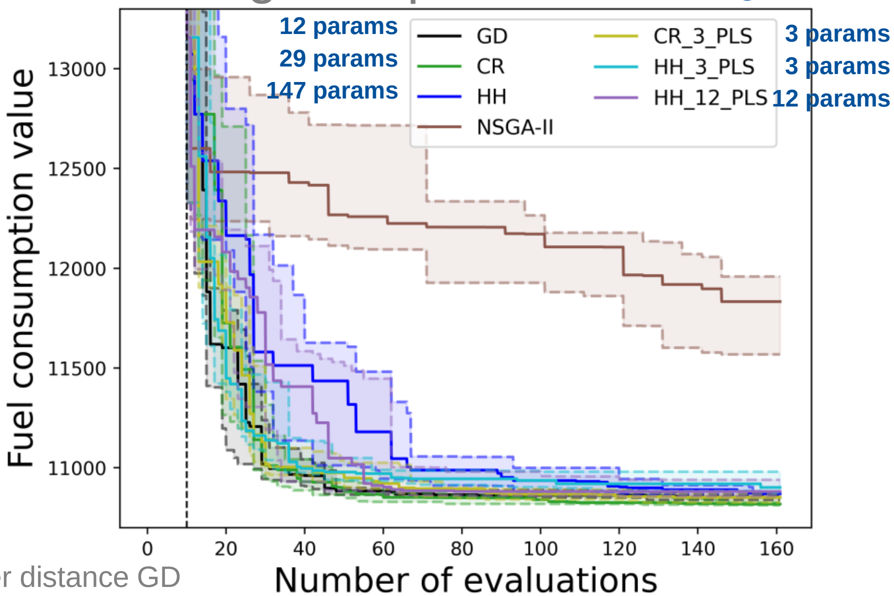


Comparison of BO with different kernels & NSGAII

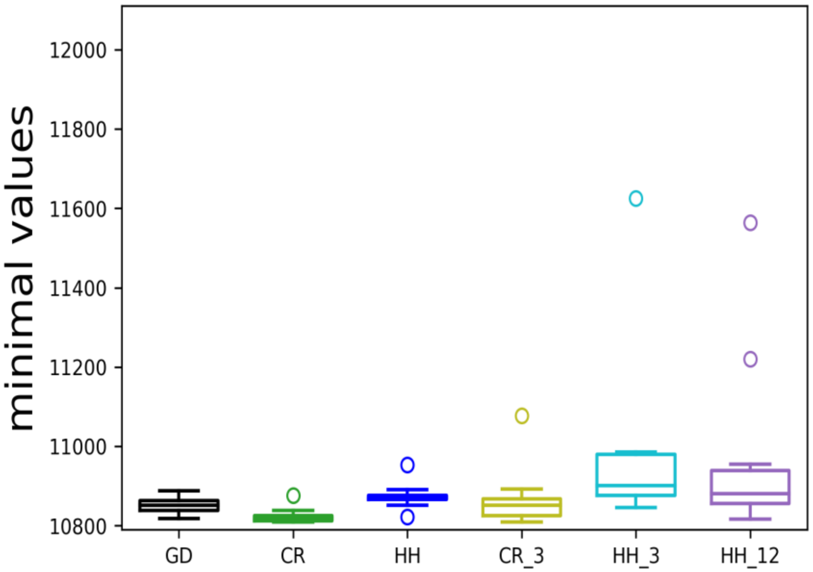
10 runs of (10 + 150) iterations

Convergence plots

Categorical variants with PLS



Boxplots
after 160 evaluations



Gower distance GD
Continuous Relaxation CR
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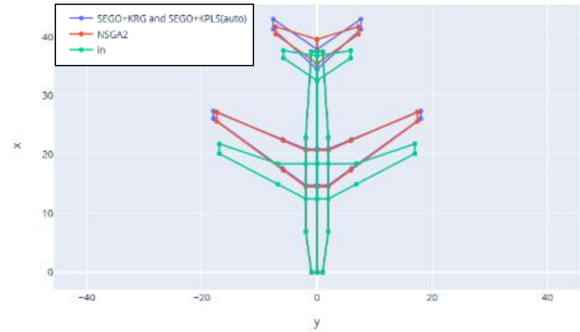
DRAGON optimization results



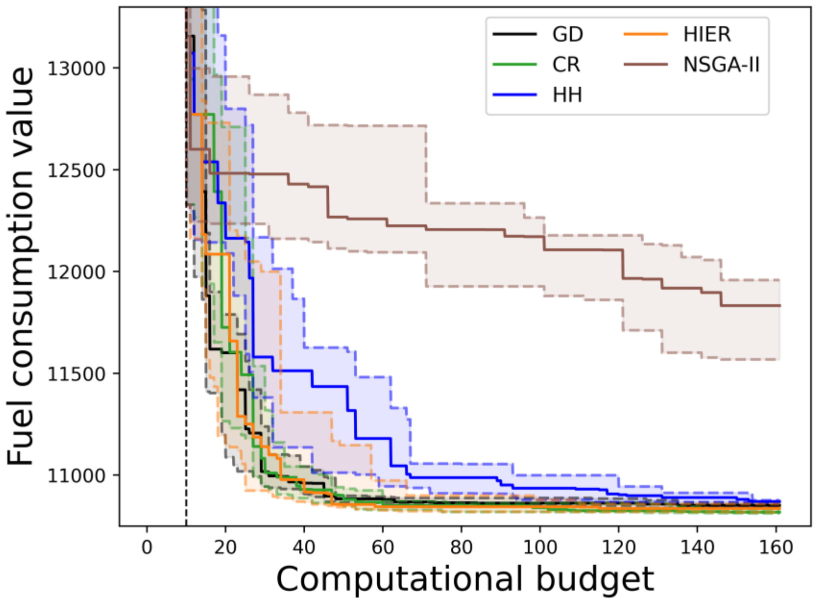
Comparison of BO with different kernels & NSGAII

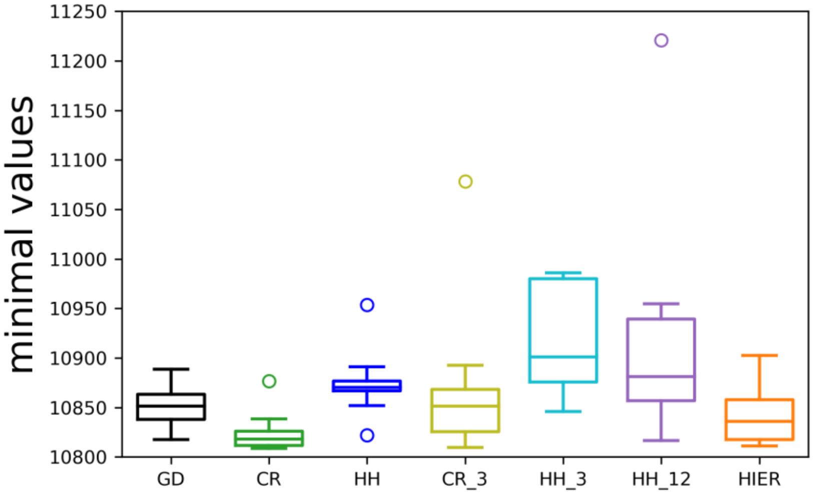
10 runs of (10 + 150) iterations

Convergence plots

Categorical or Hierarchical variants

Boxplots
after 160 evaluations





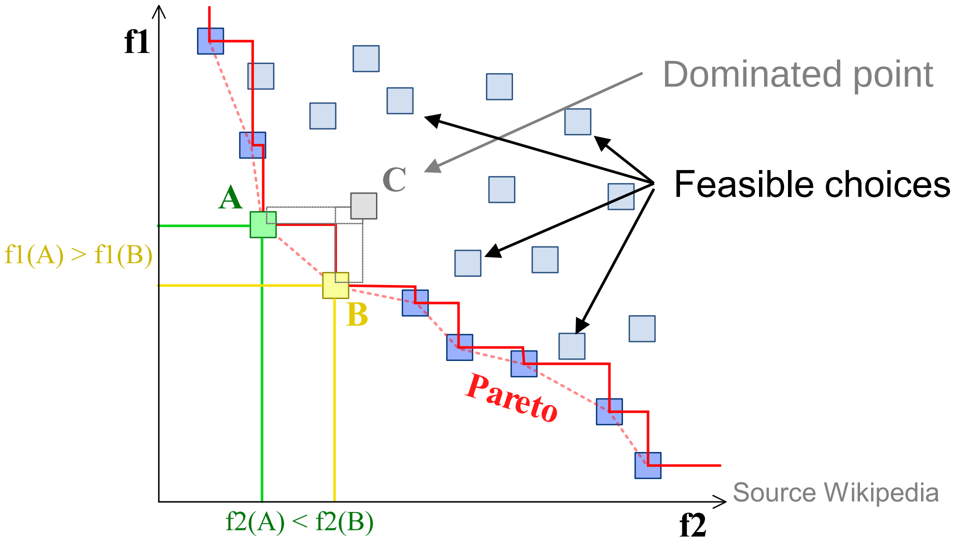
➔Hierarchical choice: best trade off convergence & CPU time

Saves, P., Bartoli, N., Diouane, Y., Lefebvre, T., Morlier, J., David, C., ... & Defoort, S. (2022). Bayesian optimization for mixed variables using an adaptive dimension reduction process: applications to aircraft design. In *AIAA SCITECH 2022 Forum* (p. 0082).

How to perform a multiobjective optimization?

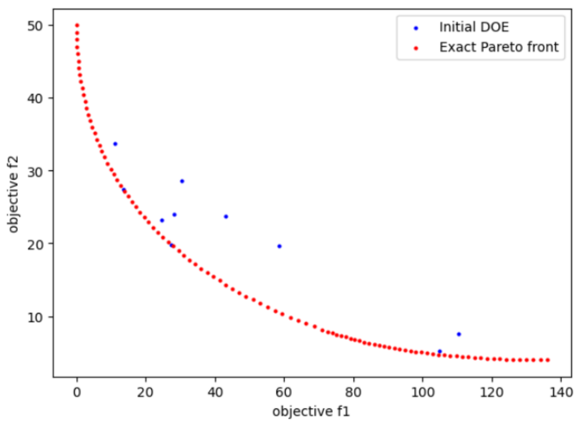
$$\begin{cases} \min\limits_{\boldsymbol{x}\in\mathbb{R}^d} \quad \boldsymbol{f} = [f_1(\boldsymbol{x}), f_2(\boldsymbol{x}), \cdots, f_n(\boldsymbol{x})] \\ \text{s.t.} \\ c_1(\boldsymbol{x}) \leq 0 \\ \vdots \\ c_m(\boldsymbol{x}) \leq 0 \end{cases}$$

***n* objectives**



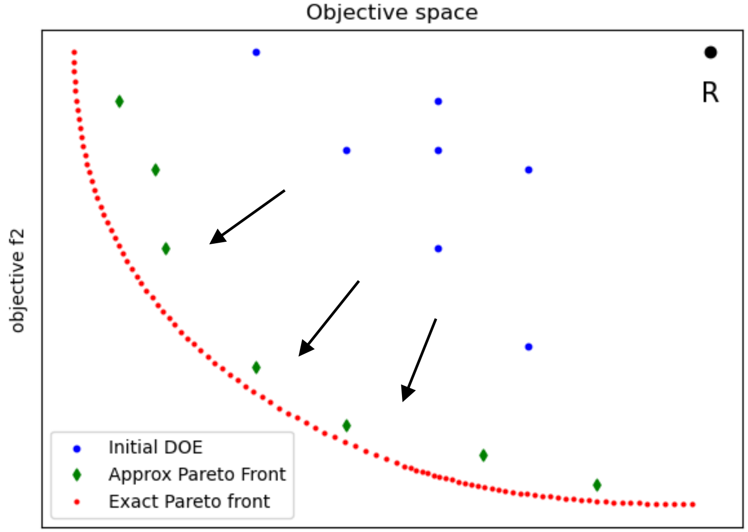
Source Wikipedia

Build a Pareto Front (non dominated points)



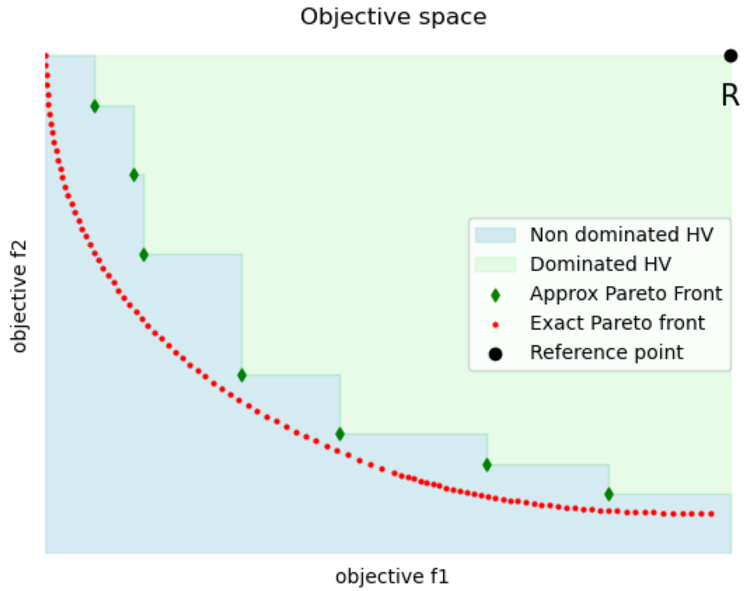
Internship R. Grapin 2021-2022

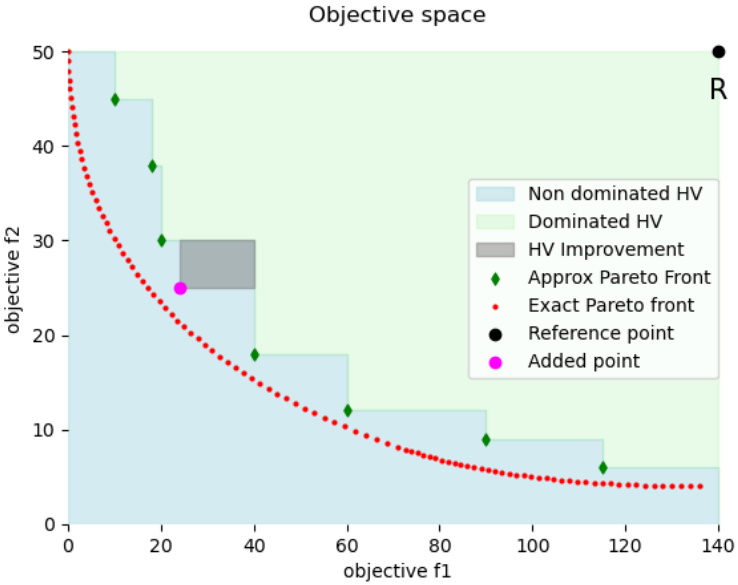
Multi objective: HyperVolume Improvement



From the initial DOE
add new points in order to
improve the Hyper Volume

Infill criterion based on Gaussian Process each objective i: $\mathcal{N}(\hat{y}_i(x), s_i^2(x))$





New infill criterion proposed for Multi-objective

$$f(\mathrm{x}) \Rightarrow Y(x) = \mathcal{N}(\hat{y}(\boldsymbol{x}), s^2(\boldsymbol{x}))$$

- Mono-objective $\mathrm{WB2S}(\boldsymbol{x}) = s\,\mathrm{EI}(\boldsymbol{x}) - \hat{y}(\boldsymbol{x})$

scaling factor

- Multi-objective $\alpha_{\boldsymbol{f}}^{\mathrm{reg}}(\boldsymbol{x}) = \gamma\,\alpha_{\boldsymbol{f}}(\boldsymbol{x}) - \psi(\mu_{\boldsymbol{f}}(\boldsymbol{x}))$

Acquisition function $\alpha_{\boldsymbol{f}}(\boldsymbol{x}) = \mathrm{EHVI}(\boldsymbol{x}), \mathrm{PI}(\boldsymbol{x}), \mathrm{MPI}(\boldsymbol{x}), \ldots$

based on Hyper Volume Improvment

Regularized choices

$$\begin{cases} (\mathrm{reg} = \max) & : \quad \psi(\hat{\boldsymbol{y}}(\boldsymbol{x})) = \max_{i \leq n} \hat{y}_i(\boldsymbol{x}) \\ (\mathrm{reg} = \mathrm{sum}) & : \quad \psi(\hat{\boldsymbol{y}}(\boldsymbol{x})) = \sum_{i=1}^{n} \hat{y}_i(\boldsymbol{x}) \end{cases}$$

Bartoli, N., Lefebvre, T., Dubreuil, S., Olivanti, R., Priem, R., Bons, N., Martins, J. R. A. A., Morlier, J. Adaptive modeling strategy for constrained global optimization with application to aerodynamic wing design. Aerospace Science and Technology, 90:85–102, 2019.
Grapin, R., Diouane, Y., Morlier, J., Bartoli, N., Lefebvre, T., Saves, P., & Bussemaker, J. H. (2022). Constrained Multi-Objective Bayesian Optimization with Application to Aircraft Design. In AIAA AVIATION 2022 Forum (p. 4053)

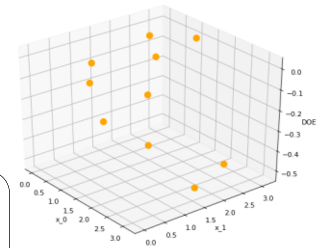
SEGOMOE algorithm – Multi objective

$$\begin{cases} \min\limits_{x \in \mathbb{R}^d} \quad f = [f_1(x), f_2(x), \cdots, f_n(x)] \\ \text{s.t.} \\ c_1(x) \leq 0 \\ \vdots \\ c_m(x) \leq 0 \end{cases}$$

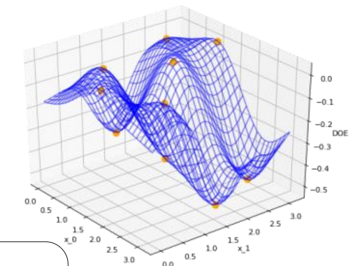
***n* objectives**

Problem definition

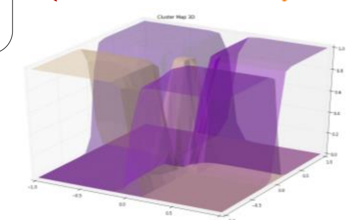
Initial DOE building



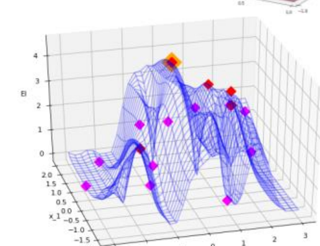
Building / Training Surrogate models



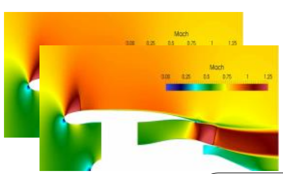
MOE SMT



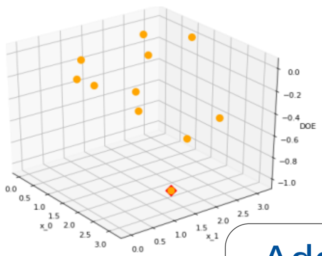
Optimization criteria



Evaluation of problem true functions



Adding new point to DOE



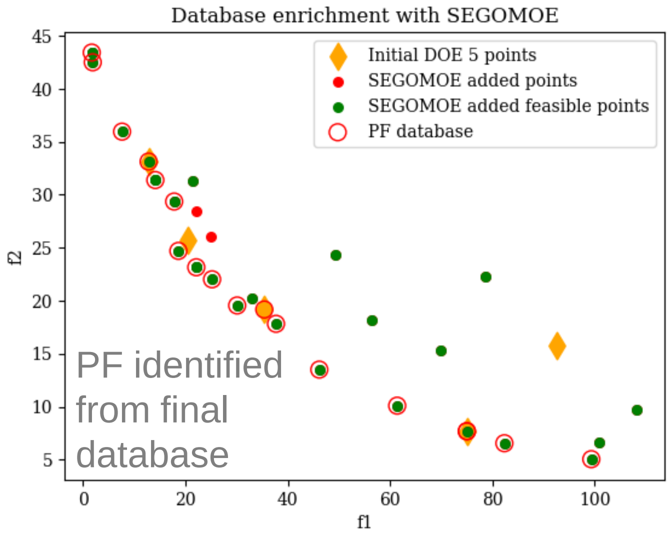
Grapin, R., Diouane, Y., Morlier, J., Bartoli, N., Lefebvre, T., Saves, P., & Bussemaker, J. H. (2022). Constrained Multi-Objective Bayesian Optimization with Application to Aircraft Design. In AIAA AVIATION 2022 Forum (p. 4053)

SEGOMOE algorithm – Multi objective

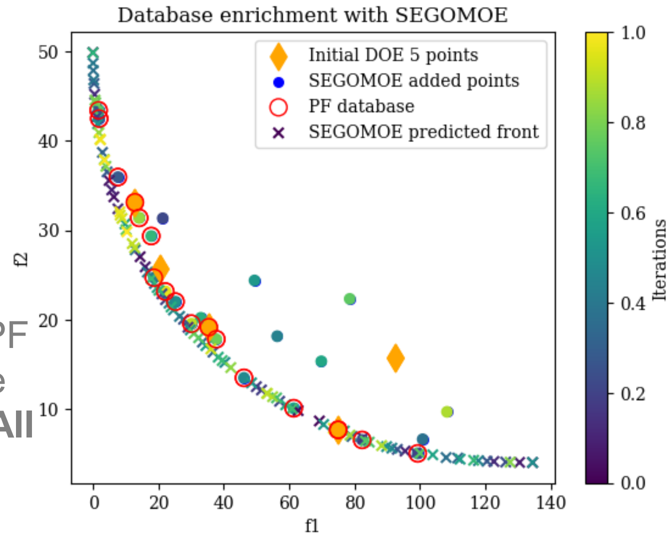
***N* iterations reached**

Initial DOE (n_{DOE} points)
+ enriched database (***N*** points)

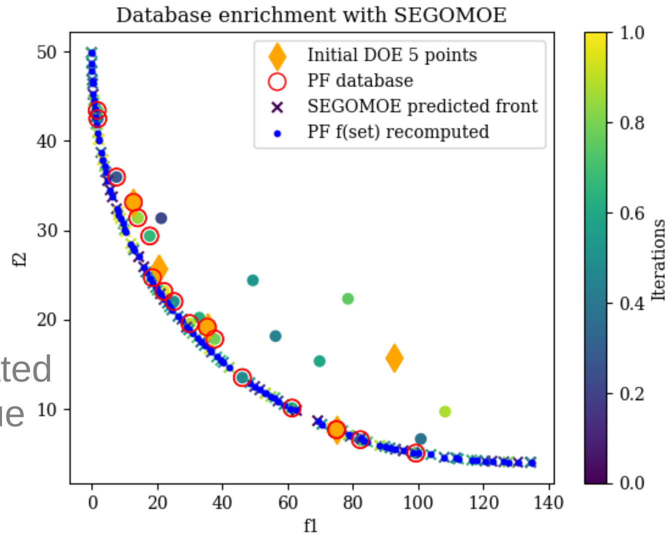
Build final Surrogate models from these (n_{DOE} + ***N***) points



→ Predicted PF from surrogate models (**NSGAII algo**)



→Re-evaluated PF from true functions



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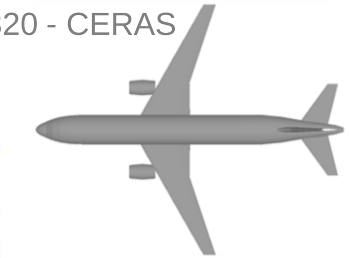
SEGOMOE validation – Multi Objective applications

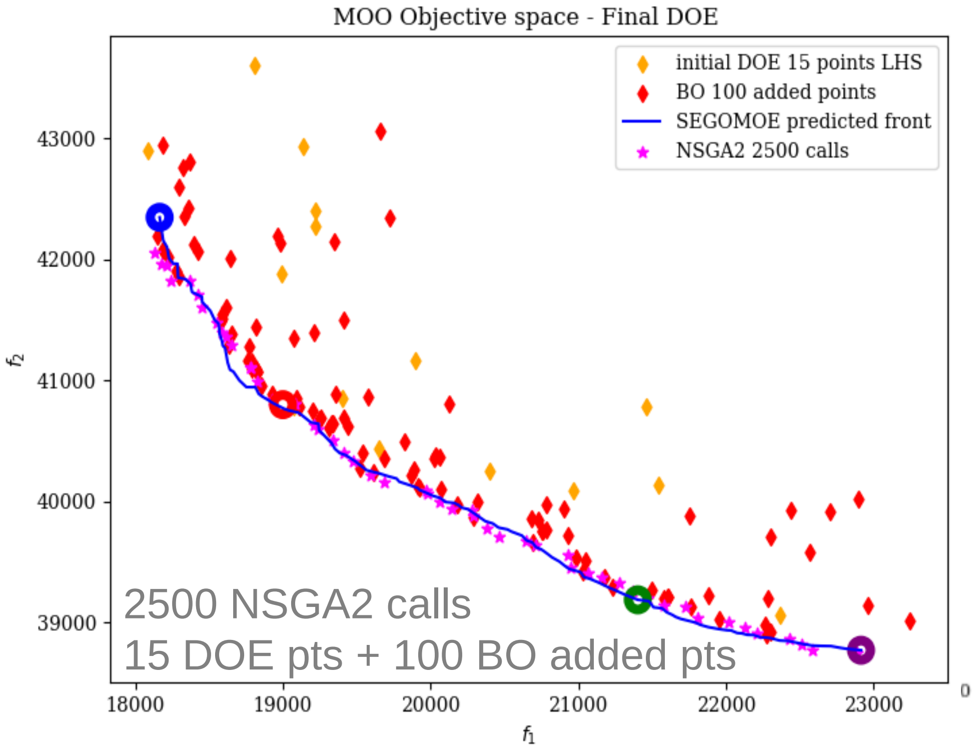
2 objectives
5 variables
3 ineq. constraints

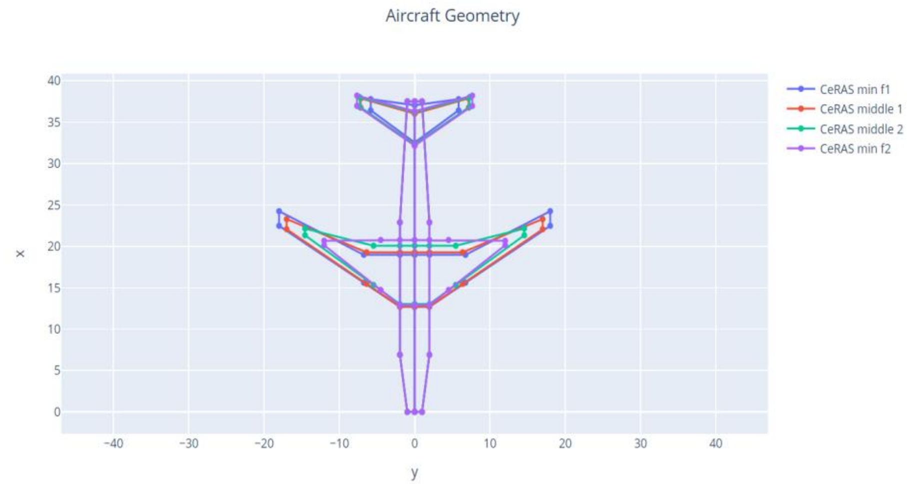
$$
\begin{cases}
\min_{x\in\mathbb{R}^5} \quad (fuel\ mass,\ operating\ weight\ empty) \\
\\
\text{with respect to} \\
\quad data : geometry : wing : MAC : at25percent : x \quad \in [16.0, 18.0] \\
\quad data : geometry : wing : aspect\_ratio \quad \in [5.0, 11.0] \\
\quad data : geometry : horizontal\_tail : aspect\_ratio \quad \in [1.5, 6.0] \\
\quad data : geometry : wing : taper\_ratio \quad \in [0., 1.0] \\
\quad data : geometry : wing : sweep\_25 \quad \in [20., 30.0] \\
\text{and such that} \\
\quad data : handling\_qualities : static\_margin < 0.1 \\
\quad data : handling\_qualities : static\_margin > 0.05 \\
\quad data : geometry : wing : span < 36
\end{cases}
$$

A320 - CERAS



FAST OAD





➔ 2500 NSGA2 calls
compared with 115 BO calls (15 DOE pts + 100 added pts)

Grapin, R., Diouane, Y., Morlier, J., Bartoli, N., Lefebvre, T., Saves, P., & Bussemaker, J. H. (2022). Constrained Multi-Objective Bayesian Optimization with Application to Aircraft Design. In AIAA AVIATION 2022 Forum (p. 4053)
Blank, J., & Deb, K. (2020). Pymoo: Multi-objective optimization in python. Ieee access, 8, 89497-89509.

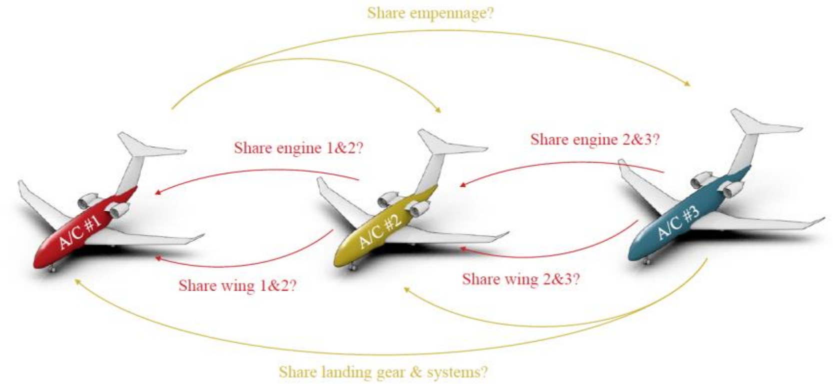
Outline

- Kriging based surrogate models
- Bayesian optimization
  - mono & multiobjective
  - mono & multifidelity
- AGILE 4.0 applications

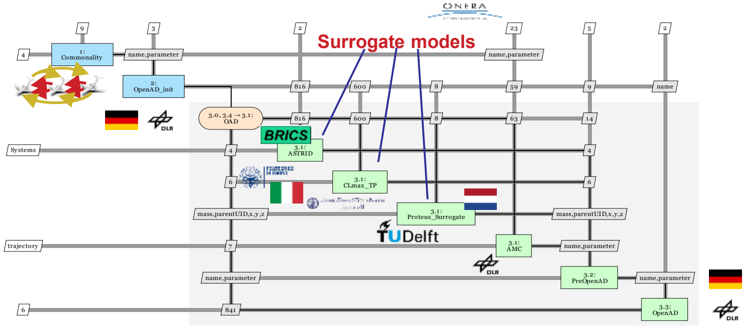
In collaboration with R. Lafage, J. H. Bussemaker, G. Donelli, J. M. Gomes de Mello,M. Mandorino, P. Della Vecchia

Family concept design

- Tradeoff between commonality and performance
- Application: business jet family
  - Use case owner: Bombardier
  - Three 8-pax business jets
  - Variations in range and cabin length



- Share systems, landing gear, wings, engines, empennage
- One wing platform per-member basis (conforming to commonality selection)



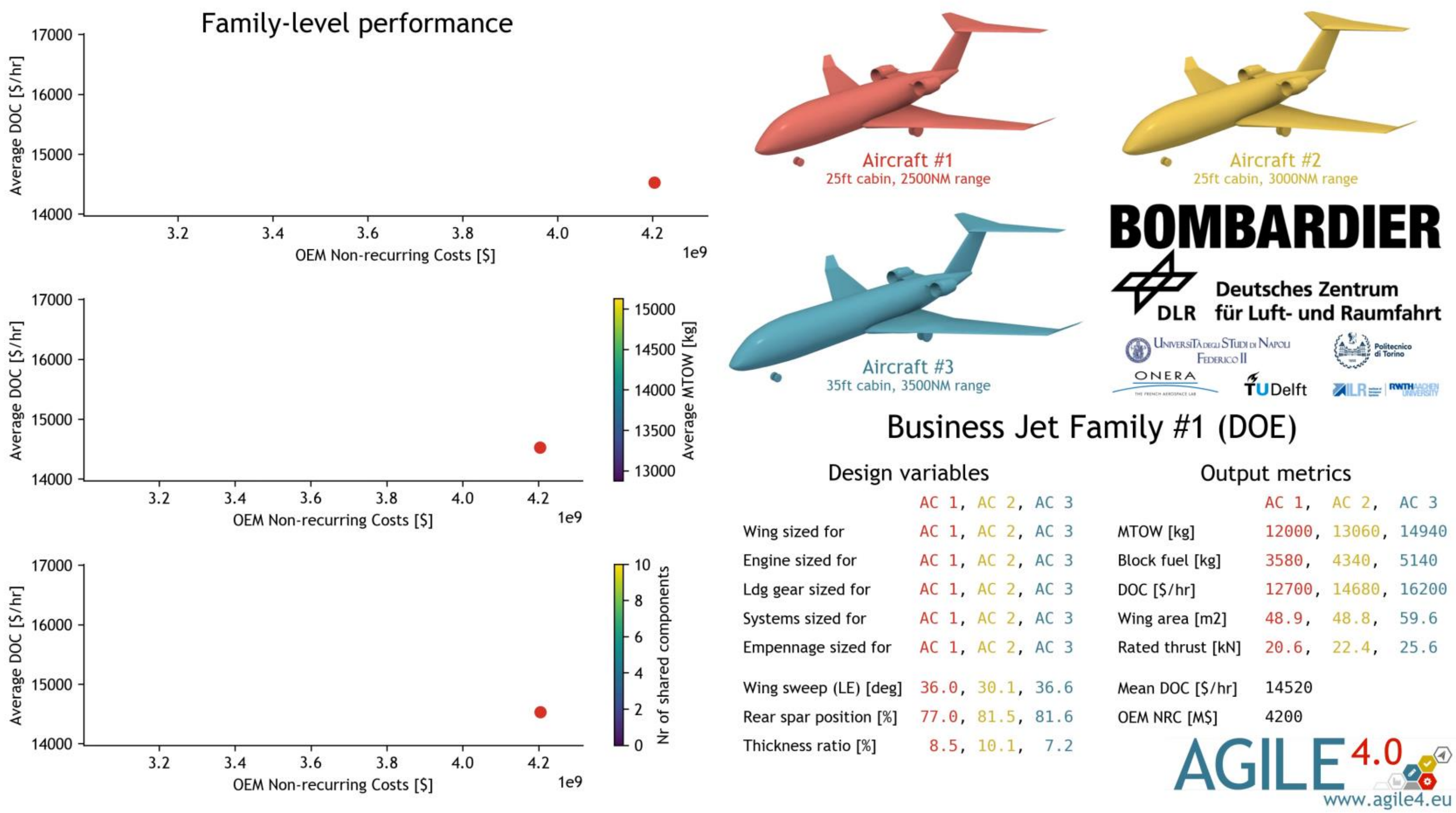
MDA: 1 hour for a family

Select the best family with commonality choices (wing, engine, empennage)

Objectives	**2 obj: Min (**Direct Operating Costs, OEM Non – Recurring Costs)
Design variables	**10 categorical**: commonality with 2 levels **9 continuous**: Leading edge sweep, rear spar location, Wing t/c for each family member
Constraints	**2 ineq. :** Balanced Field Length, Landing Field Lenght

Bussemaker, J. H., Ciampa, P. D., Singh, J., Fioriti, M., Cabaleiro De La Hoz, C., Wang, Z., ... & Mandorino, M. (2022). Collaborative Design of a Business Jet Family Using the AGILE 4.0 MBSE Environment. In AIAA Aviation 2022 Forum (p. 3934).

Family concept design



Conclusions and perspectives

- Bayesian Optimization for MDO
  - **Mixed-discrete, hierarchical**, mono and **multi-objective**, constrained
  - Subject to hidden constraints (PhD A. Tfaily McGill & Bombardier 2025, PhD J. Bussemaker DLR & TUD, 2025)
  - Extension to multi-fidelity models & data fusion (PhD M. Aguirre Castano UPHF & ONERA)
- High dimensional problem
  - Linear, random or supervised embeddings (PhD A. Durand, PolyMontréal & ONERA)
  - Cooperative strategy (PhD L. Pretsch, TUM&MTU 2025) & different acquisition functions (Internship P. Dobeli 2025)

➔ Application to more complex problems

COLOSSUS
COLLABORATIVE SYSTEM OF SYSTEMS

Wildfire fighting case

Urban air mobility

➔ Extend GP for **high dimensional** hierarchical **systems of systems** optimization

➔ Extend Bayesian optimization for high-dimensional **variable-size** multi-fidelity problems

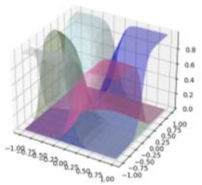
Two frameworks

SMT

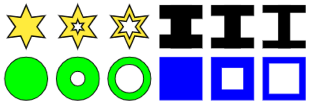
github.com/SMTorg/smt

SMT: Surrogate Modeling Toolbox

- Open source python toolbox: surrogate modeling methods, sampling techniques, and benchmarking functions
- Focus on derivatives (training derivatives used for gradient-enhanced modeling, prediction derivatives)
- New Kriging based surrogate models for higher dimension (KPLS and KPLS-K)
- Noisy Kriging to handle uncertainties on data
- Multifidelity Kriging with or without n MFKPLS)
- Mixture of experts technique for heterogeneous functions

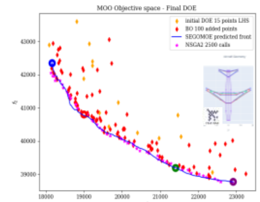


- Mixed integer Kriging to handle **discrete and categorical variables**

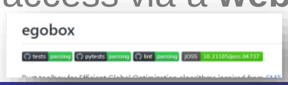


SEGOMOE

- **Mono & multi objective Bayesian optimizer**
- **Mono & Multi fidelity sources**
- Handling non linear objectives & constraints (black box, no derivative available)
- Equality & inequality constraints (1 ~ 100 constraints)
- Intermediate dimension problem (1 ~ 100 variables)



- Heterogenous variables (continuous, discrete, categorical)
- Costly evaluation (CFD, FEM, objective and/or constraints)
- Hidden constraints
- Based on SMT toolbox for surrogate models
- Remote access via a **web interface**



ONERA WhatsOpt

SEGOMOE vs EGObox

github.com/relf/egobox

JOSS
The Journal of Open Source Software
egobox, a Rust toolbox for efficient global optimization

Features	SEGOMOE	EGObox
EGO-like optimizer	✓	✓
Constrained optim	✓	✓
Mixture of experts	✓	✓
PLS dim reduction	✓	✓
Parallel Evaluation	✓	✓
CoEGO/CCBO	✓	✓
Mixed-variables optim	✓ (mixed-int kernels)	✓ (cont. relax. only)
Multi fidelity	✓	✗
Multi objective	✓	✗
Hierarchical variables	✓	✗
Trust-region EGO		✓
Licence	NDA	Open-source (Apache 2.0)
Language	Python	Rust + Python binding

Bartoli, N., Lefebvre, T., Dubreuil, S., Olivanti, R., Priem, R., Bons, N., Martins, J.R.R.A., Bouhlel, M.-A. Bouhlel & Morlier, J. (2019). Adaptive modeling strategy for constrained global optimization with application to aerodynamic wing design. Aerospace Science and technology, 90, 85-102.
Lafage, R. (2022). egobox, a Rust toolbox for efficient global optimization. Journal of Open Source Software, 7(78), 4737

Collaborative Optimization