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ONERA



THE FRENCH AEROSPACE LAB

www.onera.fr

Bayesian Optimization: mixed integer and multiobjective applications

Nathalie Bartoli (ONERA - DTIS/M2CI)

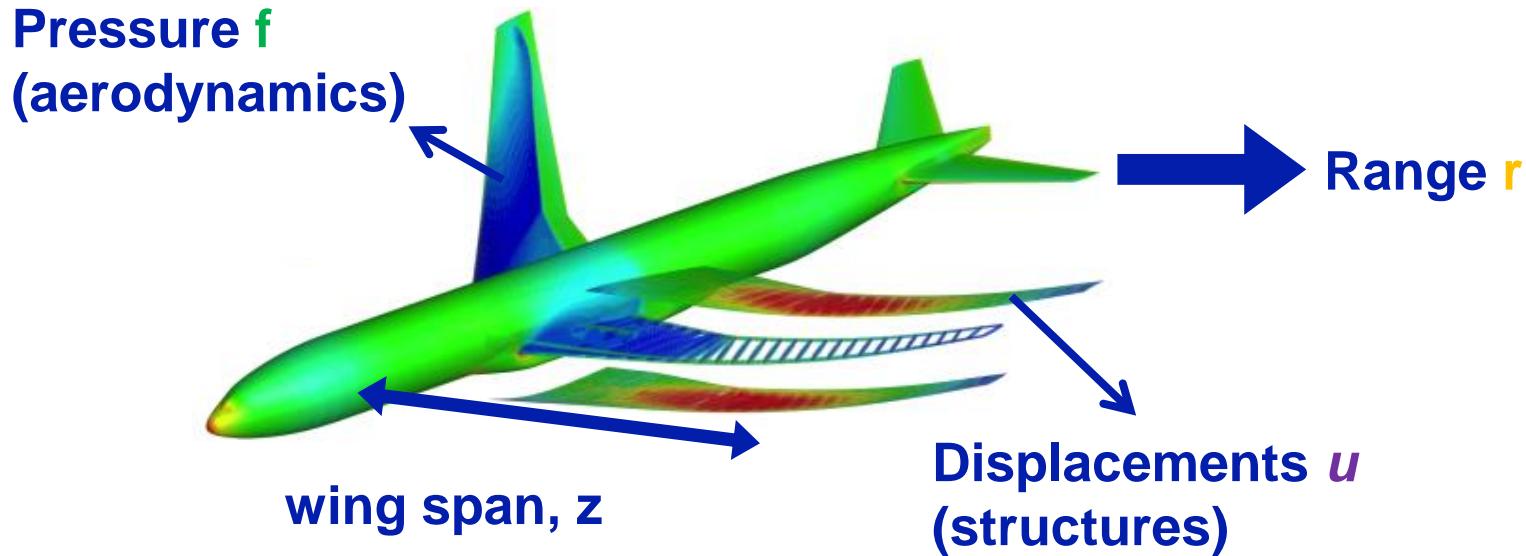
Thierry Lefebvre (ONERA - DTIS/M2CI)



Youssef Diouane
Joseph Morlier
Paul Saves



Different strategies



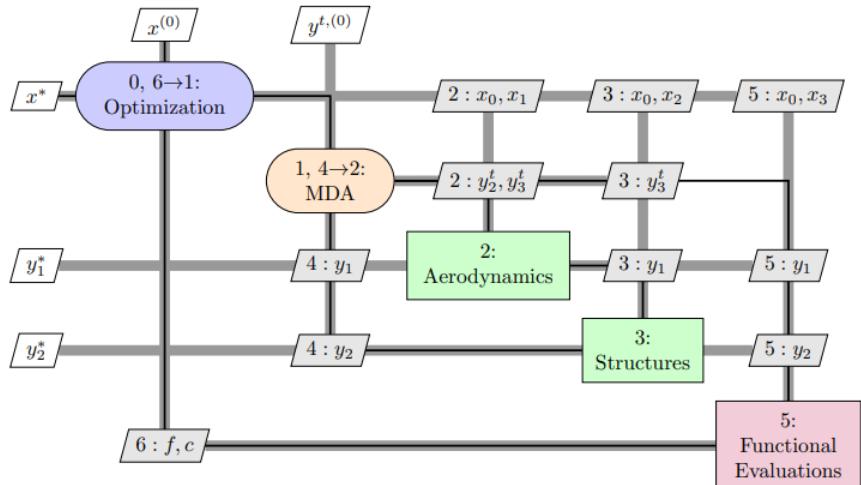
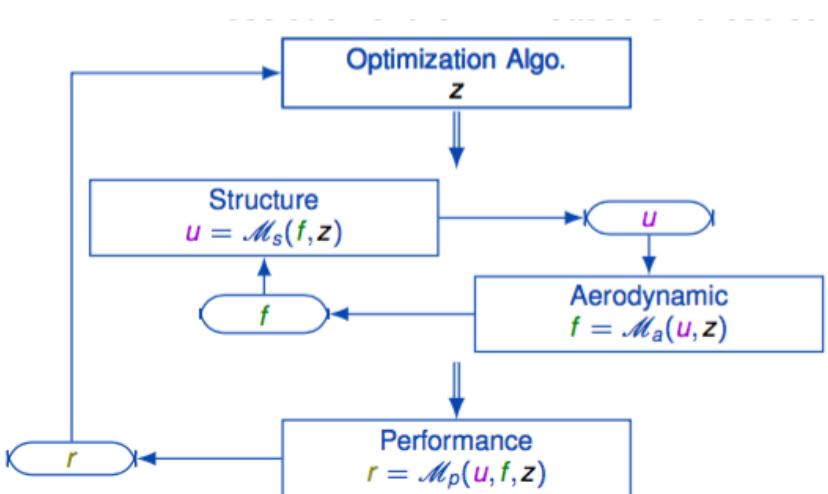
Lambe, A. B., & Martins, J. R. (2012). Extensions to the design structure matrix for the description of multidisciplinary design, analysis, and optimization processes. *Structural and Multidisciplinary Optimization*, 46(2), 273-284.

Jasa, J. P., Hwang, J. T., & Martins, J. R. (2018). Open-source coupled aerostructural optimization using Python. *Structural and Multidisciplinary Optimization*, 57(4), 1815-1827.

Hwang, J. T., & Martins, J. R. (2018). A computational architecture for coupling heterogeneous numerical models and computing coupled derivatives. *ACM Transactions on Mathematical Software (TOMS)*, 44(4), 37.

Gill, P. E., Murray, W., & Saunders, M. A. (2005). SNOPT: An SQP algorithm for large-scale constrained optimization. *SIAM review*, 47(1), 99-131.

Different strategies



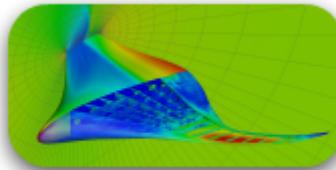
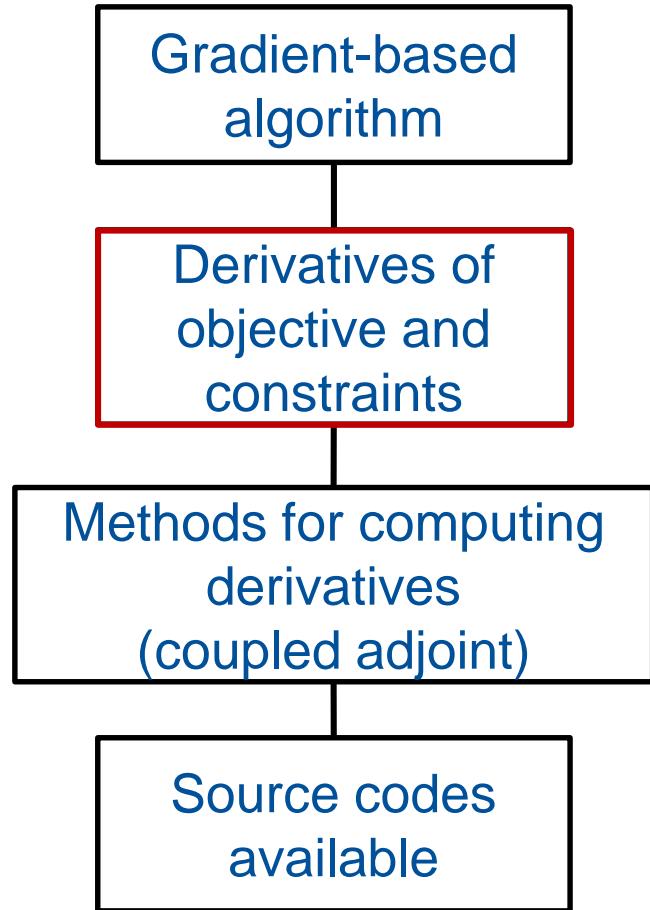
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Different strategies



MDOlab strategy within OpenMDAO

Python user script Setup up the problem: objective function, constraints, design variables, optimizer and solver options			
Optimizer interface <i>pyOptSparse</i> Common interface to various optimization software	Aerostructural solver <i>AeroStruct</i> Coupled solution methods and coupled derivative evaluation	Geometry modeler <i>DVGeometry/GeoMACH</i> Defines and manipulates geometry, evaluates derivatives	SNOPT Other optimizers Flow solver <i>ADflow</i> Governing and adjoint equations Structural solver <i>TACS</i> Governing and adjoint equations
SNOPT	Other optimizers	Flow solver <i>ADflow</i> Governing and adjoint equations	Structural solver <i>TACS</i> Governing and adjoint equations

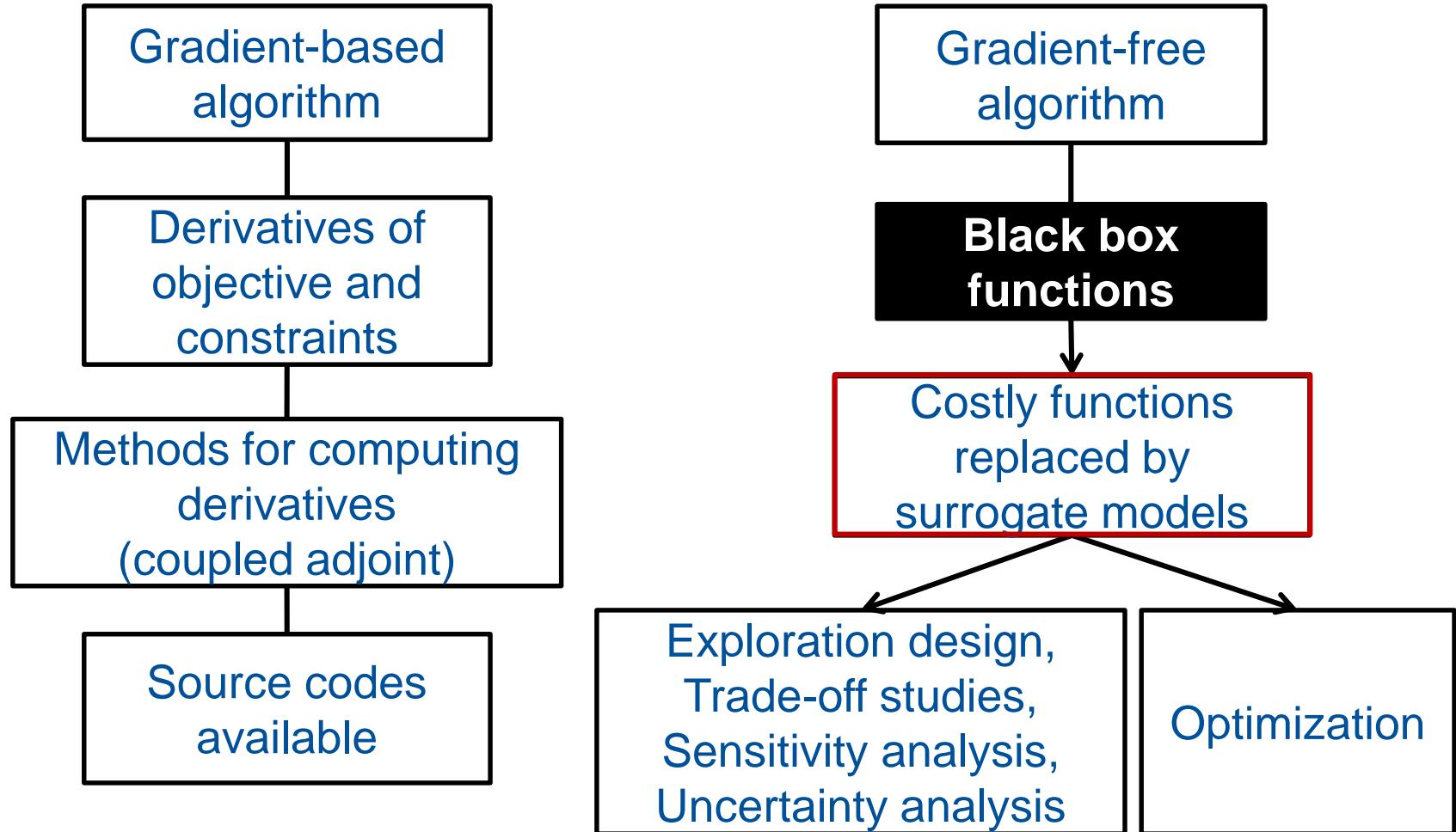
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Different strategies

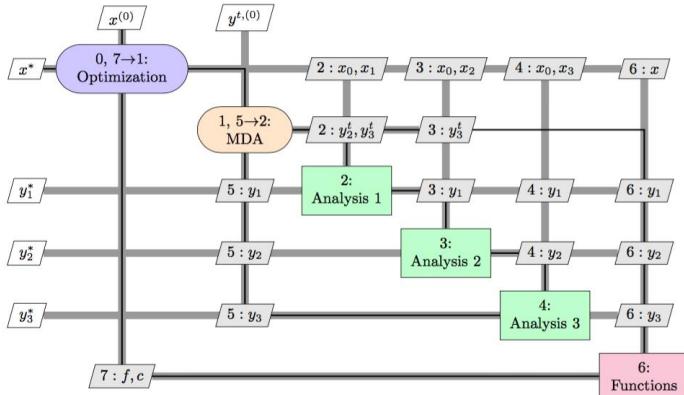


Audet, C., & Hare, W. (2017). Derivative-free and blackbox optimization. Berlin: Springer International Publishing

Powell, M. J. (1994). A direct search optimization method that models the objective and constraint functions by linear interpolation. In Advances in optimization and numerical analysis (pp. 51-67). Springer, Dordrecht.

Forrester, A., Sobester, A., & Keane, A. (2008). Engineering design via surrogate modelling: a practical guide. John Wiley & Sons

Different strategies



Generic approach
Extension to
multiple disciplines

Gradient-free
algorithm

Black box
functions

Costly functions
replaced by
surrogate models

Exploration design,
Trade-off studies,
Sensitivity analysis,
Uncertainty analysis

Optimization

Audet, C., & Hare, W. (2017). Derivative-free and blackbox optimization. Berlin: Springer International Publishing

Powell, M. J. (1994). A direct search optimization method that models the objective and constraint functions by linear interpolation. In Advances in optimization and numerical analysis (pp. 51-67). Springer, Dordrecht.

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Outline

- Kriging based surrogate models
 - Bayesian optimization
 - mono & multiobjective
 - Applications
 - DRAGON (hybrid electric aircraft)
 - EU project AGILE4.0
- & dedicated Notebook for analytical functions

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 functions**
→ Mixture of experts (MOE)
- Models to handle **heterogeneous variables**
→ Kriging based on continuous relaxation
- Models to handle multifidelity data
→ Co-Kriging (MFKPLS, MKPLS-K)
→ Co-Kriging with heteroscedastic Noise



SMT 2.0 features (June 2023):

github.com/SMTorg/smt

- 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
- Bayesian optimization (EGO without constraint) for continuous and mixed variables

➔ Included some Jupyter notebooks



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.

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

Main steps to build a surrogate model

1. Black box to replace by a surrogate model

$$y(x^{(i)}) = f(x^{(i)}) \text{ with } x^{(i)} \in \mathbb{R}^d \text{ and } y(x^{(i)}) \in \mathbb{R}$$

where f is the model (expensive, free-derivative, noise-free) such as CFD code or FEM code

2. Data (X,y): n observation points – design of experiments

- DOE
- Design variables (inputs)
 $X^{DOE} = \{x^{(1)}, x^{(2)}, \dots, x^{(n)}\}^t$ with $x^{(i)} \in \mathbb{R}^d$
 - Observations (output responses of your expensive black box)
 $y^{DOE} = \{y(x^{(1)}), y(x^{(2)}), \dots, y(x^{(n)})\}^t$ with $y(x^{(i)}) \in \mathbb{R}$

3. Fit the surrogate model: determine parameters (training)

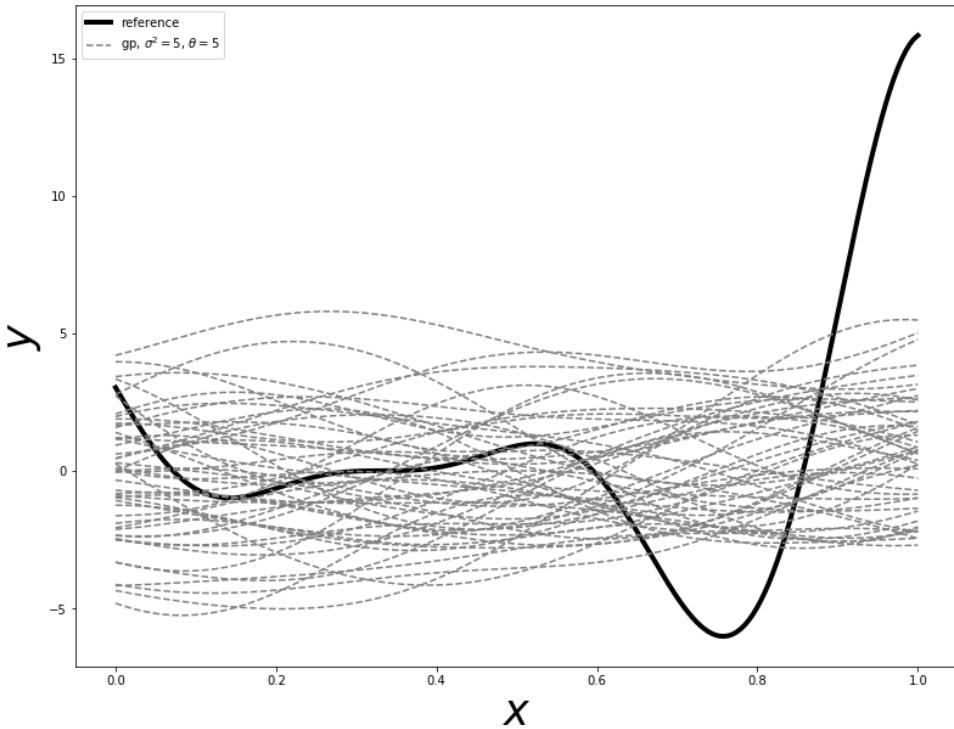
4. Predict the response at a new point $x_{new} \in \mathbb{R}^d$

5. Validate the surrogate

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (\hat{y}_i - y(x^{(i)}))^2}{n}}$$

Gaussian process or Kriging model

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



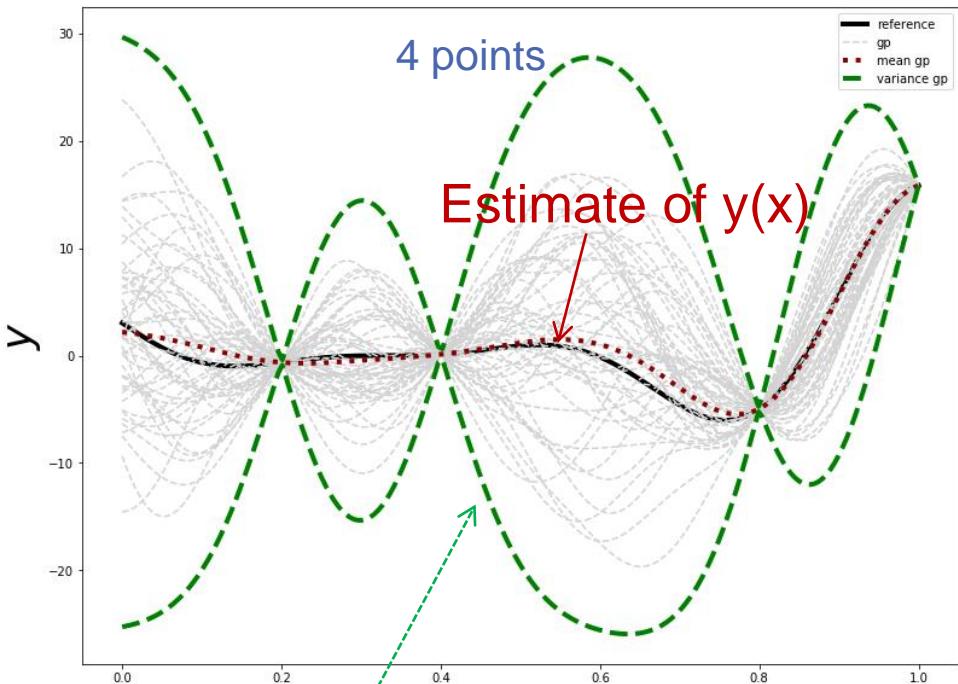
Gaussian process characterized by:

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

D. G. Krige. 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
C. E. Rasmussen and C. K. Williams. Gaussian processes for machine learning, volume 1. MIT press Cambridge, 2006.

Gaussian process or Kriging model

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



Quantification of
the uncertainties in
these estimates

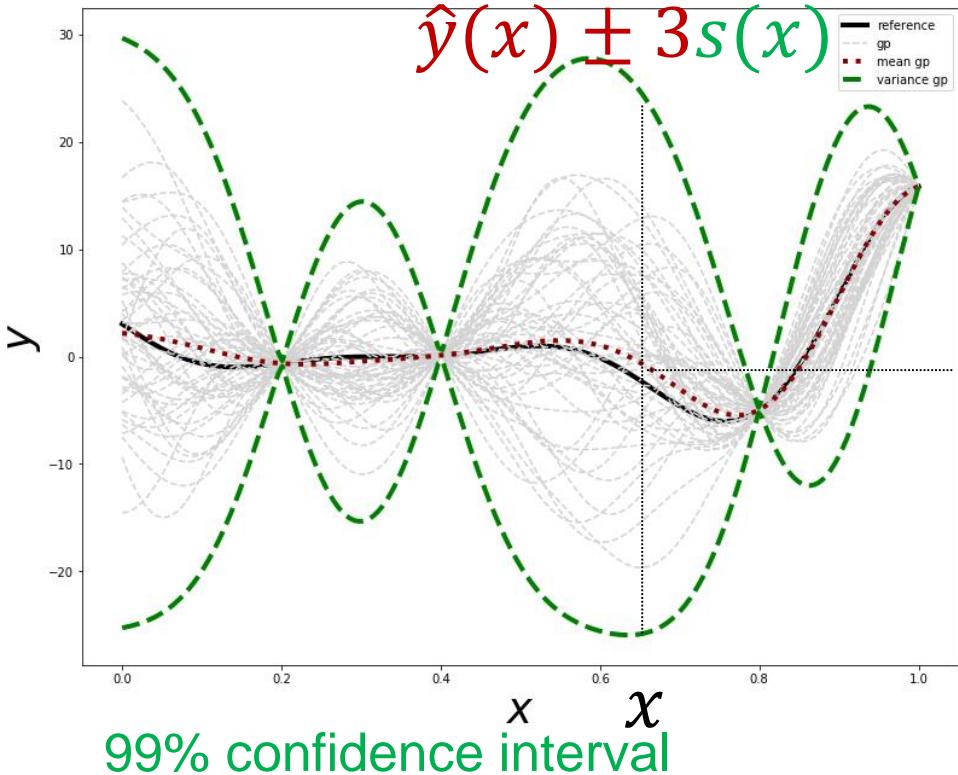
Gaussian process
characterized by:

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

+ information provided by data

D. G. Krige. 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
C. E. Rasmussen and C. K. Williams. Gaussian processes for machine learning, volume 1. MIT press Cambridge, 2006.

Gaussian process or Kriging model



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

DOE (LHS)

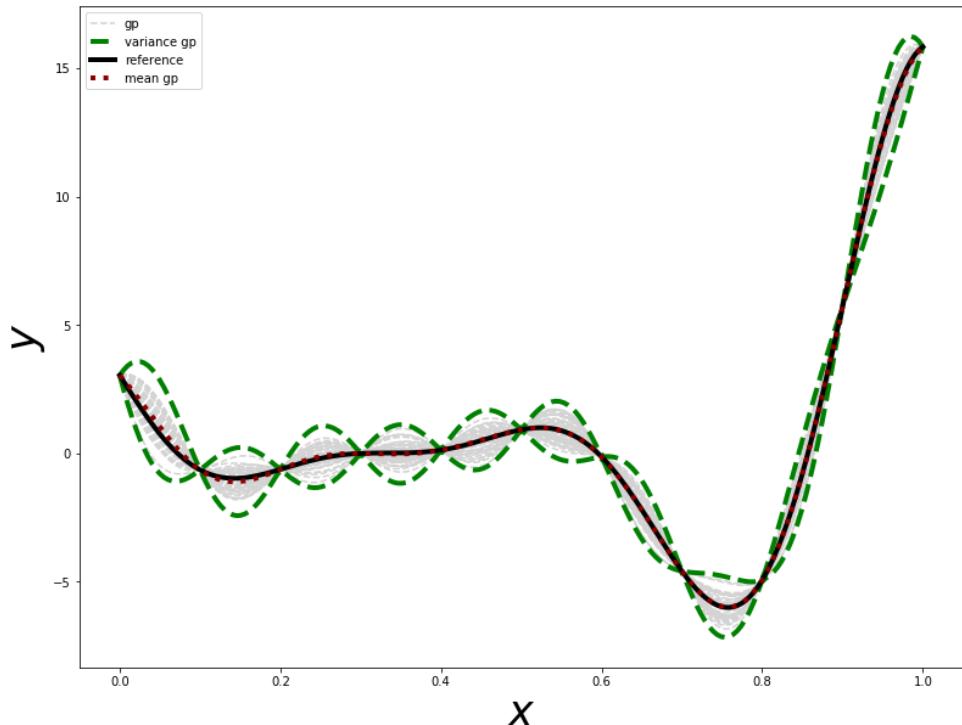
Estimation of
hyperparameters
 θ_i ($i=1, \dots, d$) by MLE

Covariance matrix

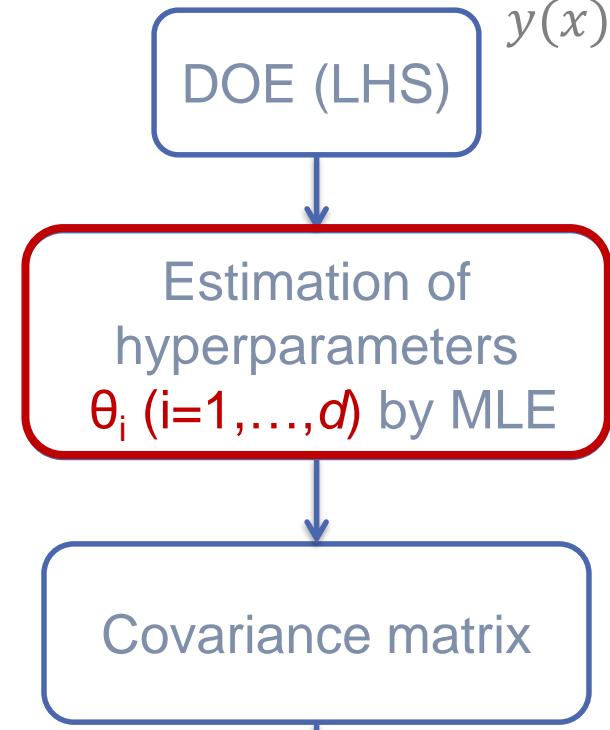
Prediction \hat{y} and variance s^2
estimations at a new point

D. G. Krige. 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

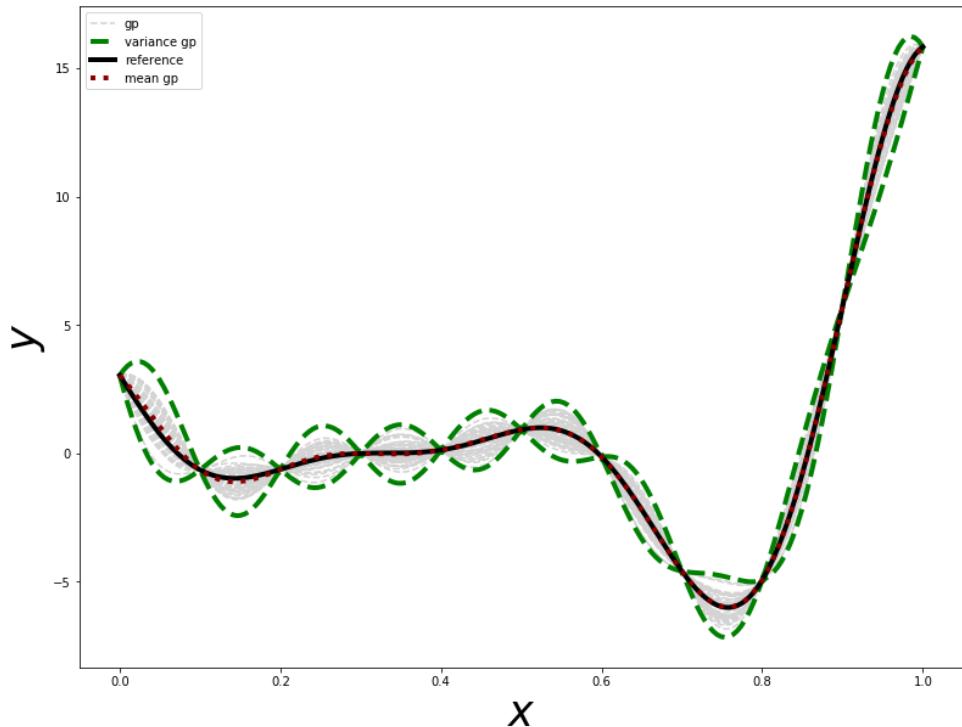


$$x \in \mathbb{R}^d$$
$$y(x) \in \mathbb{R}$$



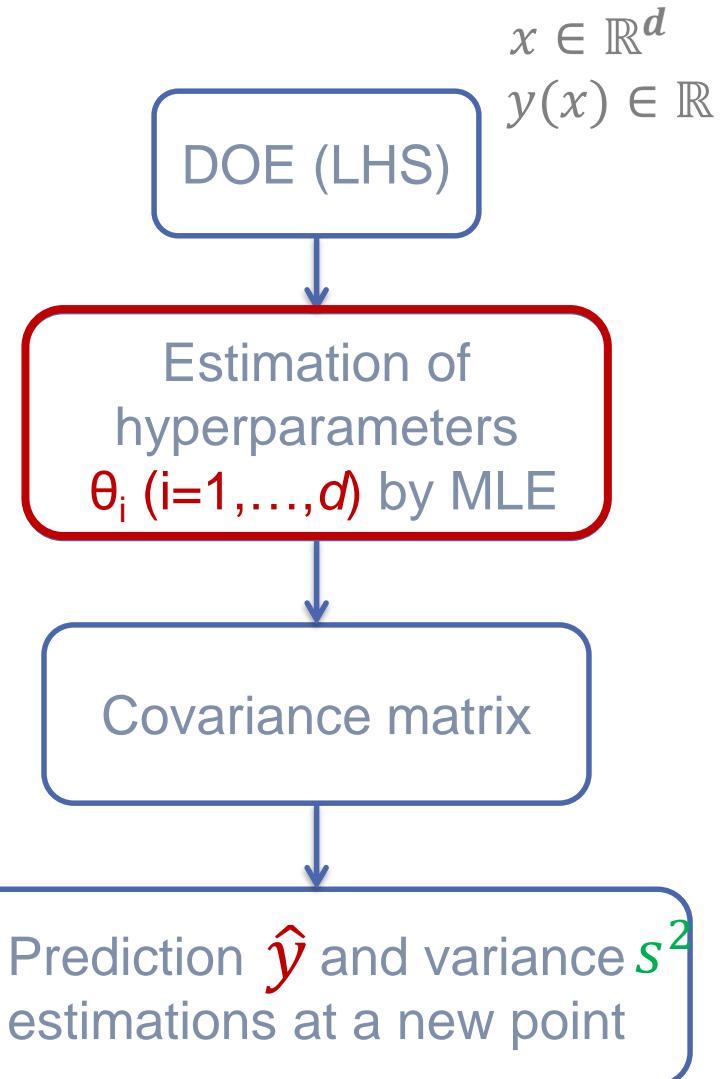
GP approach in the notebook

Gaussian process or Kriging model



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

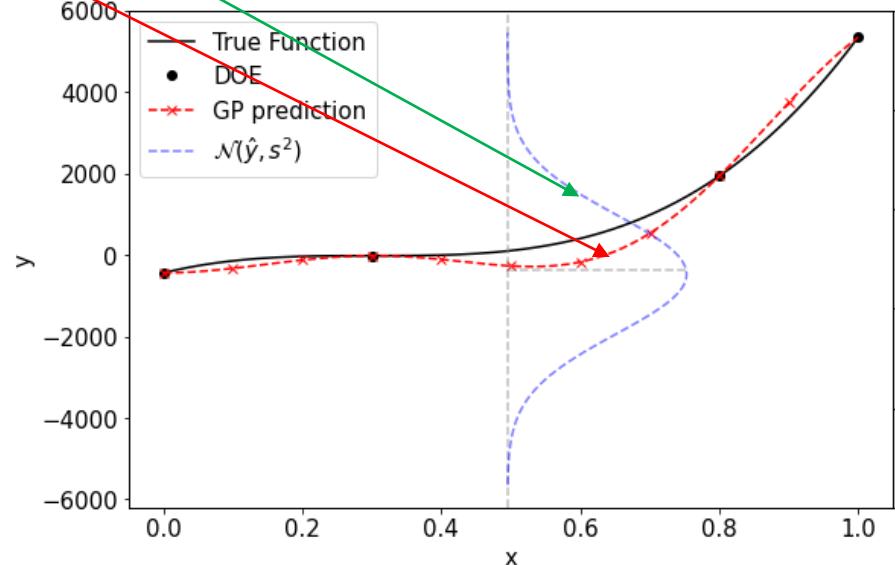
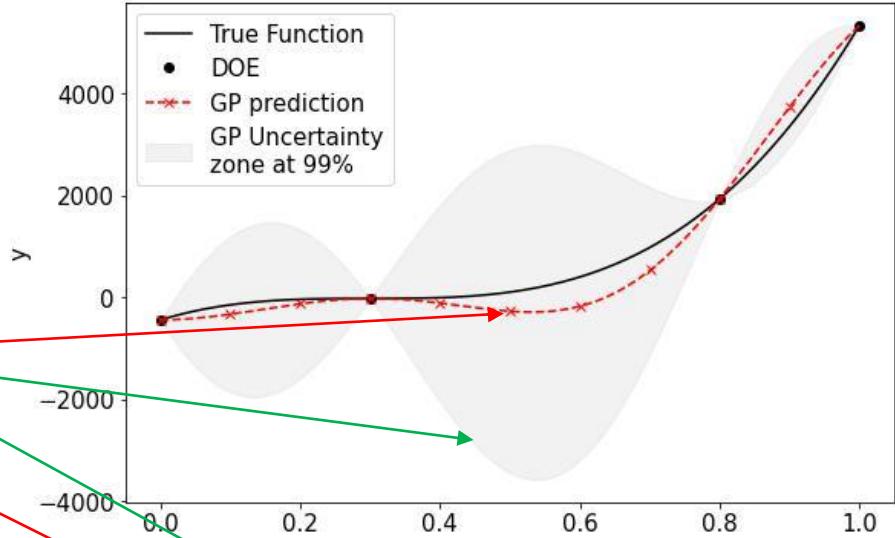
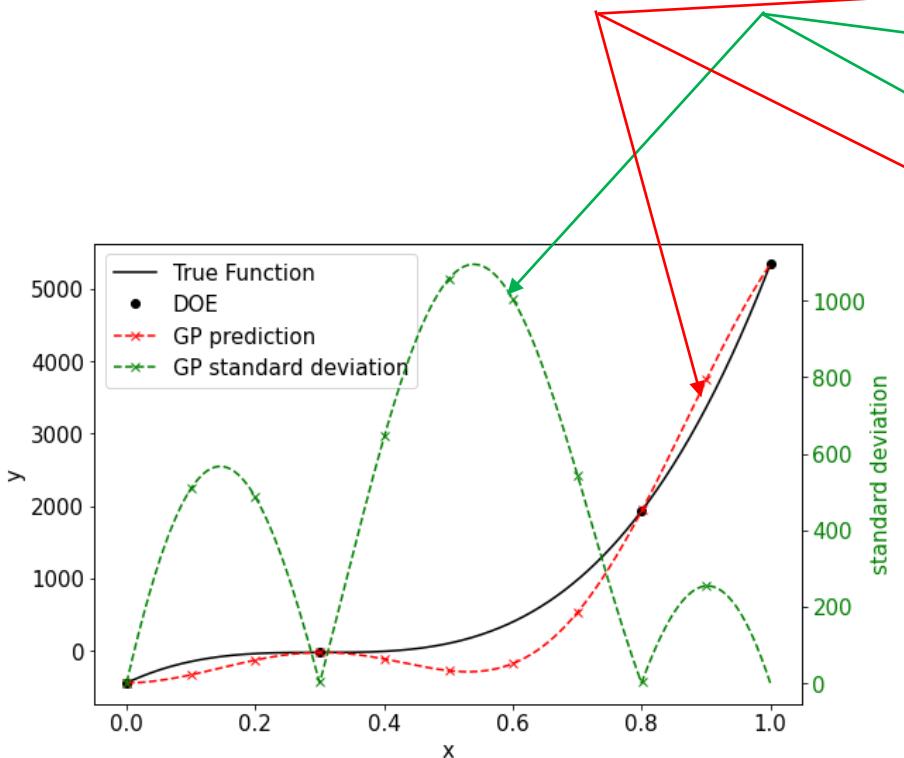
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Kriging or Gaussian process model

Initial DOE 4 points

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



D. G. Krige. 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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Models to handle a large number of design variables

New 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

$$x \in \mathbb{R}^d$$

Ordinary
Kriging

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

d parameters θ_i to evaluate

Covariance kernel



KPLS

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

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

h parameters θ_j to evaluate

- $|w_{i,j}|_{i=1,\dots,d}$ describes how sensitive the j -th principal component is to each design variable $i \rightarrow$ **PLS**
- θ_j describes how sensitive the function is to each principal component (max $h \approx 4$) \rightarrow **MLE**
- If $h = d \rightarrow$ 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

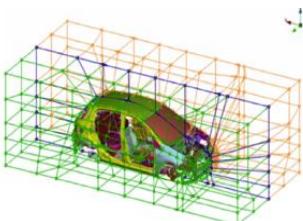
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Models to handle a large number of design variables

New Kriging models: KPLS & KPLS-K

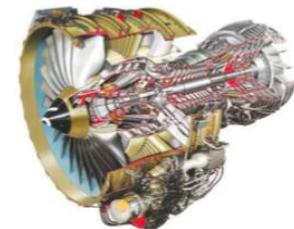
MOPTA test case function
from automotive industry



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

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

- CPU time drastically reduced: interest for adaptive enrichment optimization method
- Automatic choice for the number of PLS components

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

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

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-SUPAFRO, 2016, <https://hal.archives-ouvertes.fr/tel-01293319>

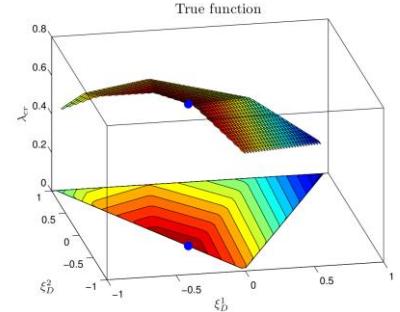
Models to handle heterogeneous functions

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.

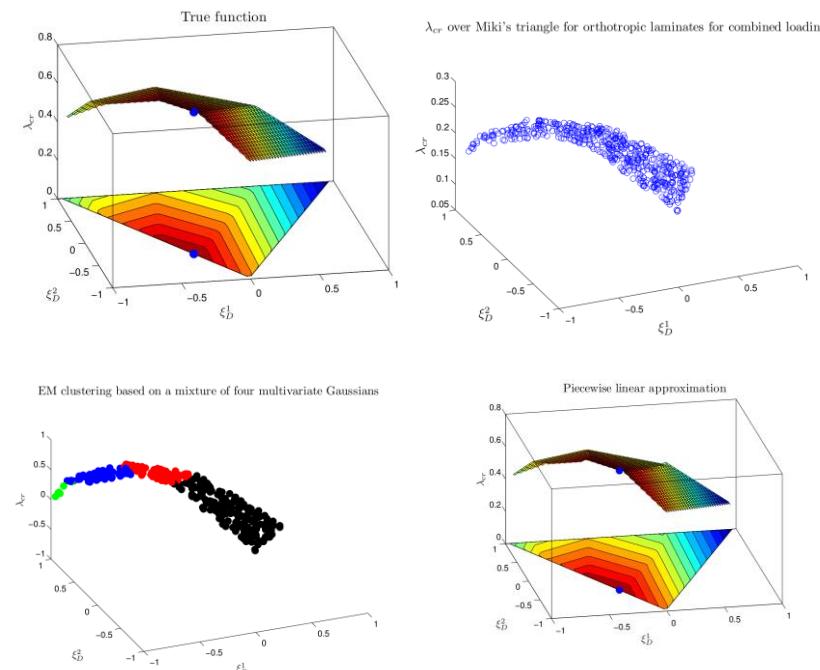
Betteghor, D., Bartoli, N., Grignon, S., Morlier, J., and Samuelides, M., "Surrogate modeling approximation using a mixture of experts based on EM joint estimation," Structural and Multidisciplinary Optimization, Vol. 43, No. 2, 2011, pp. 243–259

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

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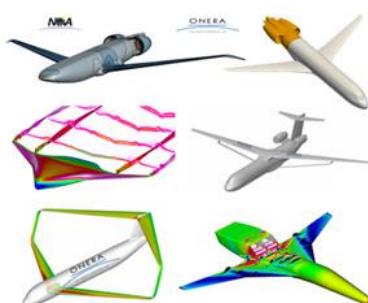
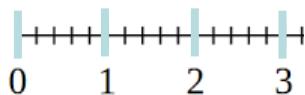
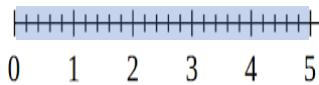
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Models to handle mixed variables (continuous, discrete, categorical)

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

State of the Art approach: Continuous Relaxation

Ex: Garrido-Merchán and Hernández-Lobato model

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

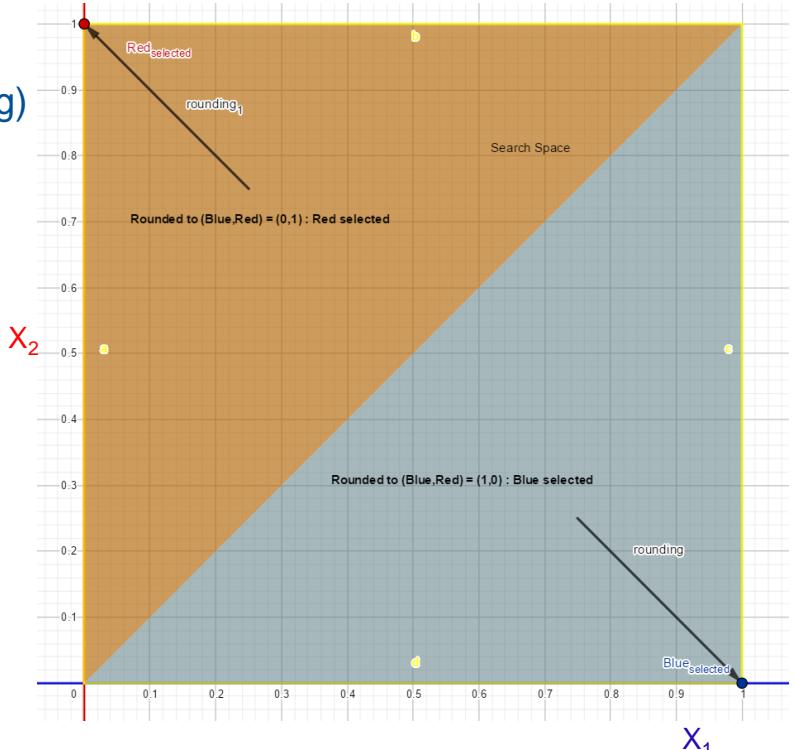
Example with 1 categorical variable X and two levels

- Red color
- Blue color

→ 1 Categorical variable replaced by 2 continuous variables denoted by X_1 and $X_2 \in [0,1]$

- If $X_1 > X_2 \Rightarrow (1., 0.) \Rightarrow$ Blue color
- If $X_1 < X_2 \Rightarrow (0., 1.) \Rightarrow$ Red color

**A continuous kernel
(in the relaxed 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
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

State of the Art approach: Continuous Relaxation

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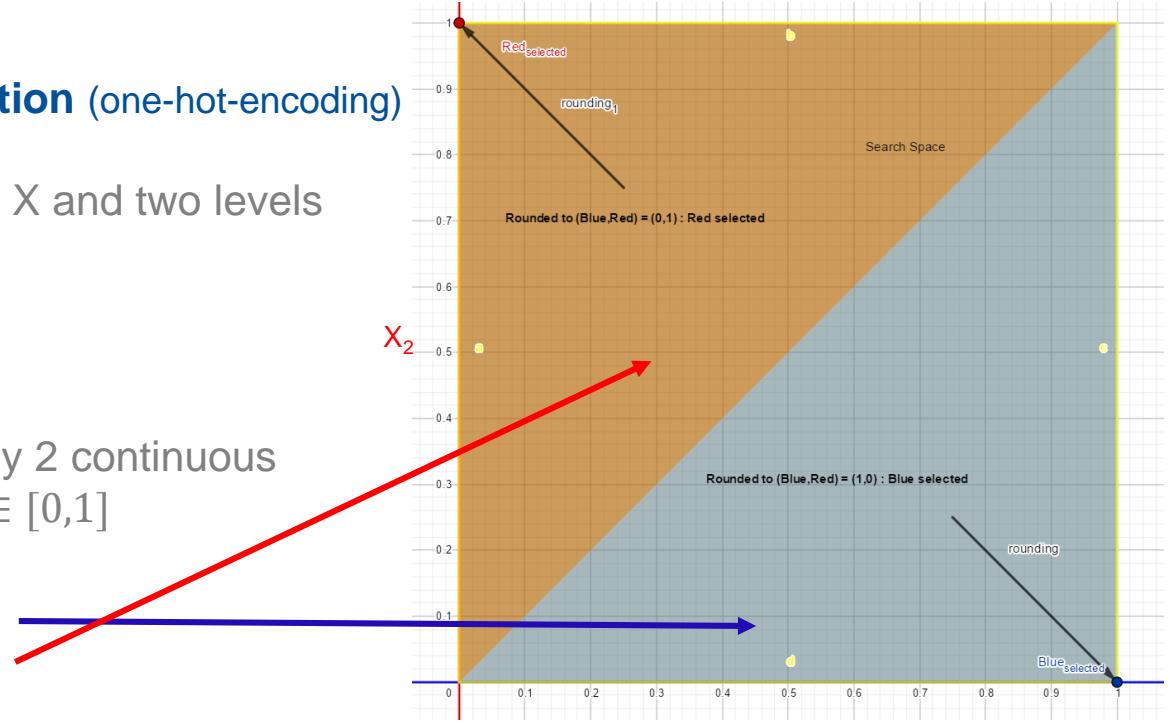
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- If $X_1 < X_2 \Rightarrow (0., 1.) \Rightarrow$ Red color

**A continuous kernel
(in the relaxed dimension)**



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

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State of the Art approach: Continuous Relaxation

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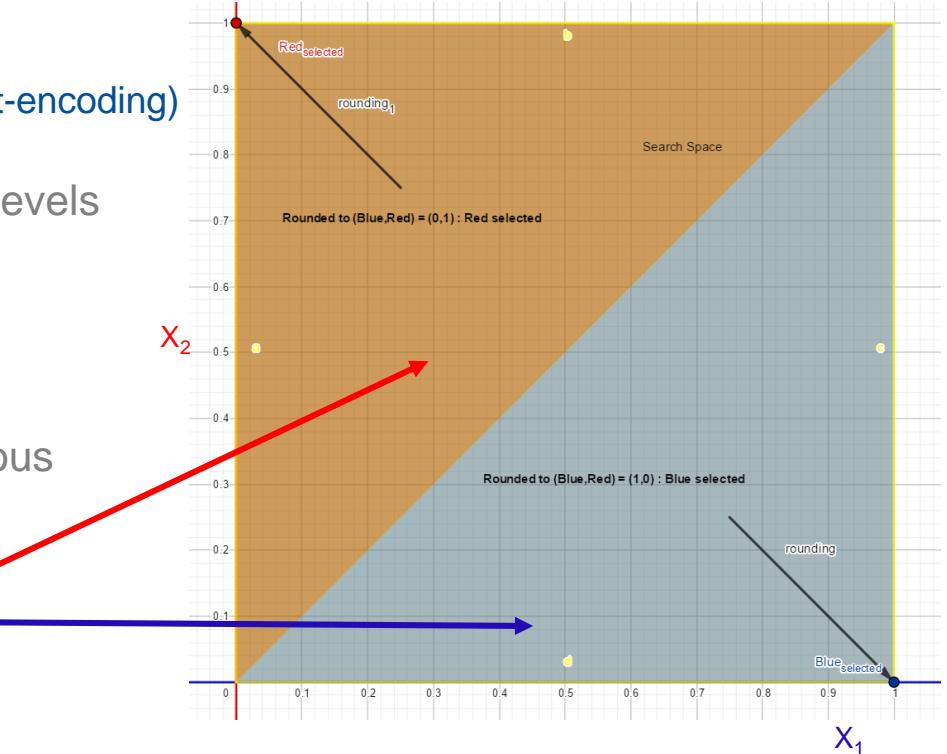
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**A continuous kernel
(in the relaxed dimension)**



→ Increase 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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State of the Art approach: Continuous Relaxation

Ex: Garrido-Merchán and Hernández-Lobato model

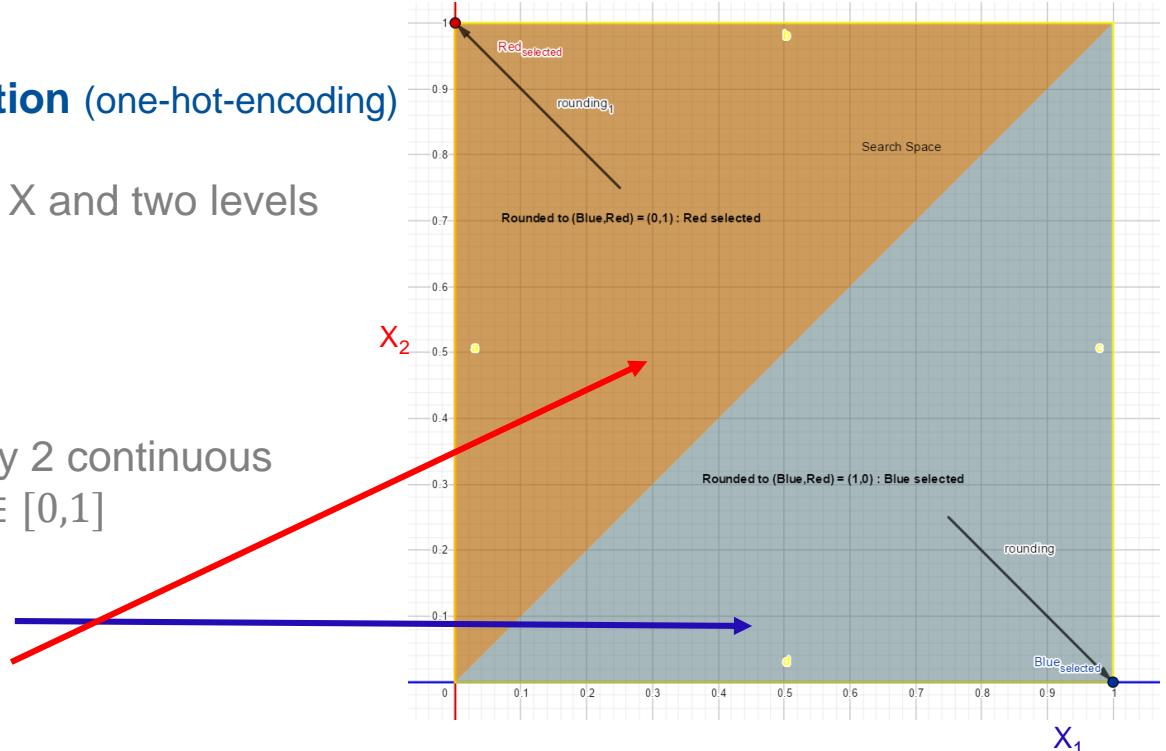
→ Model as a **Continuous Relaxation** (one-hot-encoding)

Example with 1 categorical variable X and two levels

- Red color
- Blue color

→ 1 Categorical variable replaced by 2 continuous variables denoted by X_1 and $X_2 \in [0,1]$

- If $X_1 > X_2 \Rightarrow (1., 0.) \Rightarrow$ Blue color
- If $X_1 < X_2 \Rightarrow (0., 1.) \Rightarrow$ Red color



→ Use of KPLS models to decrease the dimension

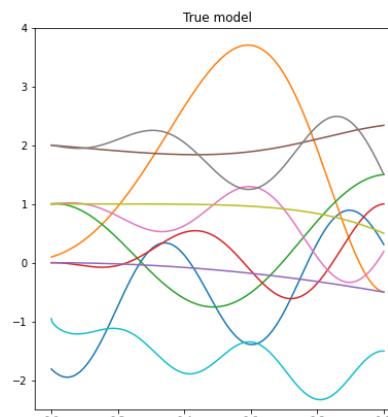
E. C. Garrido-Merchán, and D. Hernández-Lobato. "Dealing with categorical and integer-valued variables in Bayesian Optimization with Gaussian processes". Neurocomputing, vol. 380 (2020), pages 20-35
Saves, P., Bartoli, N., Diouane, Y., Morlier, J., & Lefebvre, T. (2021, March). Enhanced Kriging models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

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

Toy function with a categorical variable (10 levels)

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

Toy function surrogate



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

○ Mixed kernels integration (Phd P. Saves)

Continuous Relaxation, Gower distance,
Homoscedastic hypersphere,
Exponential Homoscedastic hypersphere
+ KPLS for dimension reduction with automatic
choice for number of PLS components

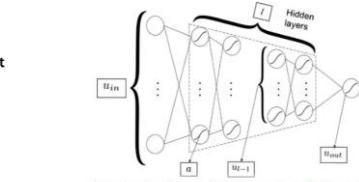
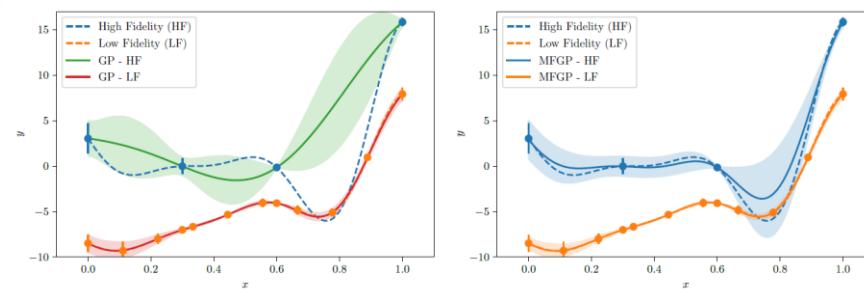
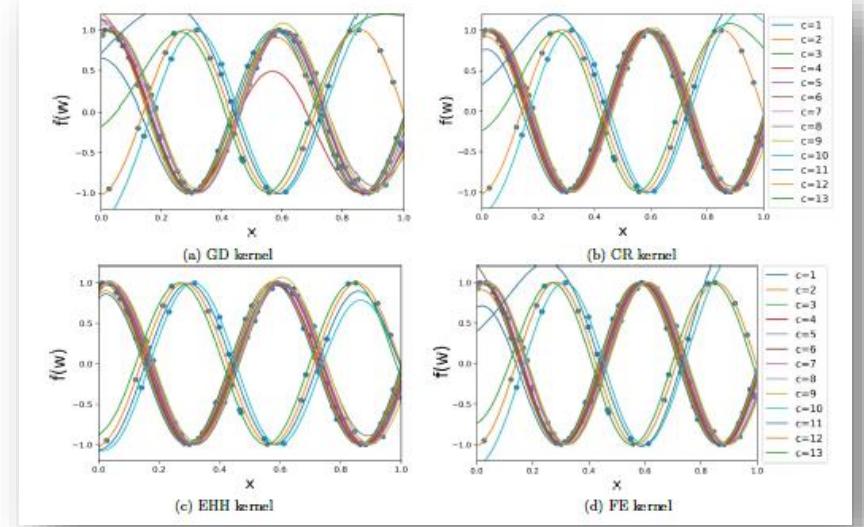
○ Multifidelity surrogates with heterogenous uncertainties on data

(Phd R. Charayron – PhD Data fusion)

○ Extension to hierarchical variables (variable-size problems)

New proposed kernels (Phd P. Saves)

New application cases (Collab. J. Bussemaker DLR)



(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, ..., 128, 256}	ORD	NEUTRAL
# of hidden layers	l	{1, 2, 3}	ORD	META
# of units hidden layer i	u_i	{50, 51, ..., 55}	ORD	DECREED

(b) Description of the variables for the problem

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

Saves, P., Diouane, Y., Bartoli, N., Lefebvre, T., & Morlier, J. (2022). A mixed-categorical correlation kernel for Gaussian process. *arXiv preprint arXiv:2211.08262*.

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).

Outline

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

Optimization problem in the field of aircraft design

$$\left\{ \begin{array}{l} \min_{\boldsymbol{x} \in \mathbb{R}^d} \quad \boldsymbol{f}(\boldsymbol{x}) = [f_1(\boldsymbol{x}), f_2(\boldsymbol{x}), \dots, f_n(\boldsymbol{x})] \\ \text{s.t.} \\ c_1(\boldsymbol{x}) \leq 0 \dots c_j(\boldsymbol{x}) = 0 \dots c_m(\boldsymbol{x}) \leq 0 \end{array} \right.$$

n objectives
d design variables
m mixed constraints
1 to *n* objectives

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

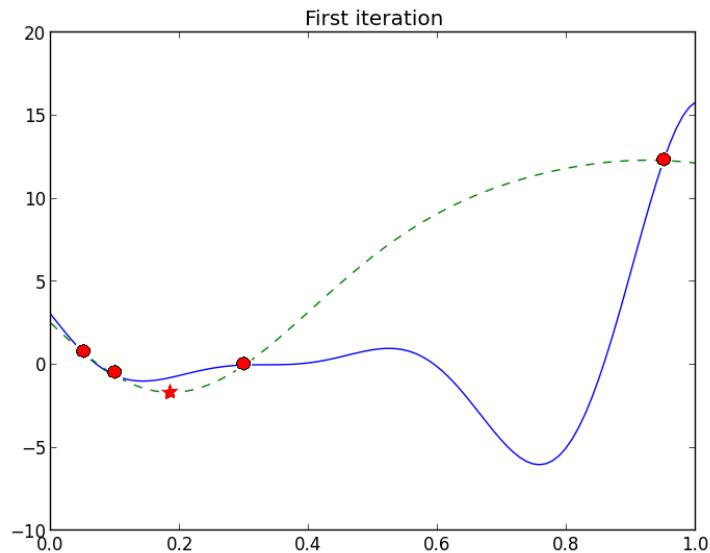
How to optimize some costly functions?

- Replace the black box function (costly code, objectif or constraints) by its surrogate approximation in the optimization process
 - Build an accurate surrogate model for the costly function
 - Replace the function by its approximation in the optimization
- Build an accurate surrogate model requires lots of function evaluations
- Use an iterative process to minimize the number of function evaluations

Minimize directly the surrogate on a 1D example

$$f(x) = (6x - 2)^2 \sin(12x - 4)$$

4 points for the initial DOE
6 iterations



How to optimize some costly functions?

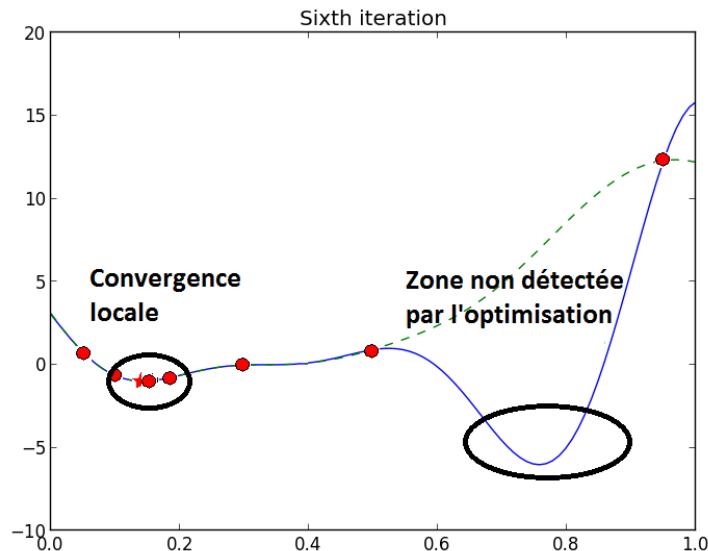
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Minimize directly the surrogate on a 1D example

$$f(x) = (6x - 2)^2 \sin(12x - 4)$$

4 points for the initial DOE
6 iterations

→ Only a local optimum

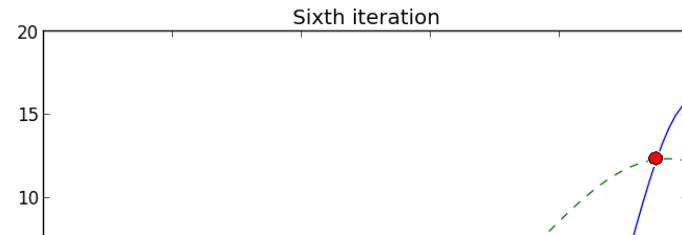


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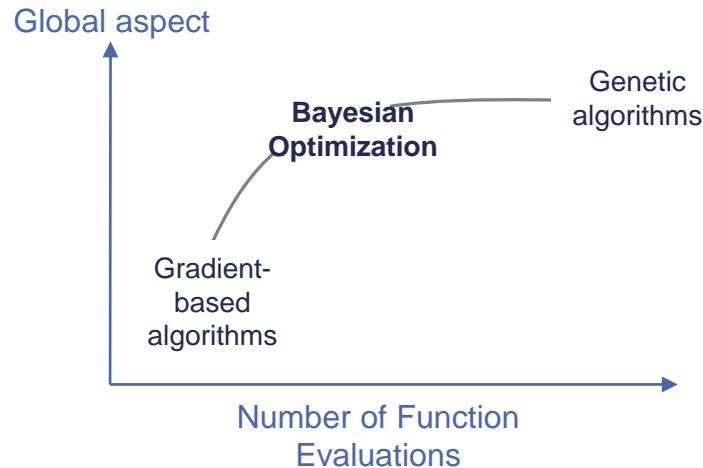
$$f(x) = (6x - 2)^2 \sin(12x - 4)$$



Surrogate Based Optim approach in the notebook

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)



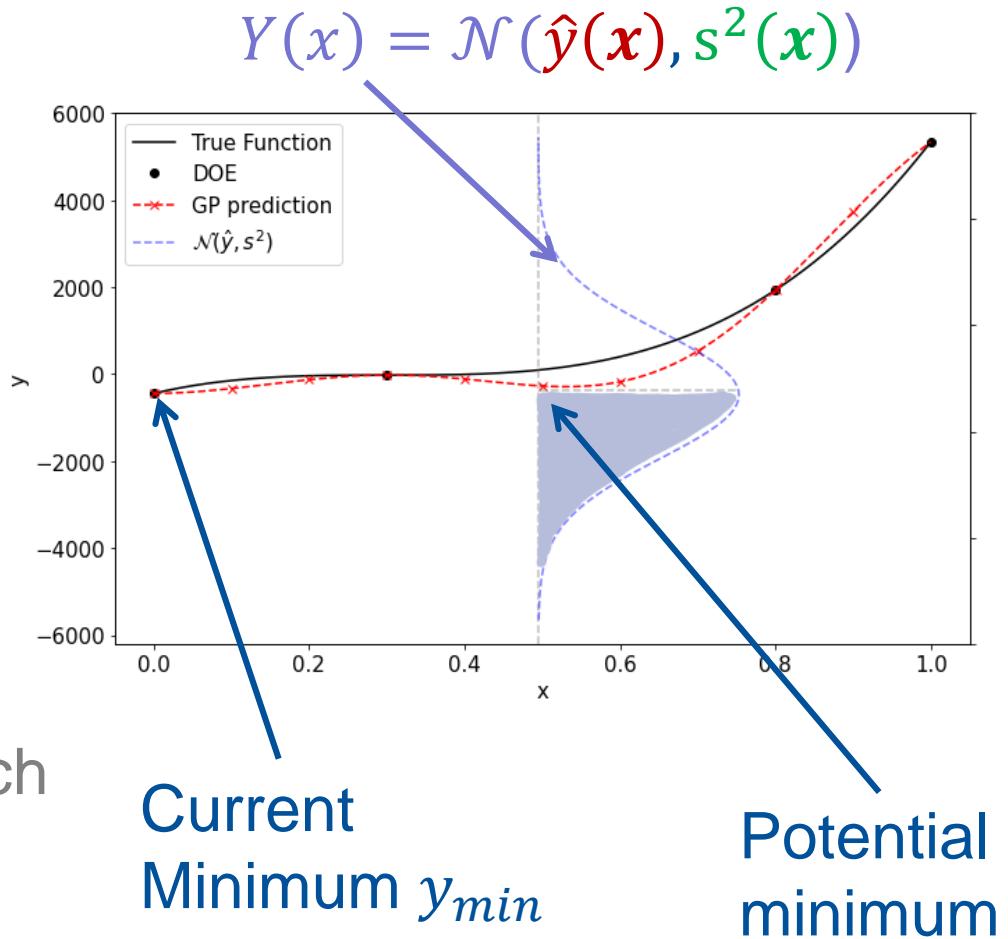
Bayesian optimization

1. Probabilistic model (surrogate model)

uses data and Bayes theorem to compute posterior distribution

2. Optimization done via an acquisition function

uses the posterior distribution to decide which data to obtain



Example: BO to tune NN hyperparameters within AlphaGo

Chen, Y., Huang, A., Wang, Z., Antonoglou, I., Schrittwieser, J., Silver, D., & de Freitas, N. (2018). Bayesian optimization in alphago. *arXiv preprint arXiv:1812.06855*.

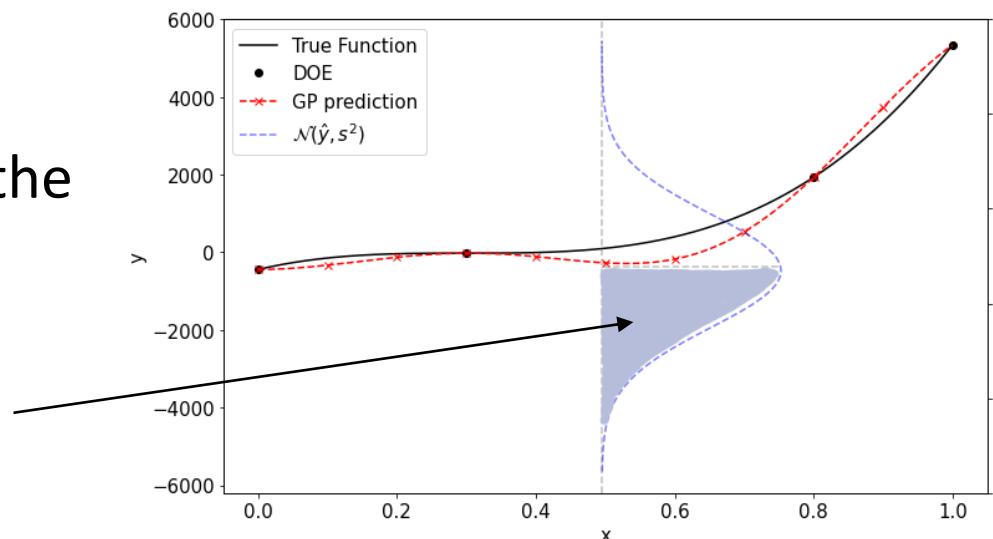
Enrichment infill sampling criterion

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

Measure of progress defined by the Improvement

$$I(x) = \max(0, y_{min} - Y(x))$$

>0 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

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

Kriging or Gaussian process of the objective function

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

Φ cumulative distribution function

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

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

|

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.

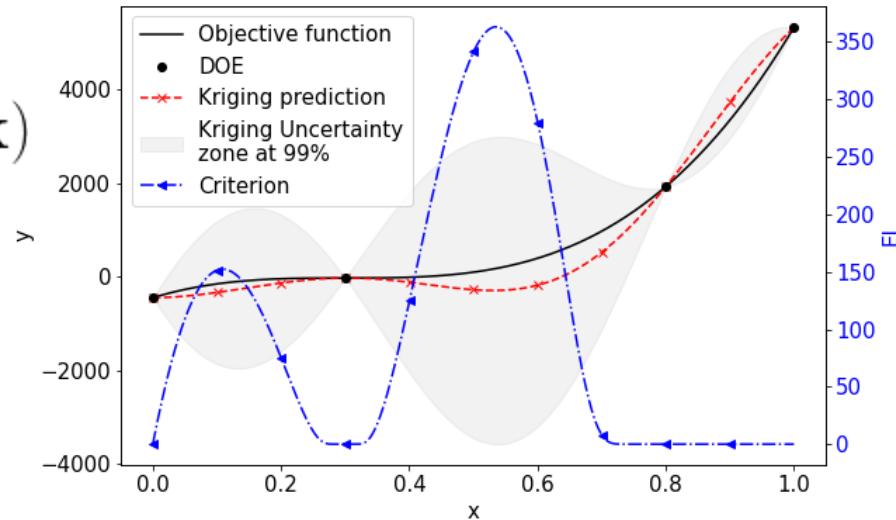
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$$f(\mathbf{x}) \Rightarrow Y(\mathbf{x}) = \mathcal{N}(\hat{y}(\mathbf{x}), s^2(\mathbf{x})) \quad \text{Expected Improvement criterion (EI)}$$

Kriging or Gaussian process of the objective function

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

$$\left\{ \begin{array}{l} \min_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x}) \\ \text{s.t.} \\ c_1(\mathbf{x}) \leq 0 \\ \vdots \\ c_m(\mathbf{x}) \leq 0 \end{array} \right. \xrightarrow{\text{Surrogate models (objective & constraints)}} \left\{ \begin{array}{l} \max_{\mathbf{x} \in \mathbb{R}^d} \text{EI}(\mathbf{x}) \\ \text{s.t.} \\ \hat{c}_1(\mathbf{x}) \leq 0 \\ \vdots \\ \hat{c}_m(\mathbf{x}) \leq 0 \end{array} \right.$$



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.

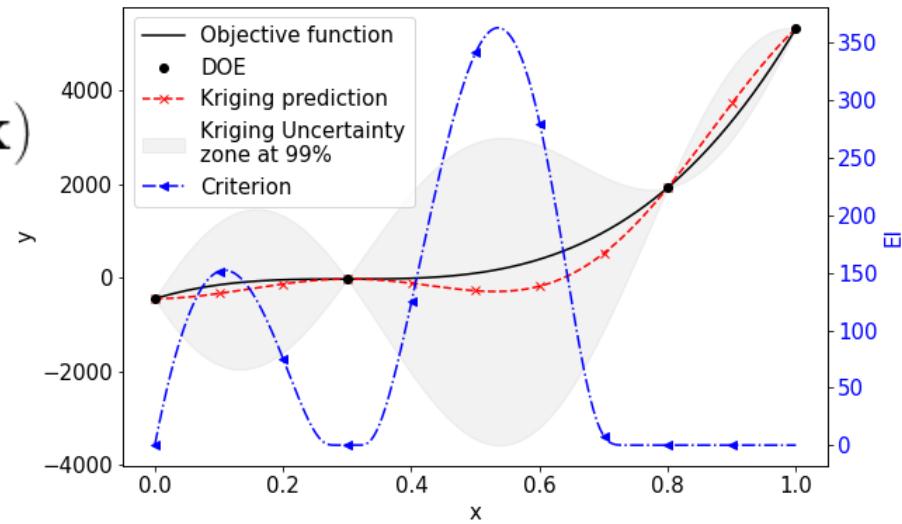
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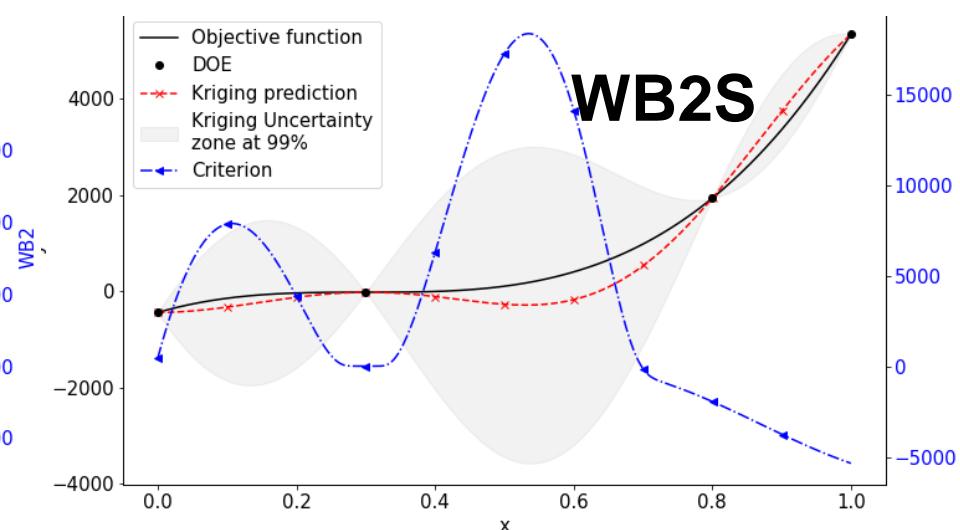
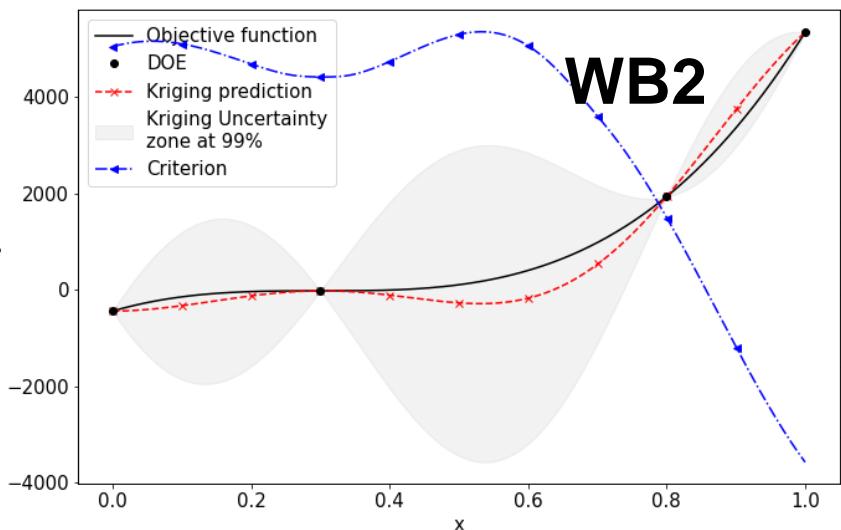
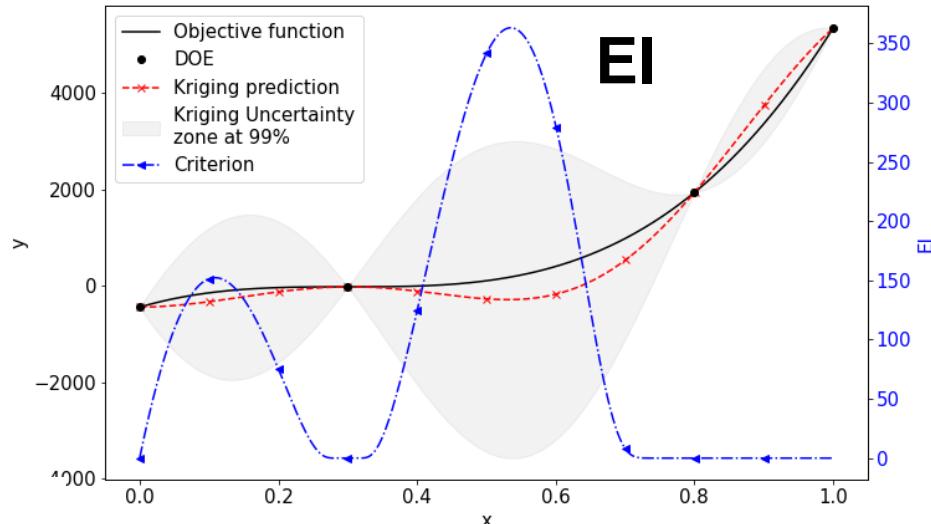
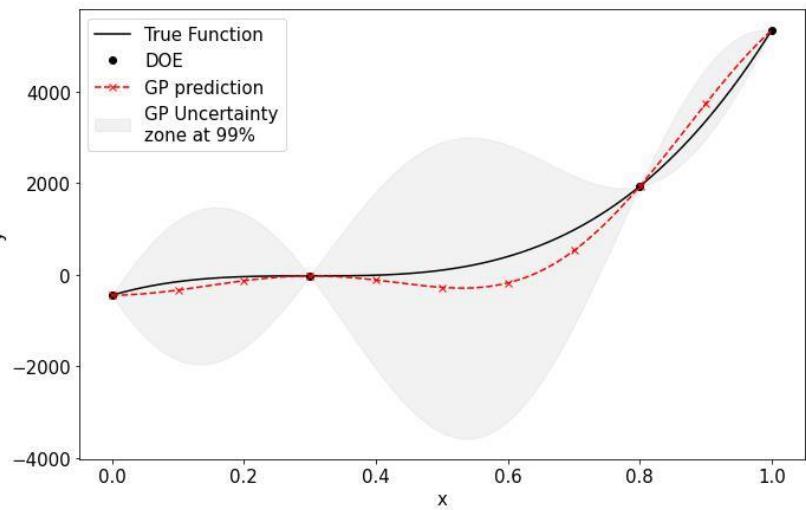


→ Different criteria available for the acquisition function (EI, WB2, WB2S)

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.

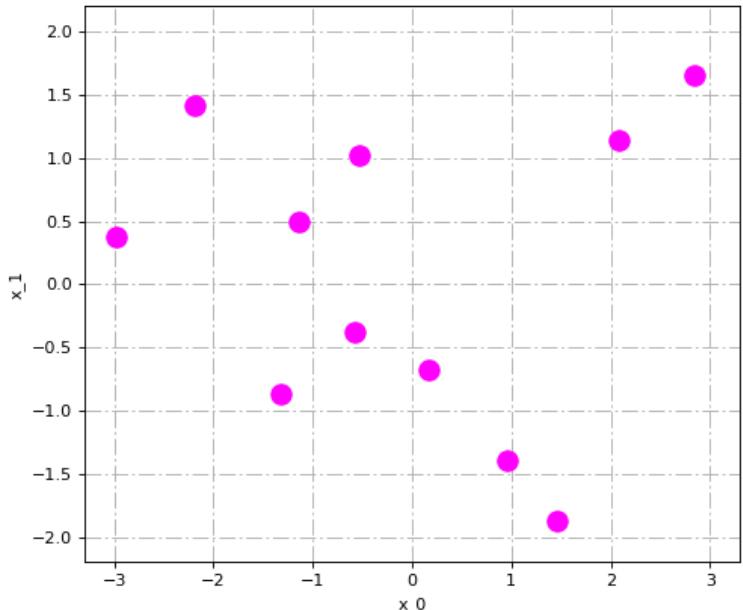
Mono objective: different criteria available



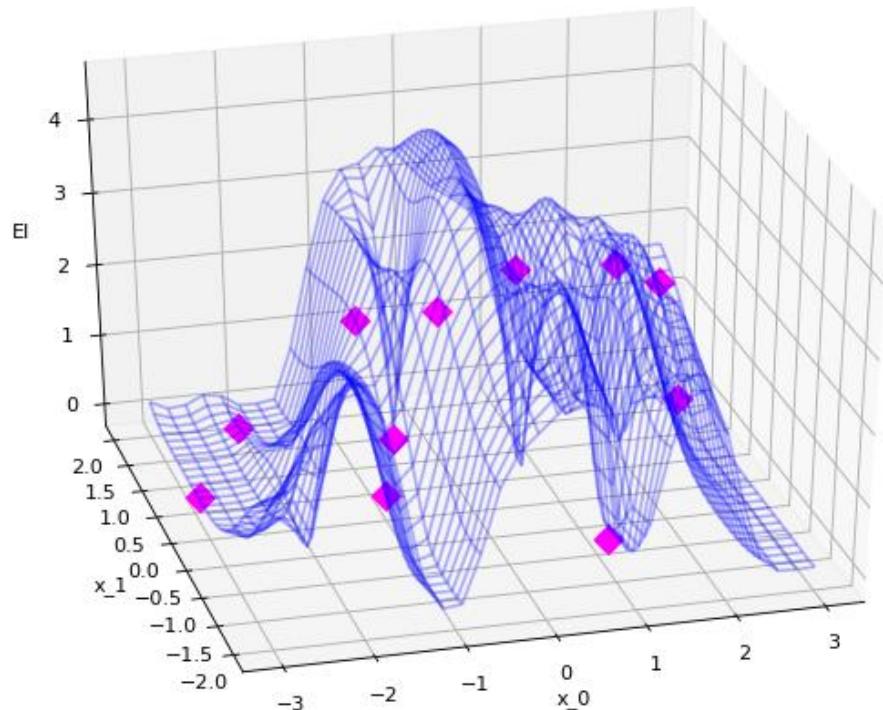
Enrichment for global optimization

$$\left\{ \begin{array}{l} \max_{x \in \mathbb{R}^d} \alpha_f(x) \quad \text{max Acquisition function} \\ \text{s.t.} \\ \hat{c}_1(x) \leq 0 \\ \vdots \\ \hat{c}_m(x) \leq 0 \end{array} \right.$$

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



● Initial DOE (LHS)

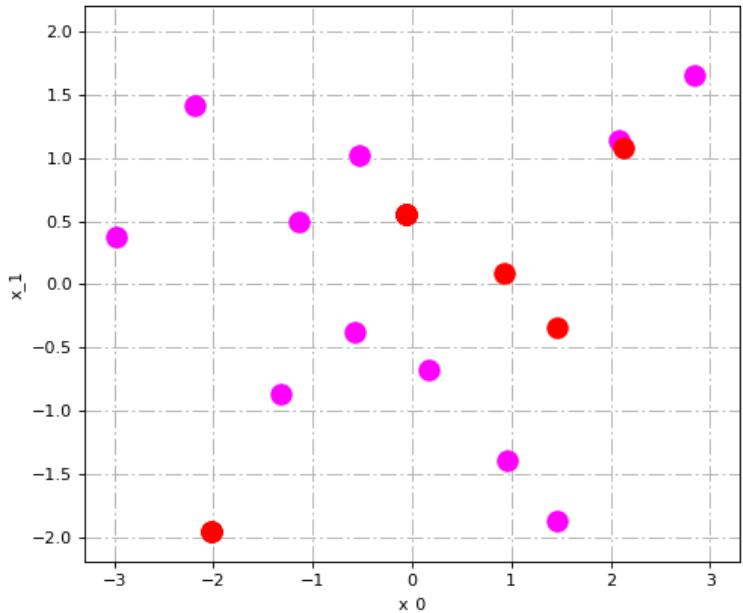


SNOPT: Sparse Nonlinear OPTimizer, Philip Gill , Walter Murray and Michael Saunders, Standford Business Software Inc.

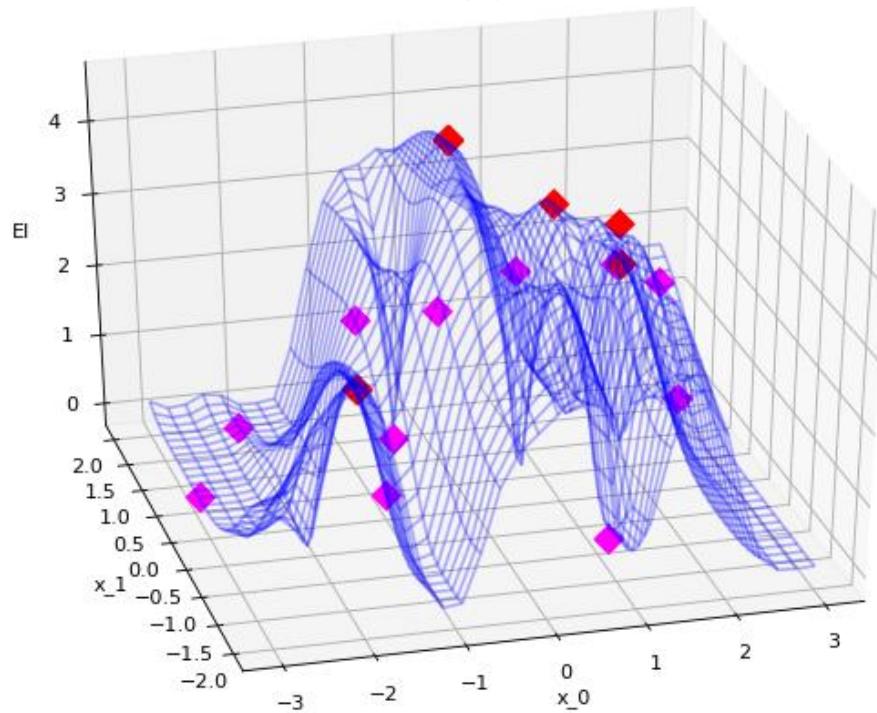
Enrichment for global optimization

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



- Initial DOE(LHS)
- Optimization results

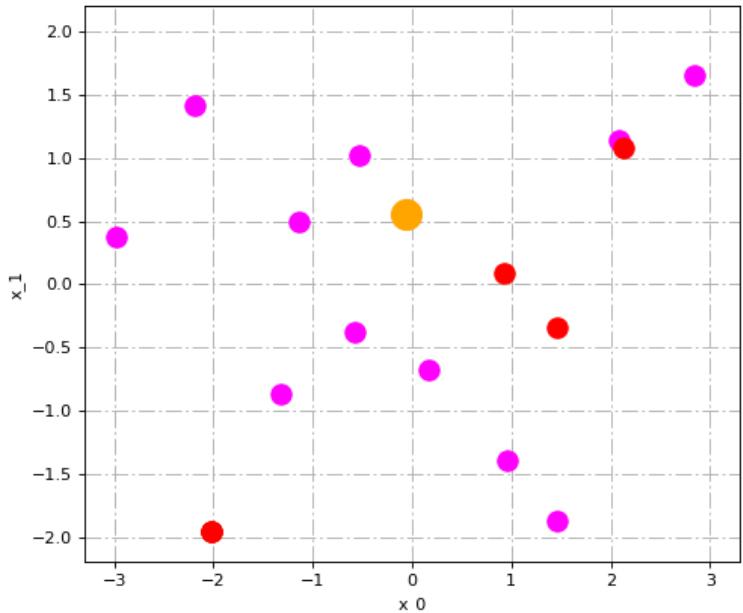


→ Sensitivity to starting points
Drives the global behaviour

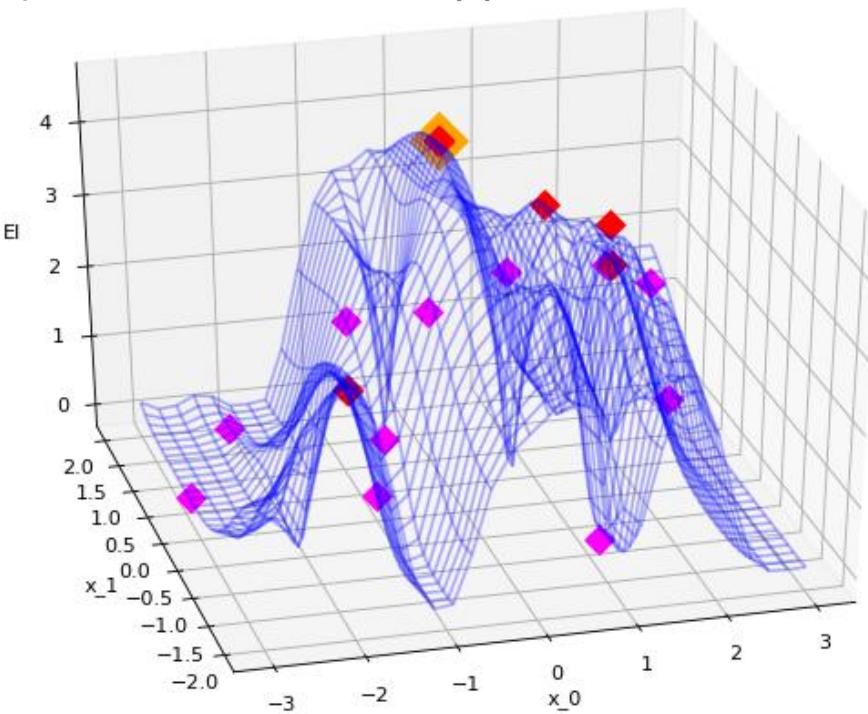
Enrichment for global optimization

$$\left\{ \begin{array}{l} \max_{x \in \mathbb{R}^d} \alpha_f(x) \\ \text{s.t.} \\ \hat{c}_1(x) \leq 0 \\ \vdots \\ \hat{c}_m(x) \leq 0 \end{array} \right.$$

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



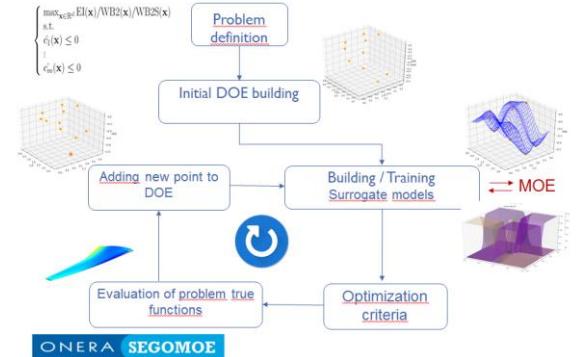
- Initial DOE(LHS)
- Optimization results
- Retained point



→ Sensitivity to starting points
Drives the global behaviour

SEGOMOE main characteristics

$$\begin{cases} \min_{\mathbf{x} \in \mathbb{R}^d} & f(\mathbf{x}) \\ \text{s.t.} & d \text{ design variables} \\ & m \text{ mixed constraints} \\ & c_1(\mathbf{x}) \leq 0 \dots c_j(\mathbf{x}) = 0 \dots c_m(\mathbf{x}) \leq 0 \end{cases}$$



- 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)
- Costly evaluation (CFD, FEM, objective and/or constraints)
- Handling non linear objectives & constraints (black box, no derivative available)
- Based on SMT toolbox for surrogate models
- Remote access via a web interface

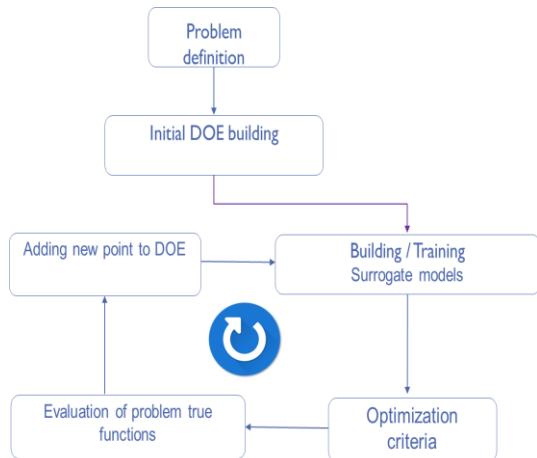


ONERA WhatsOpt®

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.

SEGO

Super Efficient Global Optimization

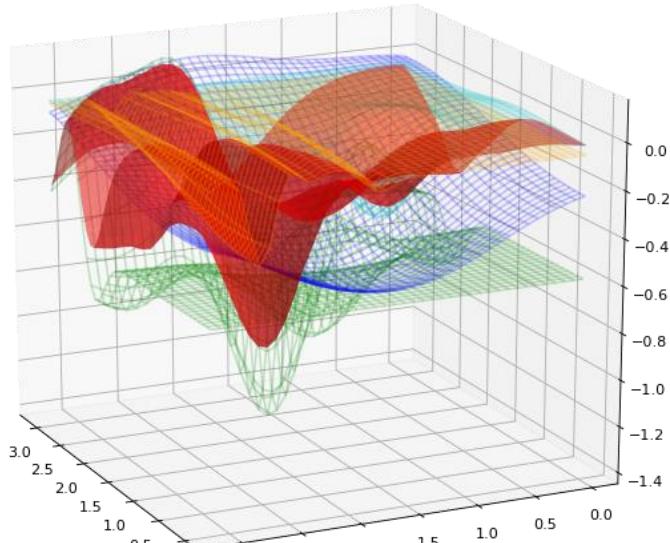


Global optimization with limited number of function evaluations

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, University of Michigan, 2002

MOE

Mixture Of Experts



Combination of GP surrogate models



Jordan, M. I., Jacobs, R. A., "Hierarchical mixtures of experts and the EM algorithm", *Neural Comput.* 6 (1994) 181–214.
 Bettebghor, D., Bartoli, N., Gribon, 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

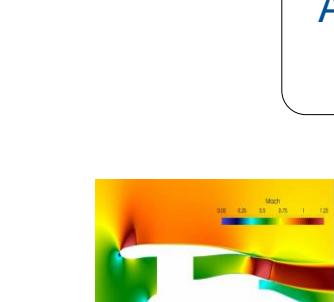
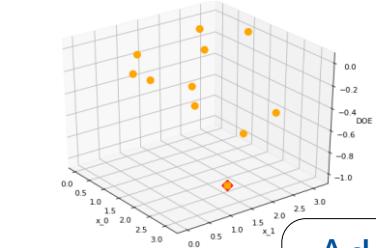
SEGOMOE algorithm – Mono objective

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

Problem
definition

SEGOMOE algorithm – Mono objective

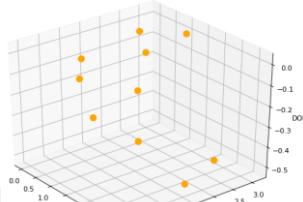
$$\begin{cases} \max_{\mathbf{x} \in \mathbb{R}^d} EI(\mathbf{x}) / WB2(\mathbf{x}) / WB2S(\mathbf{x}) \\ \text{s.t.} \\ \hat{c}_1(\mathbf{x}) \leq 0 \\ \vdots \\ \hat{c}_m(\mathbf{x}) \leq 0 \end{cases}$$



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.

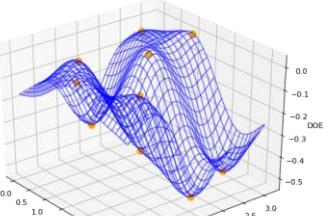
Problem definition

Initial DOE building



Adding new point to DOE

Building / Training Surrogate models

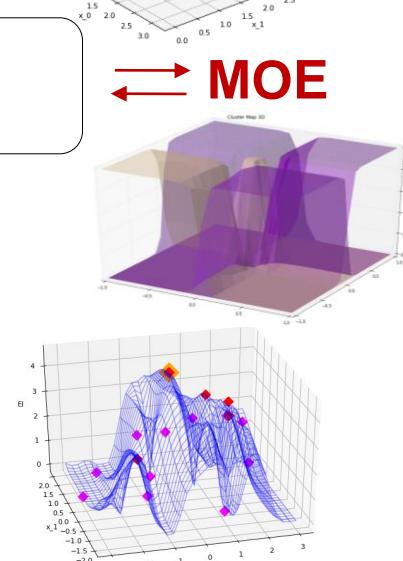


← MOE

Evaluation of problem true functions



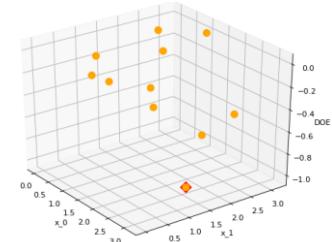
Optimization criteria



SEGOMOE algorithm – Mono objective

N iterations reached

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

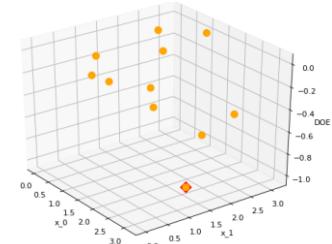


Bartoli, N., Lefebvre, T., Dubreuil, S., Olivanti, R., Priem, R., Bons, N., Martins, J.R.R.A., Bouhlel, M.-A. Bouhlel & Morlier, J. (2019). Adaptive modeling strategy for constrained global optimization with application to aerodynamic wing design. *Aerospace Science and technology*, 90, 85-102.

SEGOMOE algorithm – Mono objective

N iterations reached

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



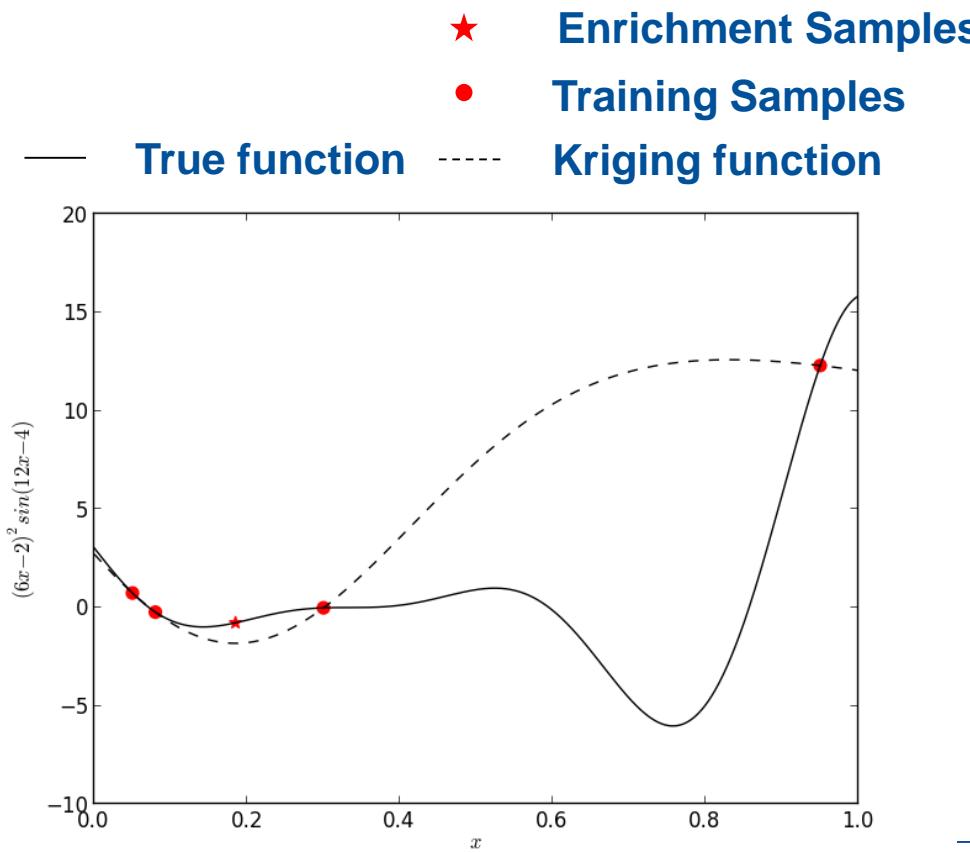
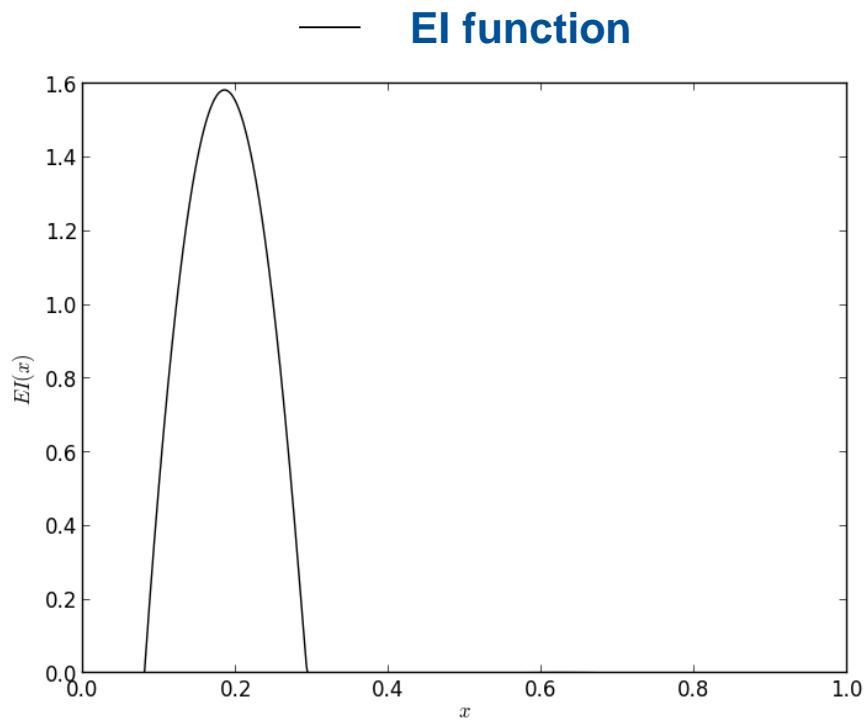
→ best point from the complete database

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.

Bayesian Optimization: Illustration on 1D example

$$\left\{ \begin{array}{l} \min (6x - 2)^2 \sin(12x - 4) \\ \text{s.t.} \\ 0 \leq x \leq 1 \end{array} \right.$$

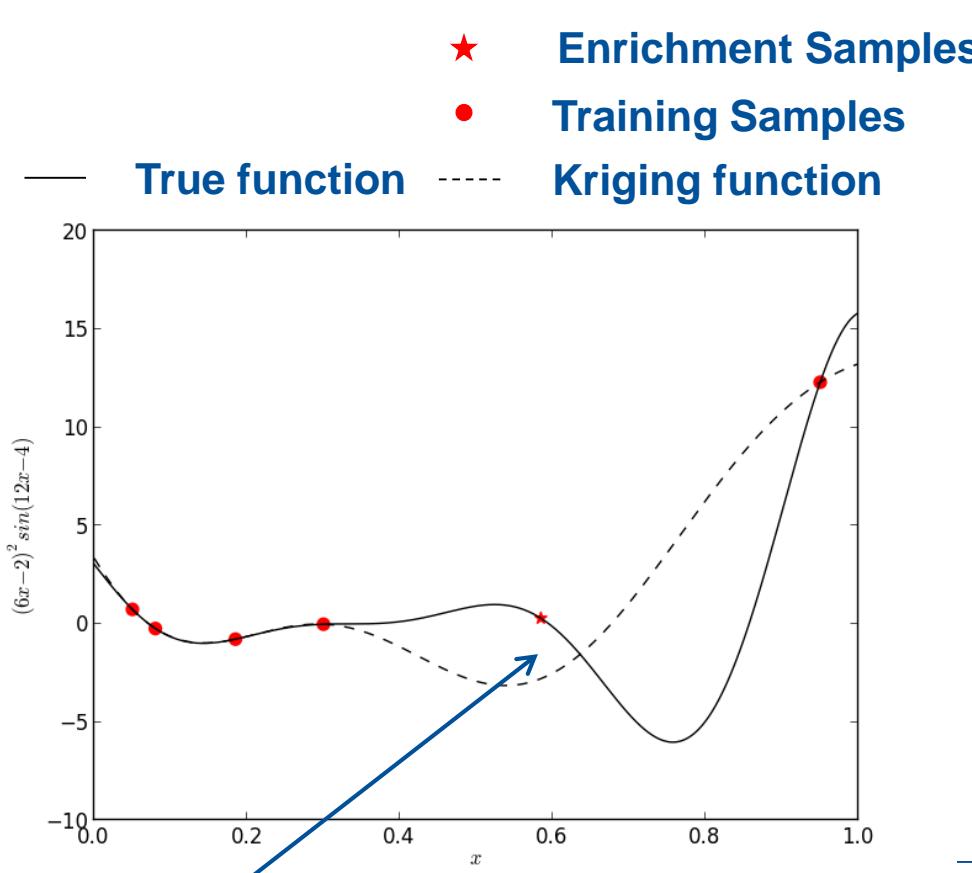
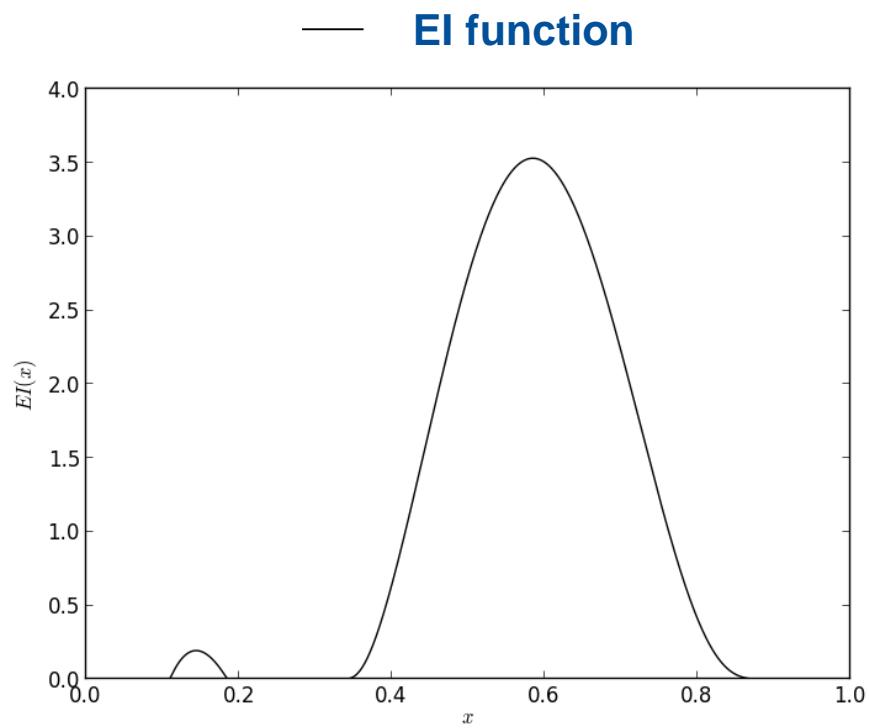
4 points for the initial DOE
6 iterations



Bayesian Optimization: Illustration on 1D example

$$\left\{ \begin{array}{l} \min (6x - 2)^2 \sin(12x - 4) \\ \text{s.t.} \\ 0 \leq x \leq 1 \end{array} \right.$$

4 points for the initial DOE
6 iterations

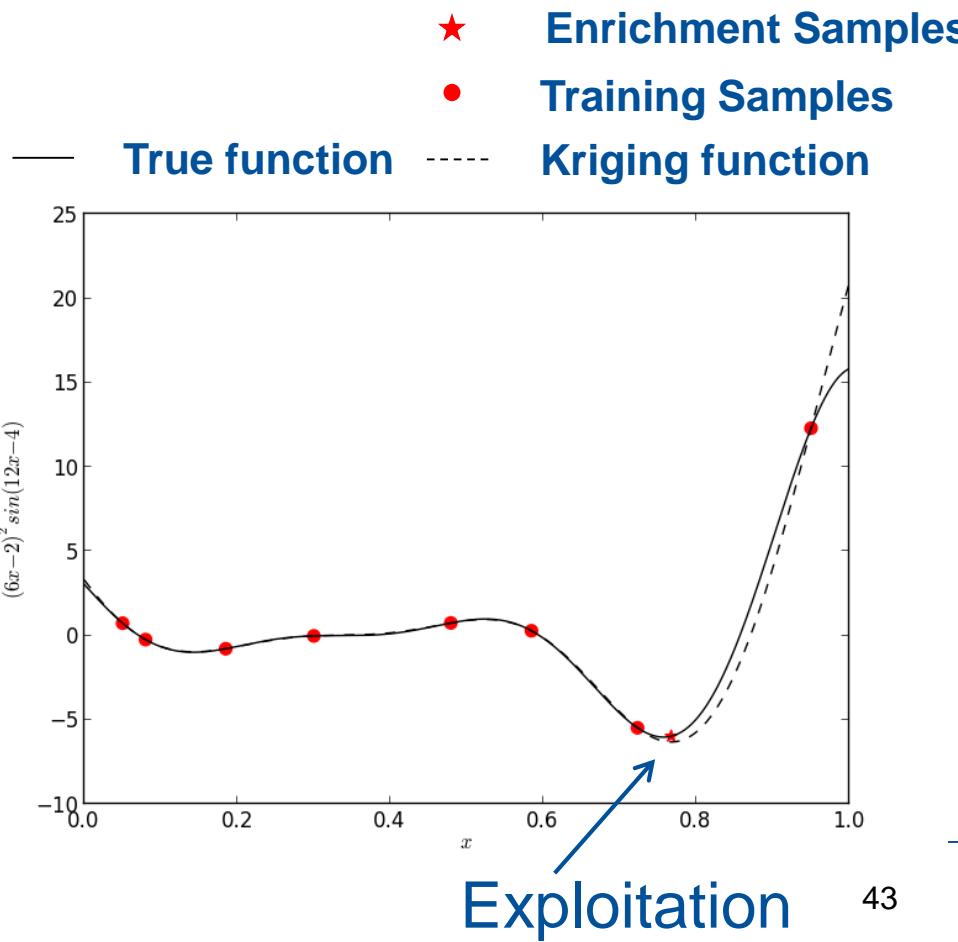
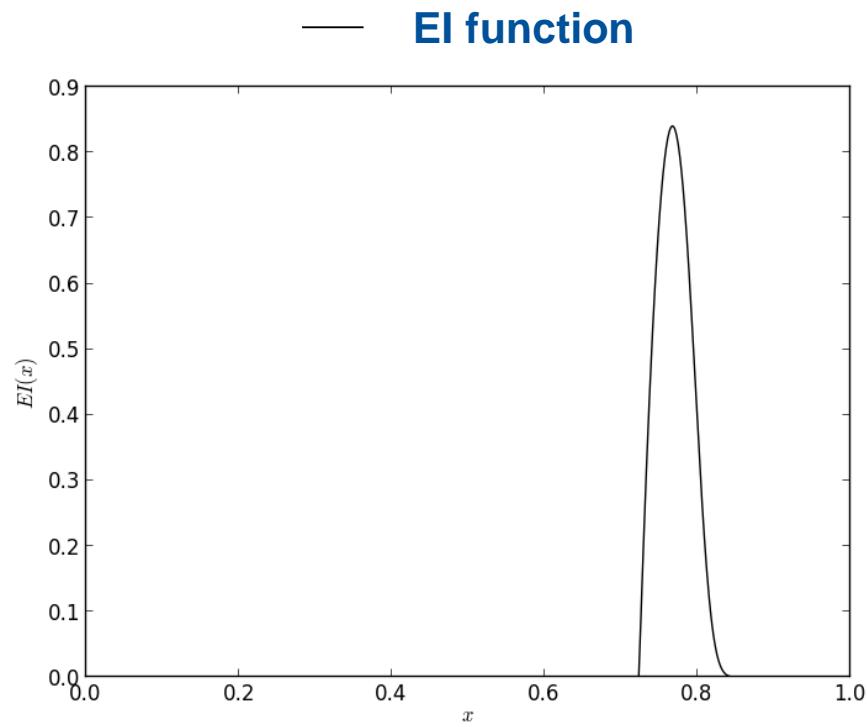


Exploration

Bayesian Optimization: Illustration on 1D example

$$\left\{ \begin{array}{l} \min (6x - 2)^2 \sin(12x - 4) \\ \text{s.t.} \\ 0 \leq x \leq 1 \end{array} \right.$$

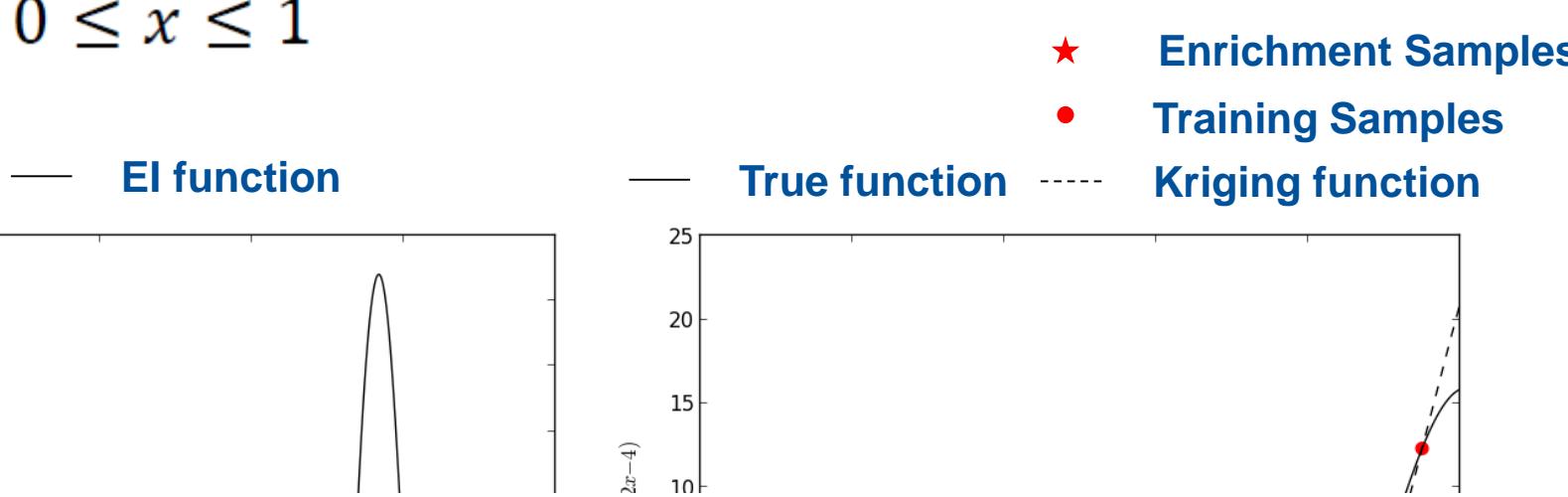
4 points for the initial DOE
6 iterations



Bayesian Optimization: Illustration on 1D example

$$\left\{ \begin{array}{l} \min (6x - 2)^2 \sin(12x - 4) \\ \text{s.t.} \\ 0 \leq x \leq 1 \end{array} \right.$$

4 points for the initial DOE
6 iterations

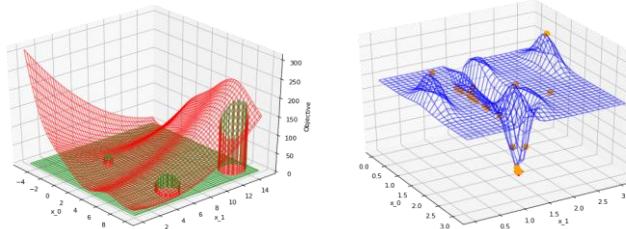


BO approach in the
notebook

SEGOMOE validation – Mono Objective applications

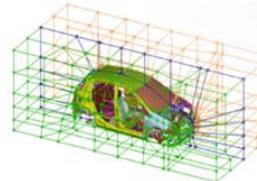
- Reference analytical functions

- Unconstrained multi-modal problems (d=2, 5, 10)
- Constrained problems (d=10, m=8)



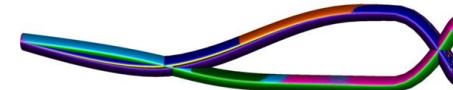
- MOPTA test case – automotive industry

d = 50, m = 68 Comparison with COBRA and COBYLA



- Wing aerodynamic optimization (ADODG6)

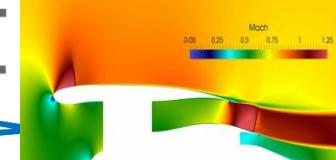
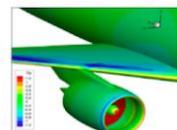
d = 17, m = 1 Global optimum found compared to SNOPT



- Nacelle optimization

d = 18, m = 2 AGILE H2020 project

Better convergence than DAKOTA



- Bombardier Research Aircraft Configuration use case

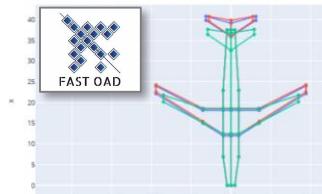
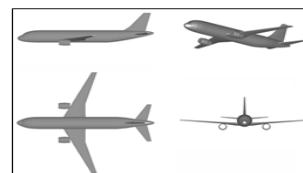
d = 12, m = 8

3h with SEGOMOE
> 8h with some internal optimizers (Isight)



- CeRAS A320 aircraft

d = 12, m=2 Comparison with SLSQP & COBYLA



CeRAS database (RWTH Aachen)

Recent methodological developments

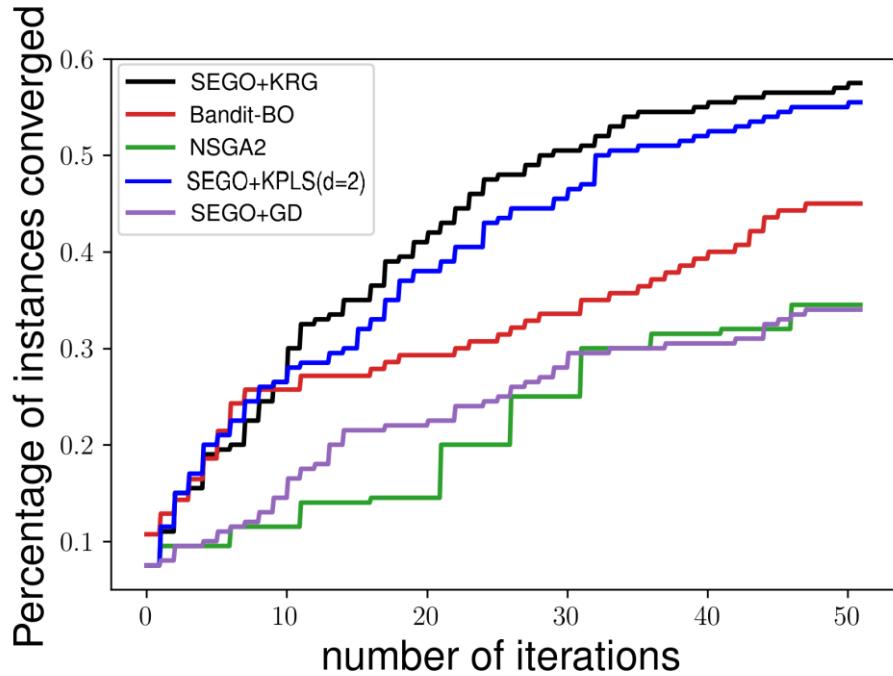
SEGOMOE capabilities

- To handle a large number of design variables
→ KPLS based models
- 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

Validation for mixed integer variables

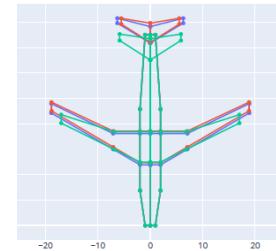
- 10 analytical tests cases (20 instances each)
⇒ 2 to 14 dimensions, with and without constraint

<https://mixed-optimization-benchmark.github.io/cases/>



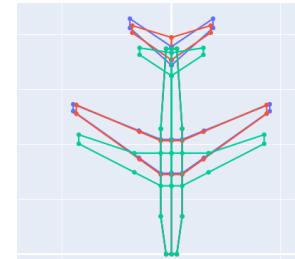
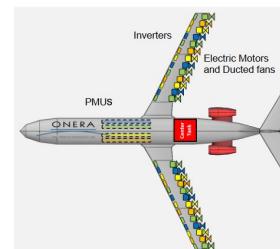
- 2 aircraft design problems with mixed continuous-categorical variables:

CeRAS: 14 dimensions



DRAGON: 29 dimensions

Distributed propulsion

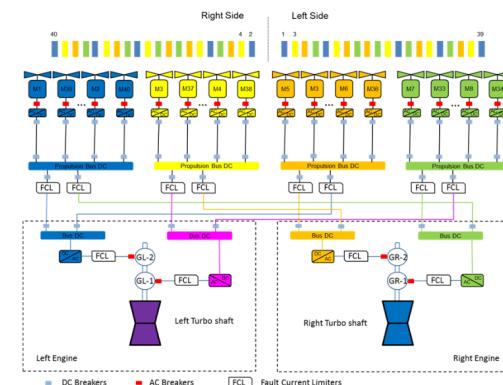
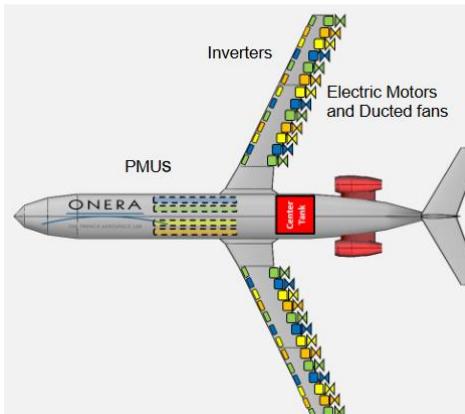
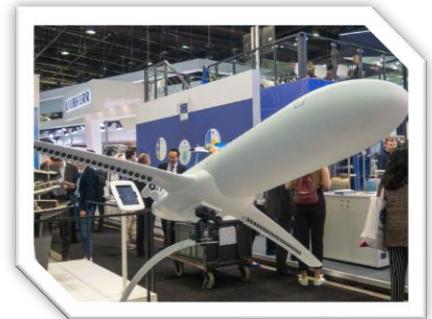


Saves, P., Bartoli, N., Diouane, Y., Lefebvre, T., Morlier, J., David, C., ... & Defoort, S. (2022). Bayesian optimization for mixed variables using an adaptive dimension reduction process: applications to aircraft design. In AIAA SCITECH 2022 Forum (p. 0082).

Application to mixed categorical

Optimization problem DRAGON green aircraft concept

- ✓ 30% reduction of CO₂ 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

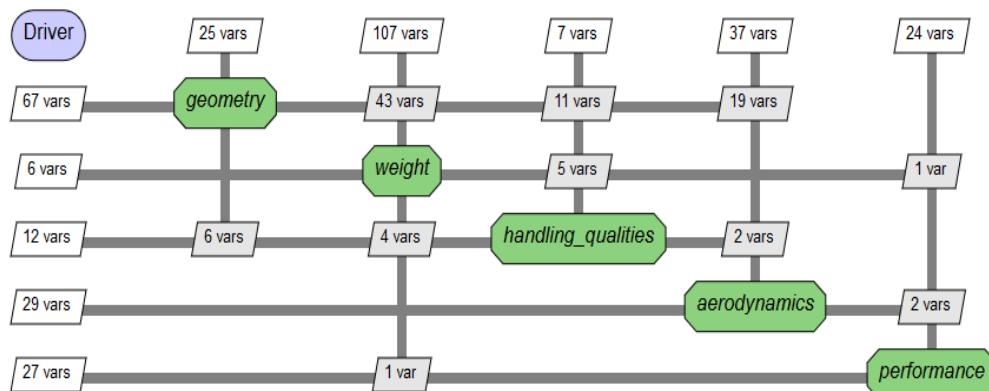
FAST-OAD: an OpenMDAO based aircraft sizing tool

Code overview



ONERA
THE FRENCH AEROSPACE LAB

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



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

FAST X OAD

Future Aircraft Sizing Tool - Overall Aircraft Design

Christophe David, Scott Delbecq, Sébastien Defoort, Peter Schmollgruber, Emmanuel Benard, Valérie Pommier-Budinger, From FAST to FAST-OAD: An open source framework for rapid Overall Aircraft Design, 2021 IOP Conf. Ser.: Mater. Sci. Eng.1024 012062.

DRAGON green aircraft concept

	Function/variable	Nature	Quantity	Range
Minimize	Fuel mass	cont	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] ($^{\circ}$)
	Wing taper ratio	cont	1	[0.2, 0.5]
	HT aspect ratio	cont	1	[3, 6]
	Angle for swept HT	cont	1	[20, 40] ($^{\circ}$)
	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	
	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	
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	



- **10 continuous design variables**
- **2 categorical design variables**

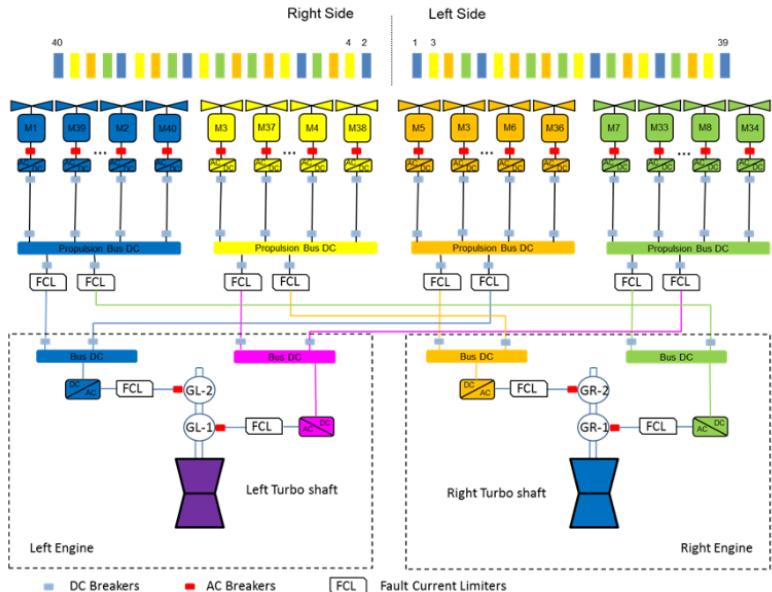
- **5 inequality constraints (MC)**
- **Fuel mass to minimize**

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 green aircraft concept

Architecture	cat	17 levels	$\{1, 2, 3, \dots, 15, 16, 17\}$
Turboshaft layout	cat	2 levels	$\{1, 2\}$
Total categorical variables	2		
Total relaxed variables	29		

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



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

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

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).

CERTIFICATE OF MERIT

2022 AIAA MULTIDISCIPLINARY DESIGN
OPTIMIZATION BEST PAPER AWARD

"Bayesian Optimization for Mixed Variables using
an Adaptive Dimension Reduction Process:
Applications to Aircraft Design"
(AIAA 2022-0082)

Authors:

Paul Saves, Eric Nguyen Van, Nathalie Bartoli, Thierry Lefebvre, Christophe David, and Sébastien Defoort, ONERA, DTIS, Université de Toulouse, and Youssef Diouane and Joseph Morlier, ISAE-Supaero ONERA, DTIS, Université de Toulouse

Paper Presentation:
AIAA 2022 Science and Technology Forum and Exposition
January 10-13, 2022, Orlando, FL



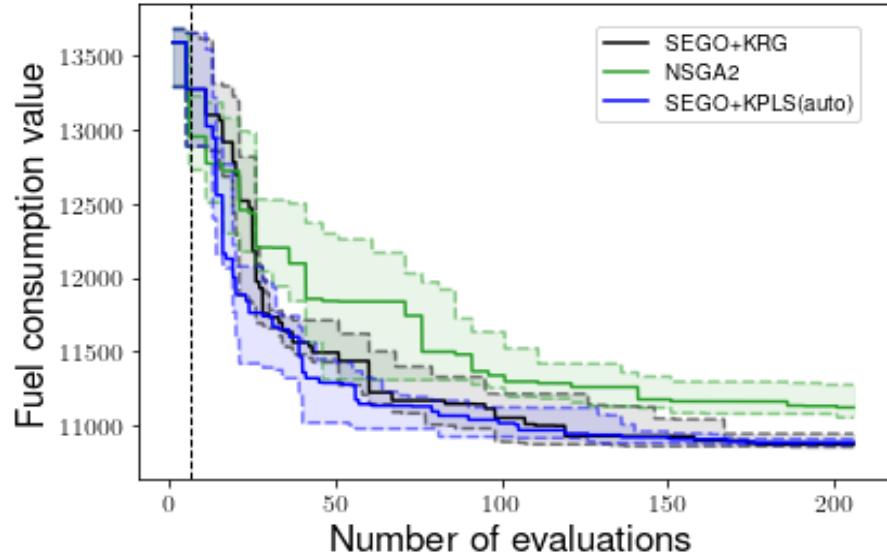
Louis J. McGill
AIAA President

Jeffrey W. Haunert
AIAA Chief Technical Activities

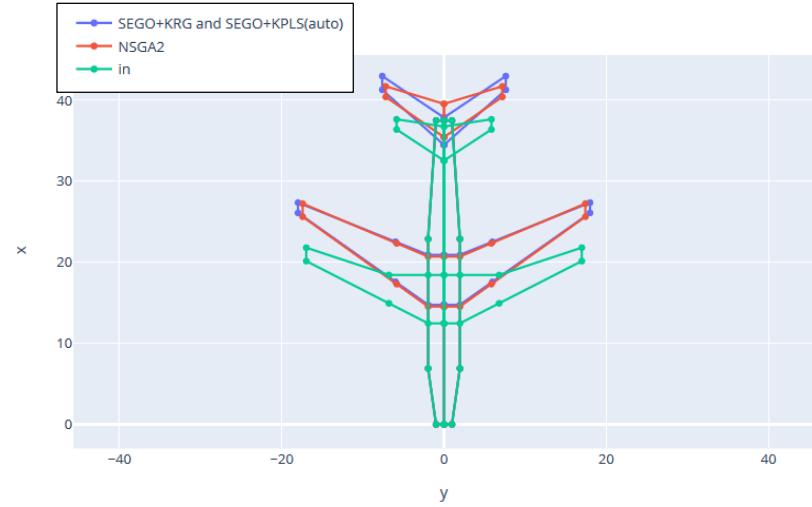
DRAGON optimization results

PhD P. Saves 2020-2023 (ISAE-ONERA)

Convergence plots for DRAGON 10 runs



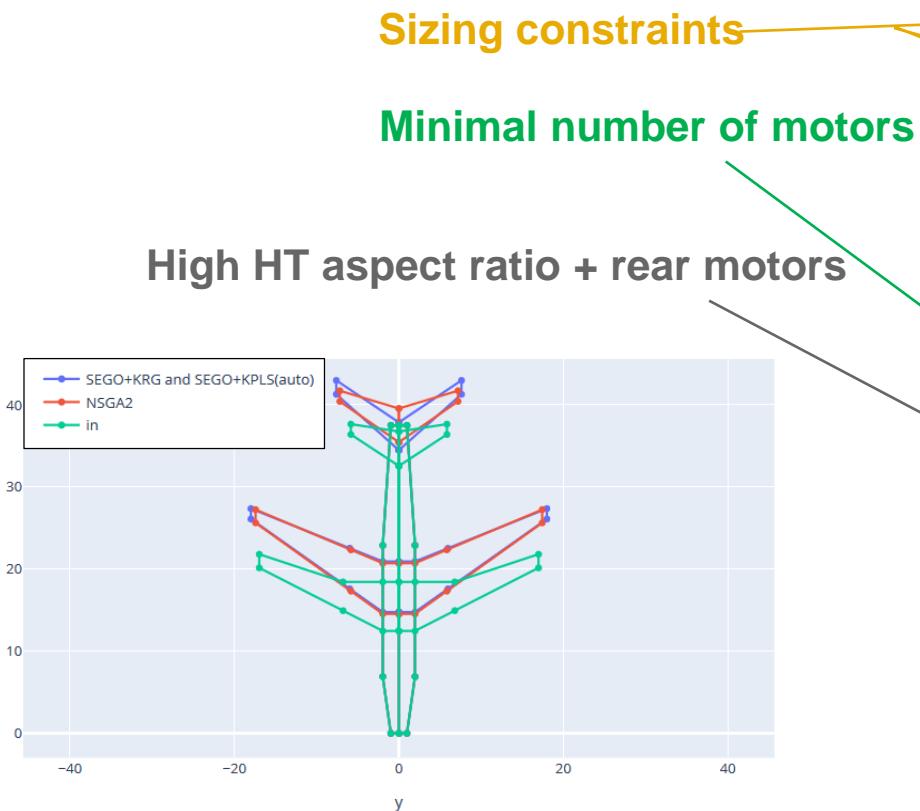
Optimal results



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DRAGON optimization results

PhD P. Saves 2020-2023 (ISAE-ONERA)



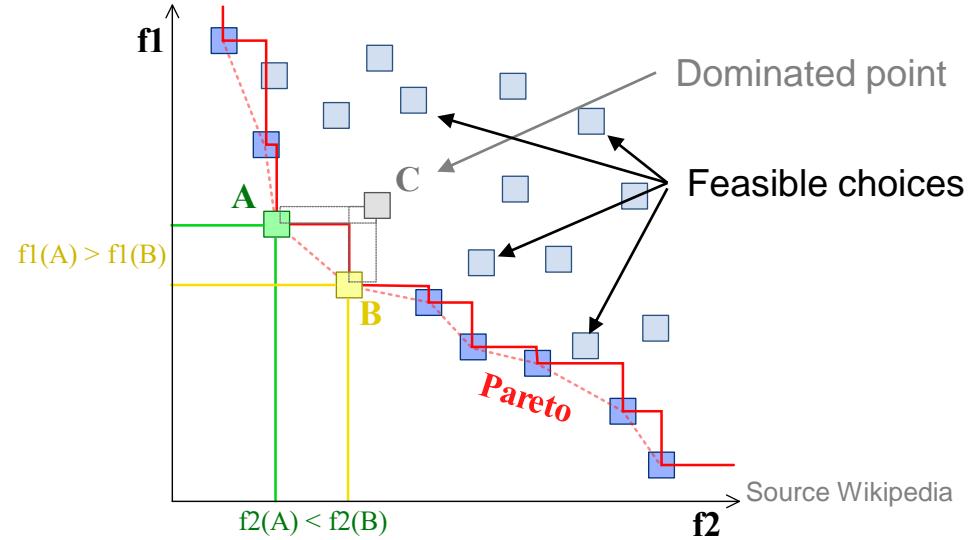
Name	Nature	Value
Fuel mass	cont	10816 kg
Wing span	cont	36 m
TOFL	cont	1722.7 m
Wing trailing edge occupied by fan	cont	10.65 m
Climb duration	cont	1735.3 s
Top of climb slope	cont	0.0108 rad
Fan operating pressure ratio	cont	1.09
Wing aspect ratio	cont	10.9
Angle for swept wing	cont	32.2°
Wing taper ratio	cont	0.235
HT aspect ratio	cont	6
Angle for swept HT	cont	40°
HT taper ratio	cont	0.3
TOFL for sizing	cont	1803 m
Top of climb vertical speed for sizing	cont	494 ft/min
Start of climb slope angle	cont	0.104 rad
Architecture	cat	10
Turboshaft layout	cat	2

- Propulsion efficiency
- Installation drag
- Space limitation

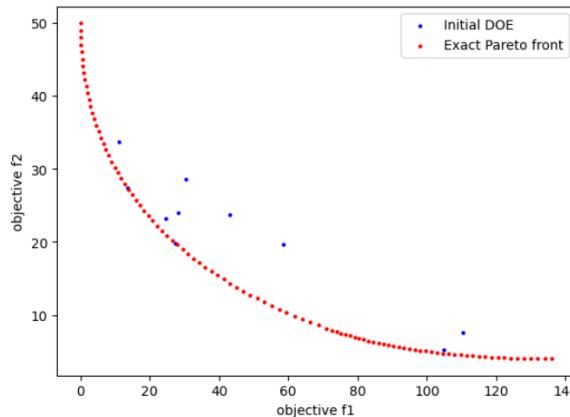
How to perform a multiobjective optimization?

$$\left\{ \begin{array}{l} \min_{\boldsymbol{x} \in \mathbb{R}^d} \quad \boldsymbol{f} = [f_1(\boldsymbol{x}), f_2(\boldsymbol{x}), \dots, f_n(\boldsymbol{x})] \\ \text{s.t.} \\ c_1(\boldsymbol{x}) \leq 0 \\ \vdots \\ c_m(\boldsymbol{x}) \leq 0 \end{array} \right.$$

n objectives

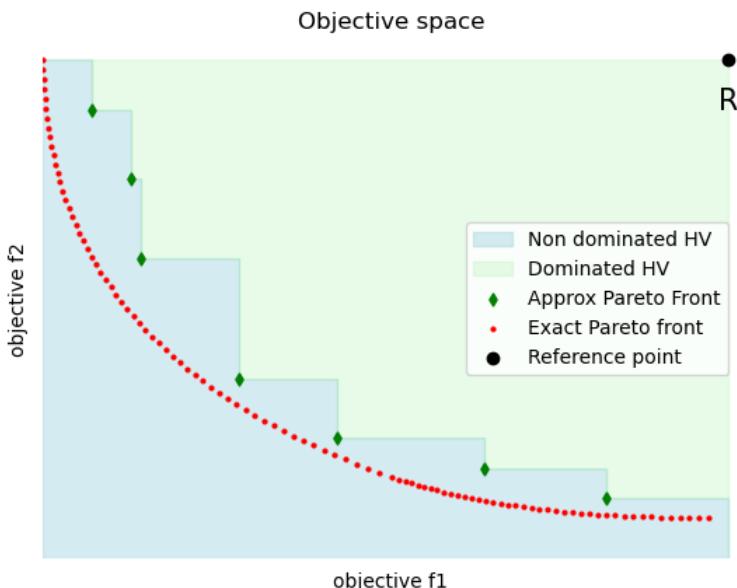
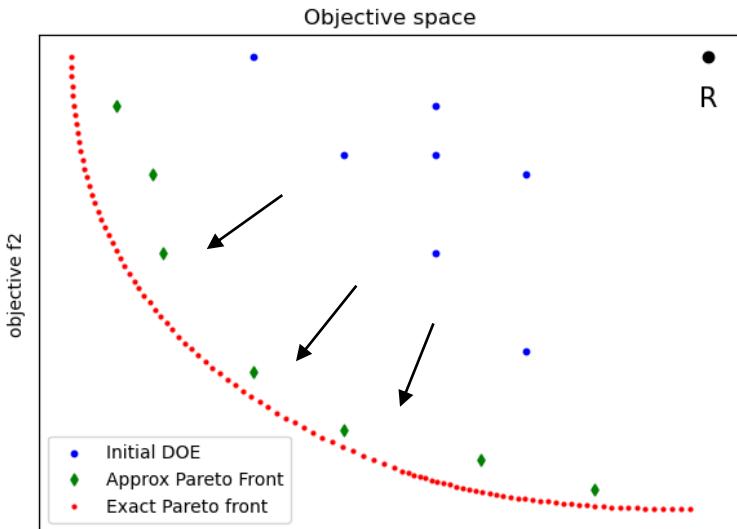


Build a Pareto Front (non dominated points)



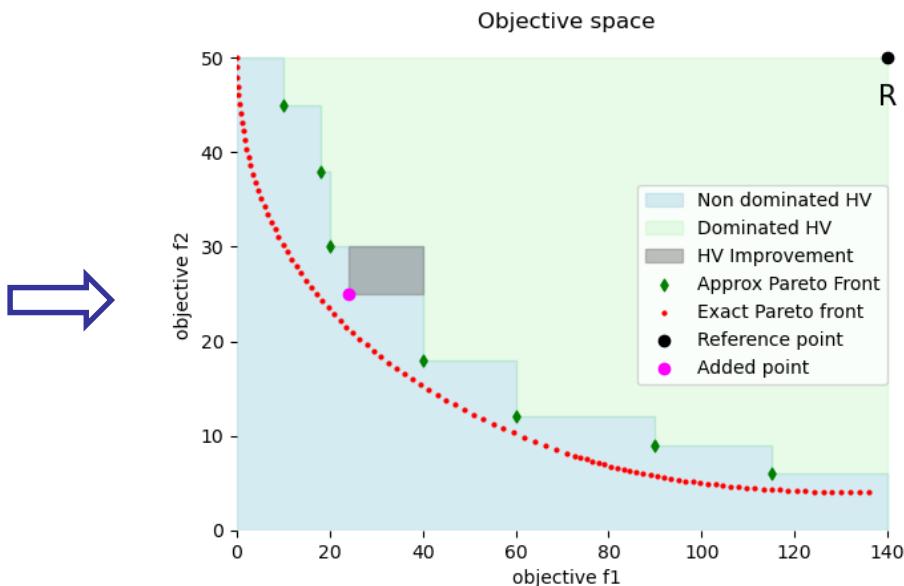
Internship R. Grapin 2021-2022

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

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

- Mono-objective

$$\text{WB2S}(\mathbf{x}) = s \text{EI}(\mathbf{x}) - \hat{\mathbf{y}}(\mathbf{x})$$

scaling factor

- Multi-objective

$$\alpha_f^{\text{reg}}(\mathbf{x}) = \gamma \alpha_f(\mathbf{x}) - \psi(\mu_f(\mathbf{x}))$$

Acquisition function

$$\alpha_f(\mathbf{x}) = \text{EHVI}(\mathbf{x}), \text{PI}(\mathbf{x}), \text{MPI}(\mathbf{x}), \dots$$

based on Hyper Volume Improvement

Regularized choices

$$\left\{ \begin{array}{l l} (\text{reg} = \max) & : \psi(\hat{\mathbf{y}}(\mathbf{x})) = \max_{i \leq n} \hat{y}_i(\mathbf{x}) \\ \\ (\text{reg} = \text{sum}) & : \psi(\hat{\mathbf{y}}(\mathbf{x})) = \sum_{i=1}^n \hat{y}_i(\mathbf{x}) \end{array} \right.$$

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.

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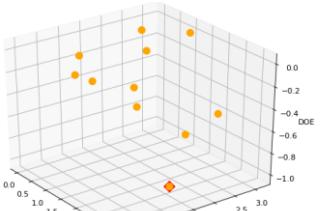
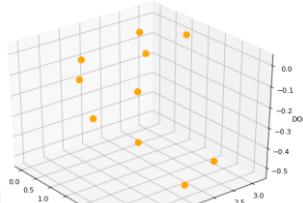
SEGOMOE algorithm – Multi objective

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

n objectives

Problem definition

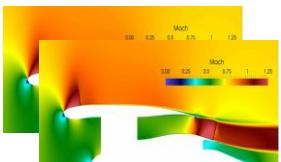
Initial DOE building



Adding new point to DOE

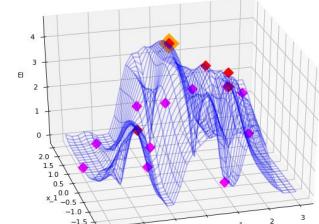
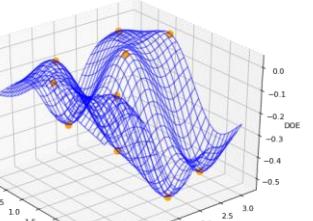
Building / Training Surrogate models

← MOE



Evaluation of problem true functions

Optimization criteria



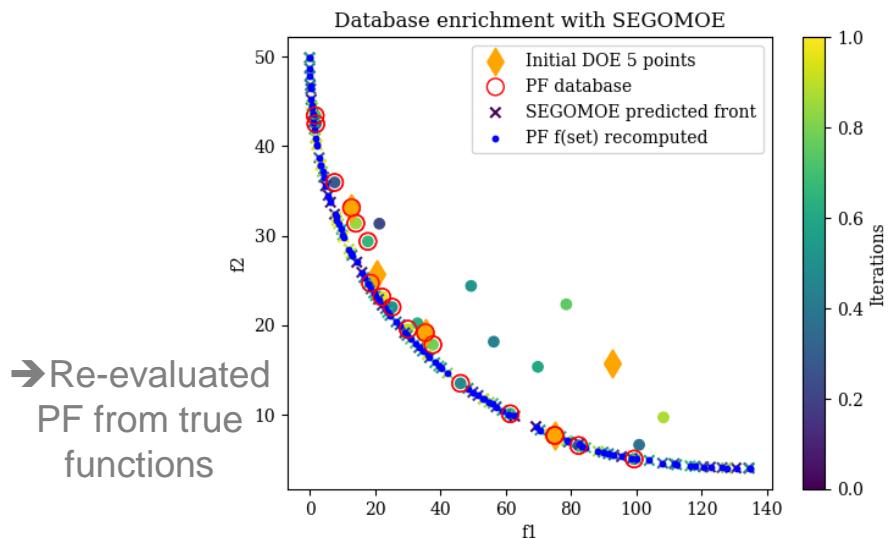
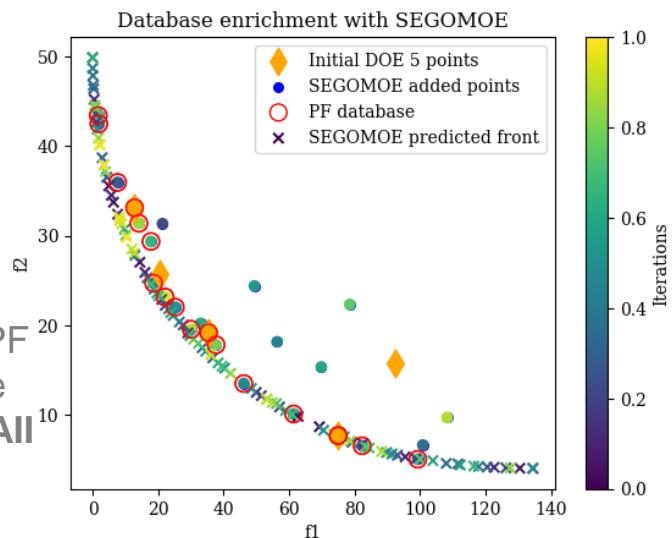
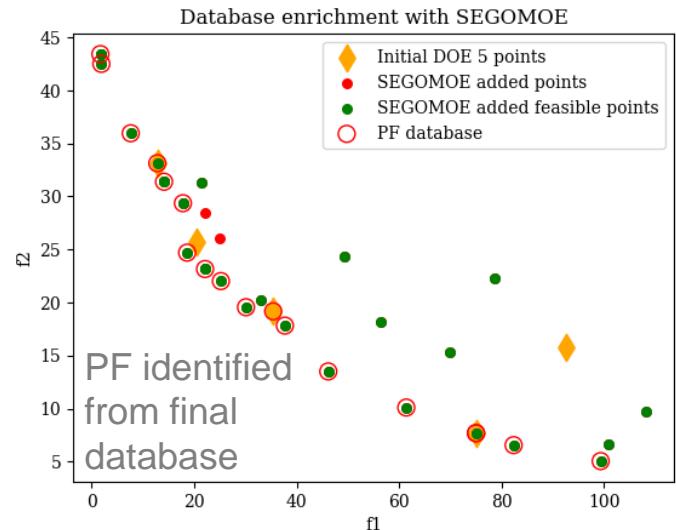
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SEGOMOE algorithm – Multi objective

N iterations reached

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

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



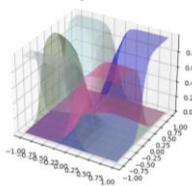
Two frameworks



github.com/SMTorg/smt

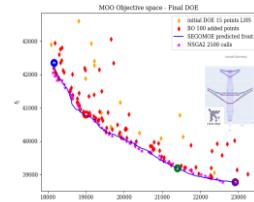


- Open source python toolbox: surrogate modeling methods, sampling techniques, and benchmarking functions
- Focus on derivatives (training derivatives used for gradient-enhanced modeling, prediction derivatives)
- New Kriging based surrogate models for higher dimension (KPLS and KPLS-K)
- Noisy Kriging 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)
- Based on SMT toolbox for surrogate models
- Remote access via a **web interface**



ONERA **WhatsOpt**

Objectifs du BE

- Partie 1 : Optimisation des hyper-paramètres du GP
- Partie 2 : Mise en place de l'algorithme EGO et comparaison de critères sur un exemple 1D
- Partie 3 : Mise en place de SEGO
- Bonus: optimisation sur un exemple 2D