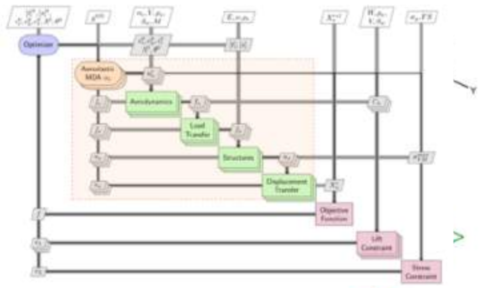
On some new [French] recipes for surrogate modeling, Bayesian and topology Optimization

If we have time …

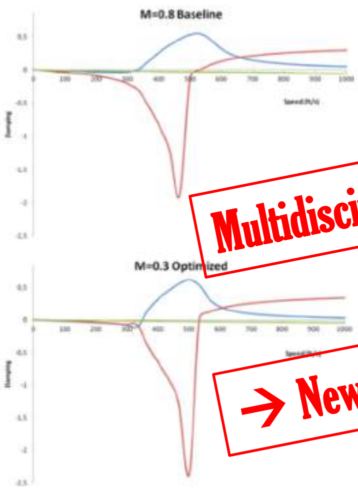
Prof.Joseph Morlier

My Research Group (Joint research with ONERA on MDO)

- 4 PhDs, 1 postdoc, 1 research assistant, 4 MsCs

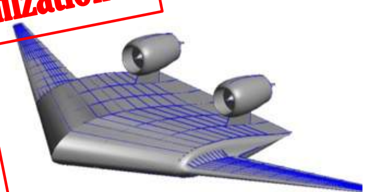


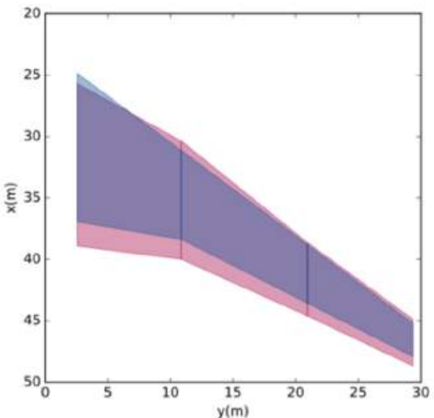
AEROSPACE ENGINEERING



Multidisciplinary Design Optimization

→ New Aircraft Concept



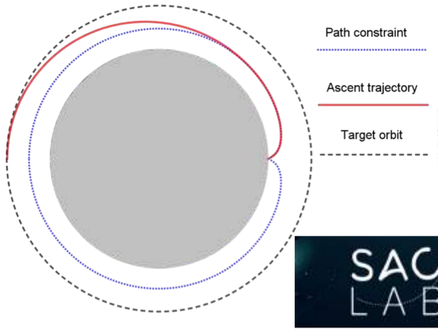


AIRBUS

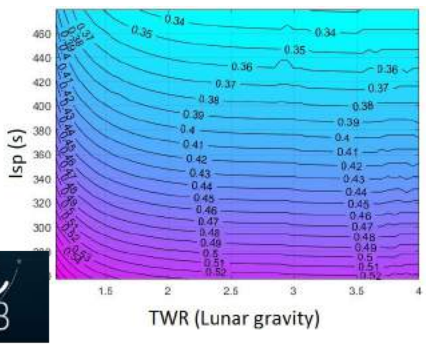
CHAIR FOR ECO DESIGN OF AIRCRAFT

ONERA

THE FRENCH AEROSPACE LAB



SAC LAB



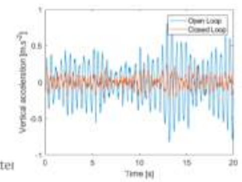
→ New disciplines such as trajectory or control

minimize $f(x) = w_1 k_h + w_2 \bar{h}_{max}(t, V_f^{CL})$

with $x = (k_h, Q, R)^{[4]}$

subject to
$$\begin{cases} V_f^{CL} > 1.2\, V_{f x_0}^{OL} \\ \left|\beta_{max}(t, V_f^{CL})\right| < \beta_{ref} \\ f_{max}^{i} < 3 f_{max\, x_0}^{i} \end{cases}$$

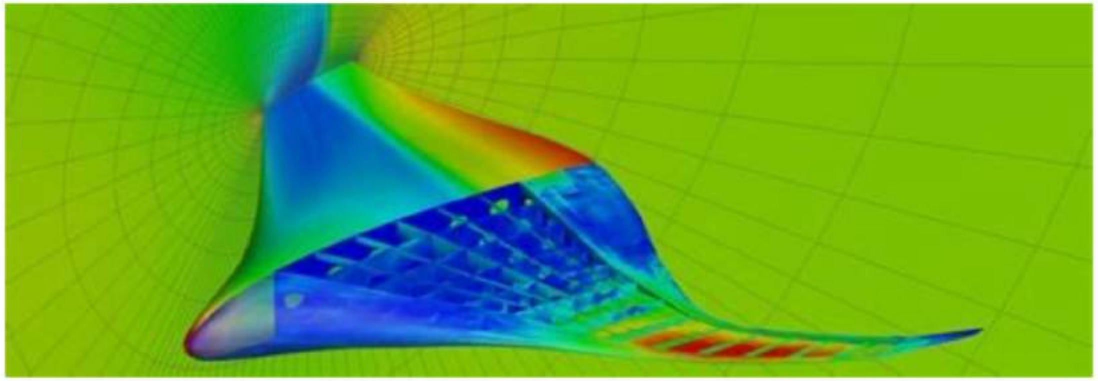
where V_f^{XL} is the open loop (OL) or closed loop (CL) flutter
β_{ref} is the maximum control surface deflection
f_{max}^{i} is the maximum frequency of mode i
$V_{f x_0}^{OL}$ is the open-loop flutter velocity at the starting point
Q, R are the LQR weight matrix to compute K



AIRBUS

Popularization

https://www.linkedin.com/pulse/optimization-mdo-connecting-people-joseph-morlier/



http://mdolab.engin.umich.edu

Optimization [MDO] for connecting people?

Publié le 14 février 2019 | Modifier l'article | Voir les stats

joseph morlier
Professor in Structural and Multidisciplinary Design Optimization, ... any idea?
2 articles

74 31 3 0

Our Goal: Embed efficient optimization algorithms in the design process of Aerostructures

- Reduce in a « smart way » the computational time of optimization for coupled simulations
- Global Optimization using surrogate modeling → fixed budget (enriching process) to deal with INDUSTRIAL problems
- Specialized surrogate models for HD (engineering) problems and UQ
- Taking into account different levels of fidelity

→Methods applied to AD Aircraft Design: Put the aircraft structure / aeroelasticity in the loop at the early stage of MDO process

→Methods applied to SLD Space Launcher Design: Put the control/trajectory/propulsion in the preliminary design loop

→ compatible with

openMDAO

http://openmdao.org

Outlines for today

multidisciplinary Design optimization

multidisciplinary optimization

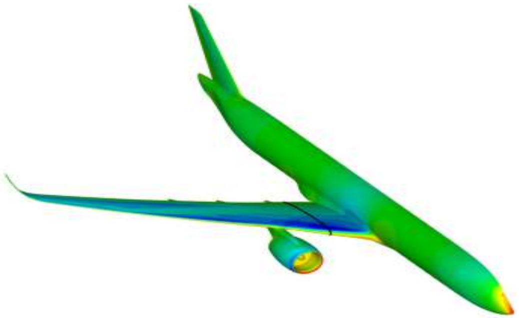
1. Surrogate modeling
2. Bayesian Optimization
3. Topology Optimization

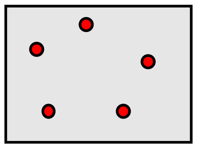
1,2: Common researches with
N. Bartoli, T. Lefebvre (ONERA/DTIS)

Outlines for today

1. Surrogate modeling
2. Bayesian Optimization
3. Topology Optimization

Surrogate modeling Recipes

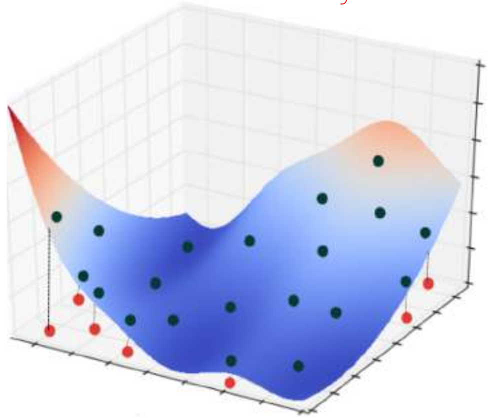


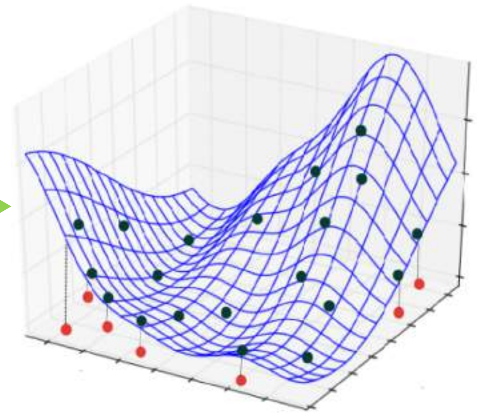


DOE

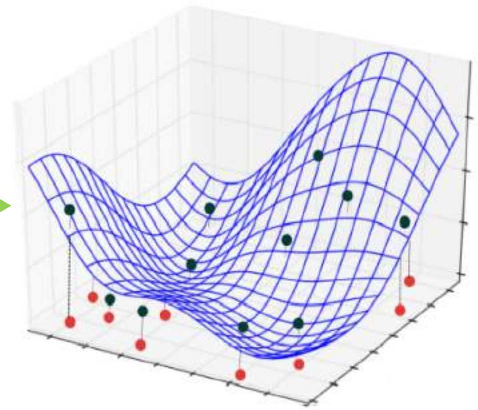
True Function Evaluation

This is costly!





Interpolant model



Regression model

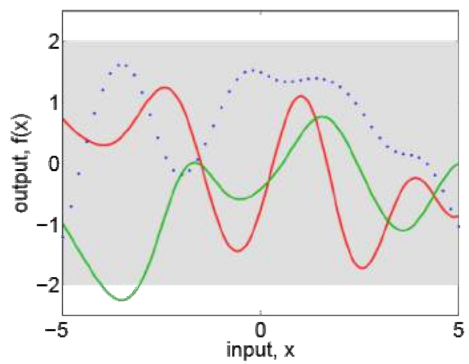
$$MSE = \frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2$$

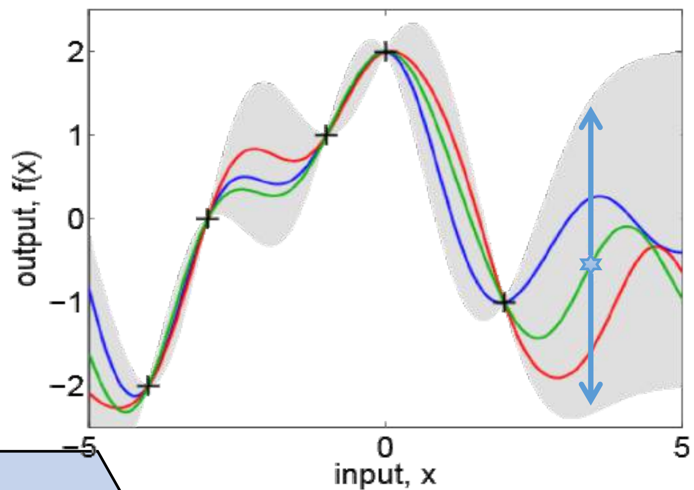
$$LOF = \frac{MSE}{Var(y)}$$

$\boldsymbol{n}$ is the number of samples
$\hat{\boldsymbol{y}}$ is the predictions of the n samples
$\boldsymbol{y}$ is the true outputs of the n samples

Gaussian Process (aka Kriging)

Image Source: http://mlg.eng.cam.ac.uk/teaching/4f13/1314/





Prior
f|x

$GP(0, K)$

X

Y

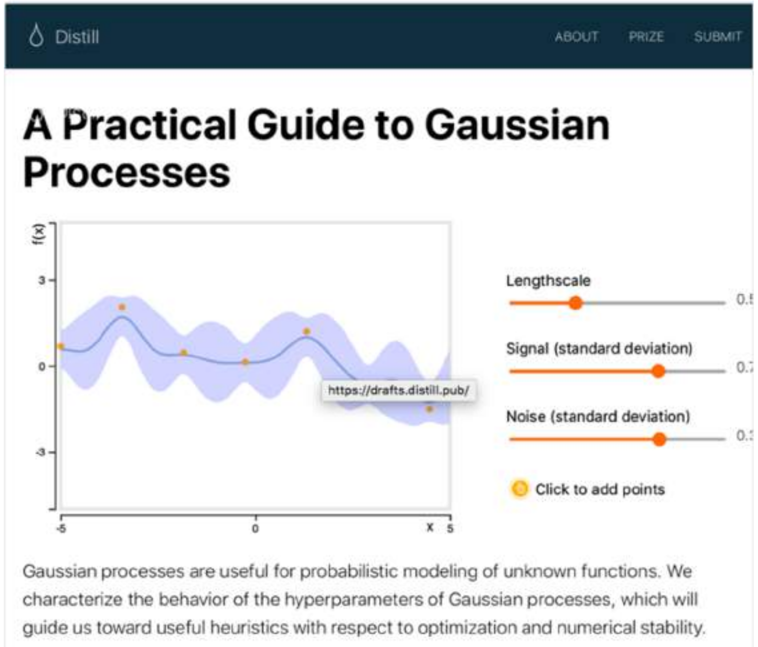
Training
y|x
$GP(0, K + \sigma_n^2 I)$
Optimize: for a better hyperparameters and better prior

Posterior on y
$\boldsymbol{y}^* | \boldsymbol{x}^*, \boldsymbol{y}, \boldsymbol{x}$

GP ($K_*[K + \sigma_n{}^2 I]^{-1}$y, $K_{**} + \sigma_n^2 I - K_*^T[K + \sigma_n{}^2 I]^{-1} K_*$)

A good starting point x_0=Rasmussen's book

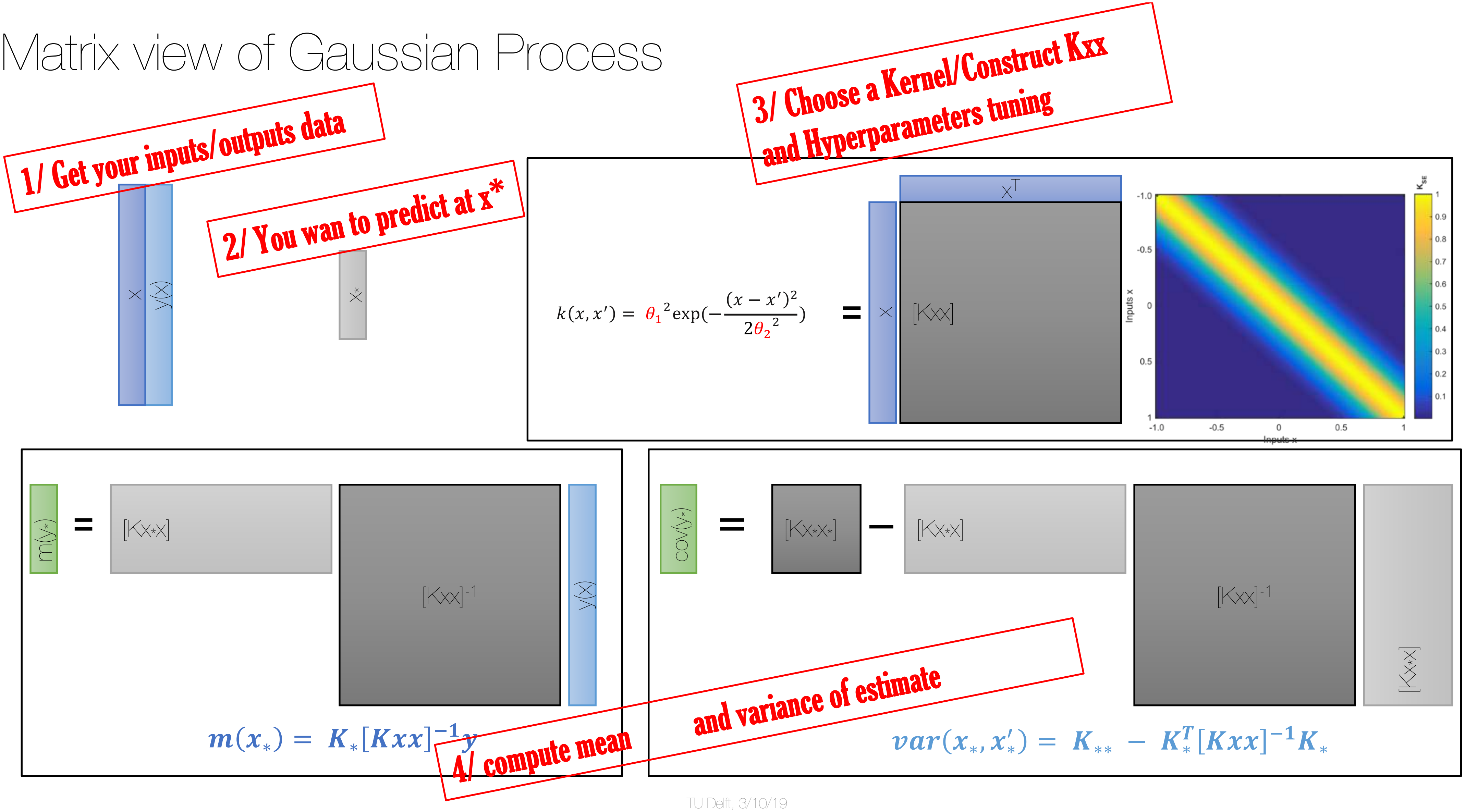
- https://drafts.distill.pub/gp/



C. E. Rasmussen & C. K. I. Williams, Gaussian Processes for Machine Learning, the MIT Press, 2006, ISBN 026218253X. © 2006 Massachusetts Institute of Technology. www.GaussianProcess.org/gpml

Gaussian Processes for Machine Learning

Matrix view of Gaussian Process



$$k(x,x') = \theta_1^{\,2}\exp\left(-\frac{(x-x')^2}{2\theta_2^{\,2}}\right)$$

$$m(x_*) = K_*[Kxx]^{-1}y$$

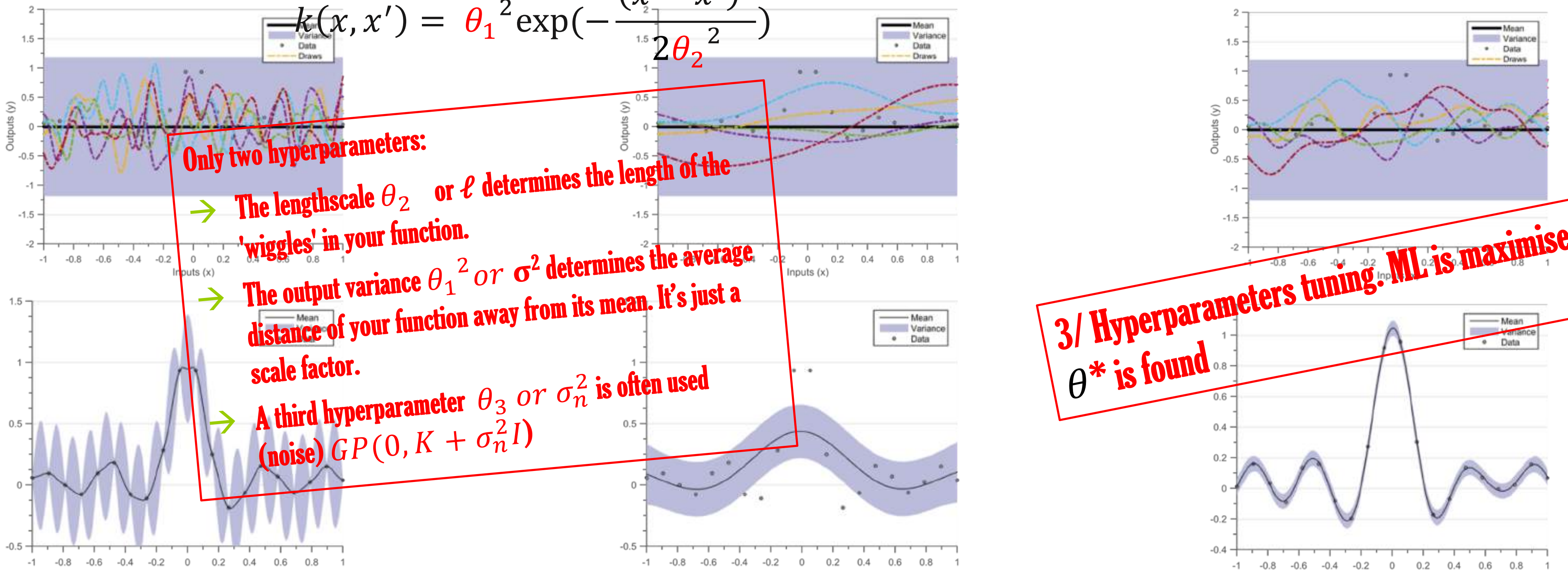
$$var(x_*,x_*') = K_{**} - K_*^T[Kxx]^{-1}K_*$$

Optimizing Marginal Likelihood (ML)

$$\text{ML} = log\left(p(y|X,\theta)\right) = -\frac{1}{2}y^T K^{-1} y - \frac{1}{2}log|K| - \frac{n}{2}log(2\pi)$$

- It is a combination of data-fit term, a complexity penalty term and a normalization term

$$k(x,x') = \theta_1{}^2 \exp\left(-\frac{(x-x')^2}{2\theta_2{}^2}\right)$$



Only two hyperparameters:

→ The lengthscale θ_2 or ℓ determines the length of the 'wiggles' in your function.

→ The output variance $\theta_1{}^2$ or σ^2 determines the average distance of your function away from its mean. It's just a scale factor.

→ A third hyperparameter θ_3 or σ_n^2 is often used (noise) $GP(0, K + \sigma_n^2 I)$

3/ Hyperparameters tuning. ML is maximised, θ^* is found

ML = -8.2

ML = -35.3

ML = 6,04

Surrogate Model Toolbox: SMT

AEROSPACE ENGINEERING
UNIVERSITY of MICHIGAN

NASA

isae SUPAERO

ONERA
THE FRENCH AEROSPACE LAB

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Focus on derivatives
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SMT: Surrogate Modeling Toolbox

The surrogate model toolbox (SMT) is an open-source Python package consisting of libraries of surrogate modeling methods (e.g., radial basis functions, kriging), sampling methods, and benchmarking problems. SMT is designed to make it easy for developers to implement new surrogate models in a well-tested and well-document platform, and for users to have a library of surrogate modeling methods with which to use and compare methods.

The code is available open-source on GitHub.

Focus on derivatives

SMT is meant to be a general library for surrogate modeling (also known as metamodeling, interpolation, and regression), but its distinguishing characteristic is its focus on derivatives, e.g., to be used for gradient-based optimization. A surrogate model can be represented mathematically as

$$y = f(\mathbf{x}, \mathbf{xt}, \mathbf{yt}),$$

where $\mathbf{xt} \in \mathbb{R}^{nt \times nx}$ contains the training inputs, $\mathbf{yt} \in \mathbb{R}^{nt}$ contains the training outputs, $\mathbf{x} \in \mathbb{R}^{nx}$ contains the prediction inputs, and $y \in \mathbb{R}$ contains the prediction outputs. There are three types of derivatives of interest in SMT:

1. Derivatives (dy/dx): derivatives of predicted outputs with respect to the inputs at which the model is evaluated.
2. Training derivatives (dyt/dxt): derivatives of training outputs, given as part of the training data set, e.g., for gradient-enhanced kriging.
3. Output derivatives (dy/dyt): derivatives of predicted outputs with respect to training outputs, representing how the prediction changes if the training outputs change and the surrogate model is re-trained.

Not all surrogate modeling methods support or are required to support all three types of derivatives; all are optional.

Surrogate modeling in HD, focus on derivatives

https://github.com/SMTorg/SMT

M.-A. Bouhlel, J. T. Hwang, N. Bartoli, R. Lafage, J. Morlier, J .R.R.A Martins (2019), A Python surrogate modeling framework with derivatives, Advances in Engineering Software

Prediction derivatives (dy/dx) are derivatives of predicted outputs with respect to the inputs at which the model is evaluated. These are computed together with the prediction outputs when the surrogate model is evaluated. These are required for gradient-based optimization algorithms based on surrogate models.

Training derivatives (dy_t/dx_t) are derivatives of the training outputs with respect to the corresponding inputs. These are provided by the user and are used to improve the model accuracy in GE-KPLS. When the adjoint method is used to compute training derivatives, a high-quality surrogate model can be constructed with a low relative cost, because the adjoint method computes these derivatives at a cost independent of the number of inputs.

Output derivatives (dy/dy_t) are derivatives of predicted outputs with respect to training outputs, which is a measure of how the prediction changes with a change in training outputs, accounting for the re- training of the surrogate model. These post-training derivatives are used when the surrogate model is trained within an optimization iteration.

Given its focus on derivatives, SMT is synergistic with the OpenMDAO framework , which is a software framework for gradient-based multidisciplinary analysis and optimization. SMT can provide the derivatives that OpenMDAO requires from its components to compute the coupled derivatives of the multidisciplinary model.

Outlines for today

1. Surrogate modeling

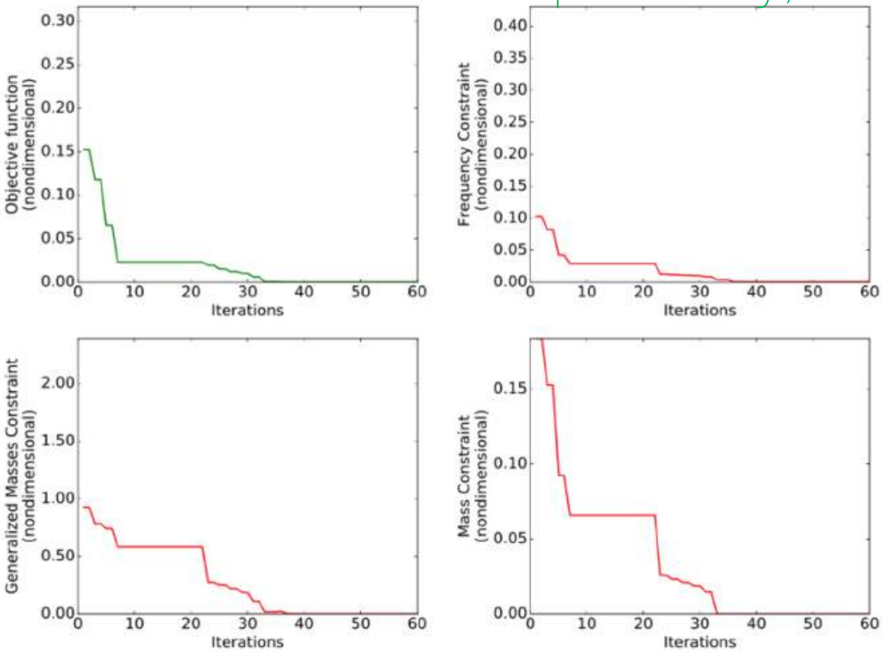
2. Bayesian Optimization

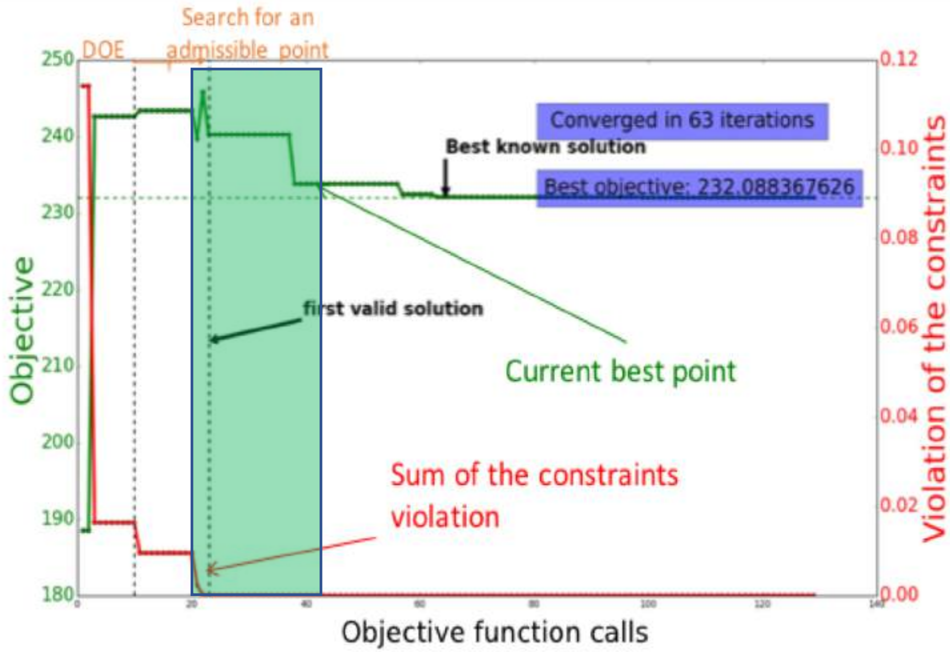
3. Topology Optimization

New paradigm for Surrogate Based Optimization (SBO)

Gradient based Optimality, Feasibility

SBO Exploration, Exploitation





Stopping criteria: tolfun, tolx, maxiter

Stopping criteria: Max Budget (Function calls)

A good starting point X_0=Forrester's book

Engineering Design via Surrogate Modelling

A Practical Guide

Alexander I. J. Forrester, András Sóbester and Andy J. Keane

University of Southampton, UK

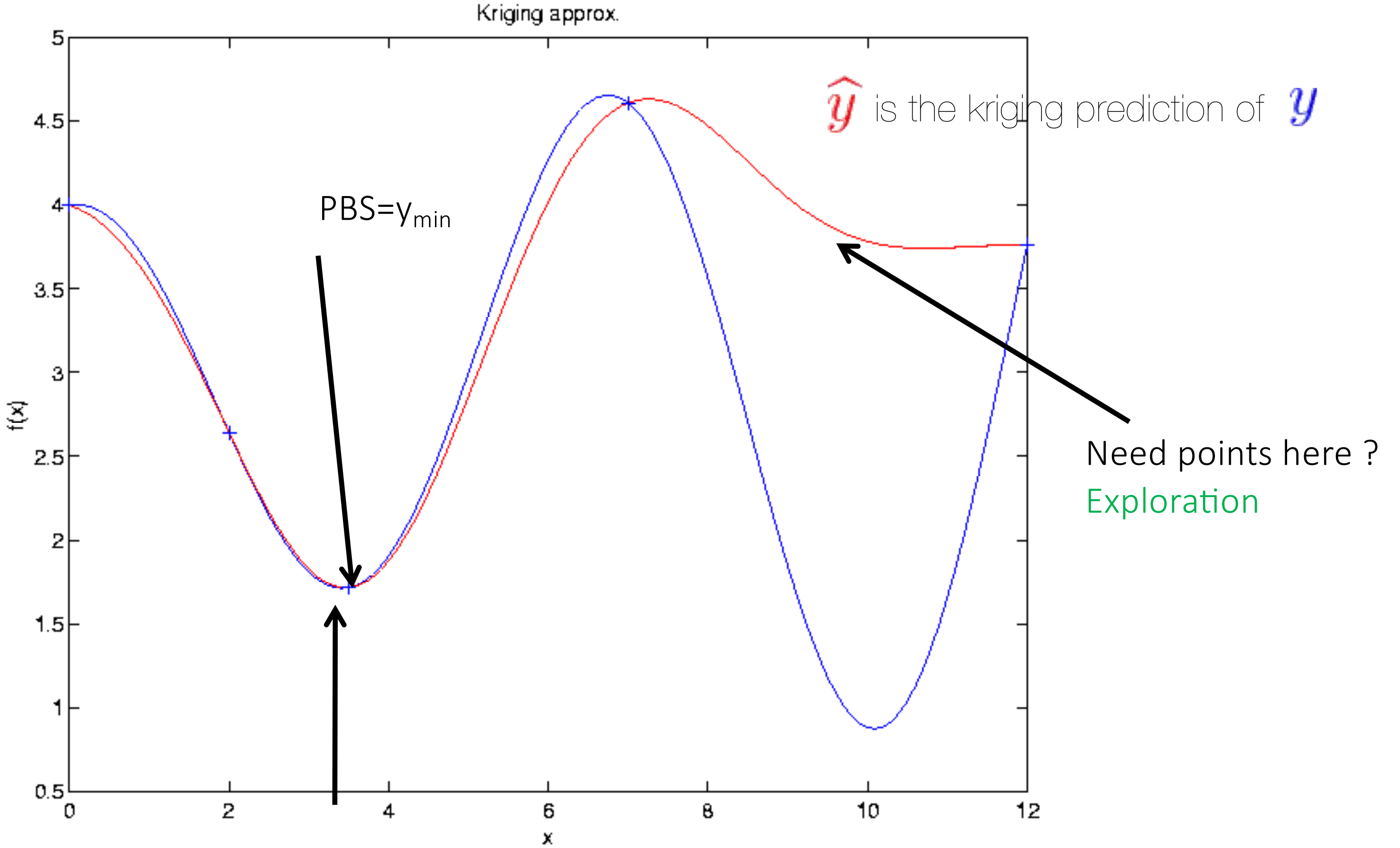
The goal is: find min of f(x) by sampling + and Kriging updating

Where do I need to update my sampling?

We note the present best solution (PBS=y_{min})

At every x there is some chance of improving on the PBS.

Then we ask: Assuming an improvement over the PBS, where is it likely be largest?

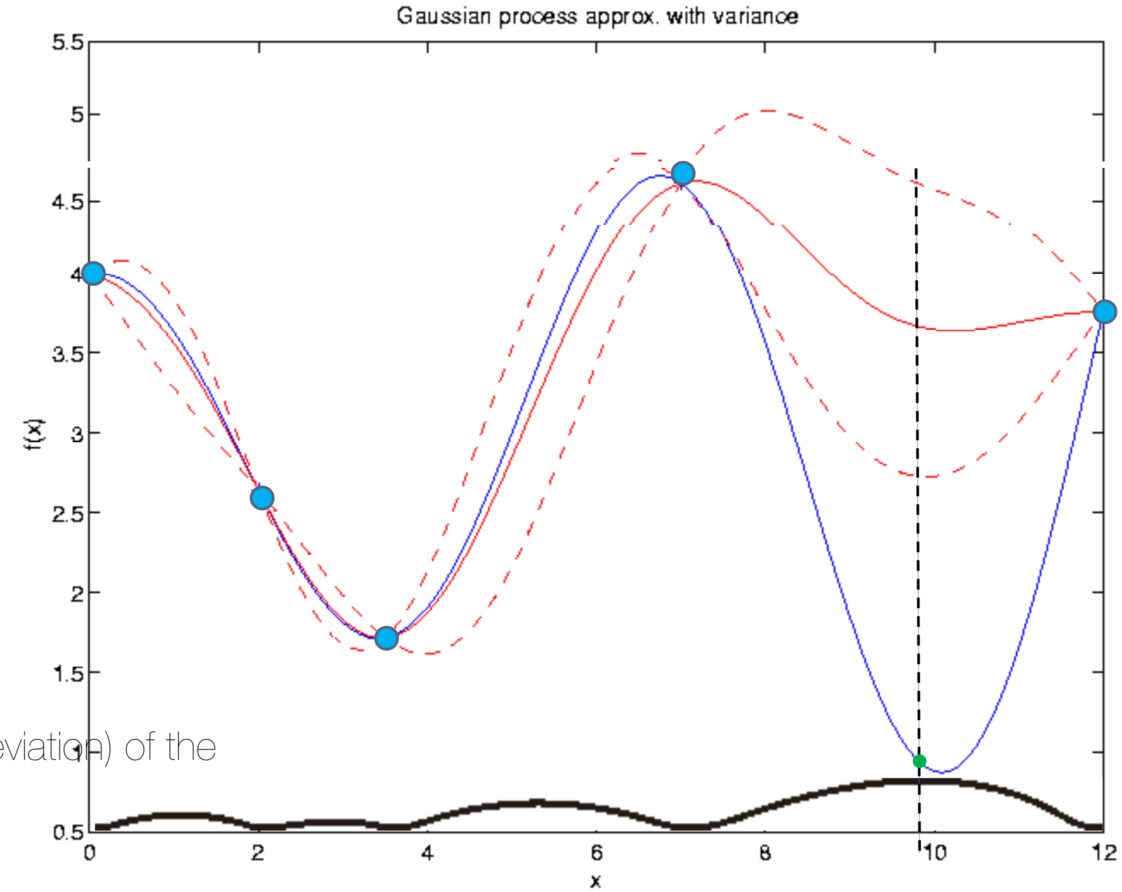


Exploitation may drive the optimization to a local optimum

In supervised mode … have a look to max(RMSE)

Impossible to compute the error: we don't know for each x the true value of the function

But…. Can we use GP properties ?

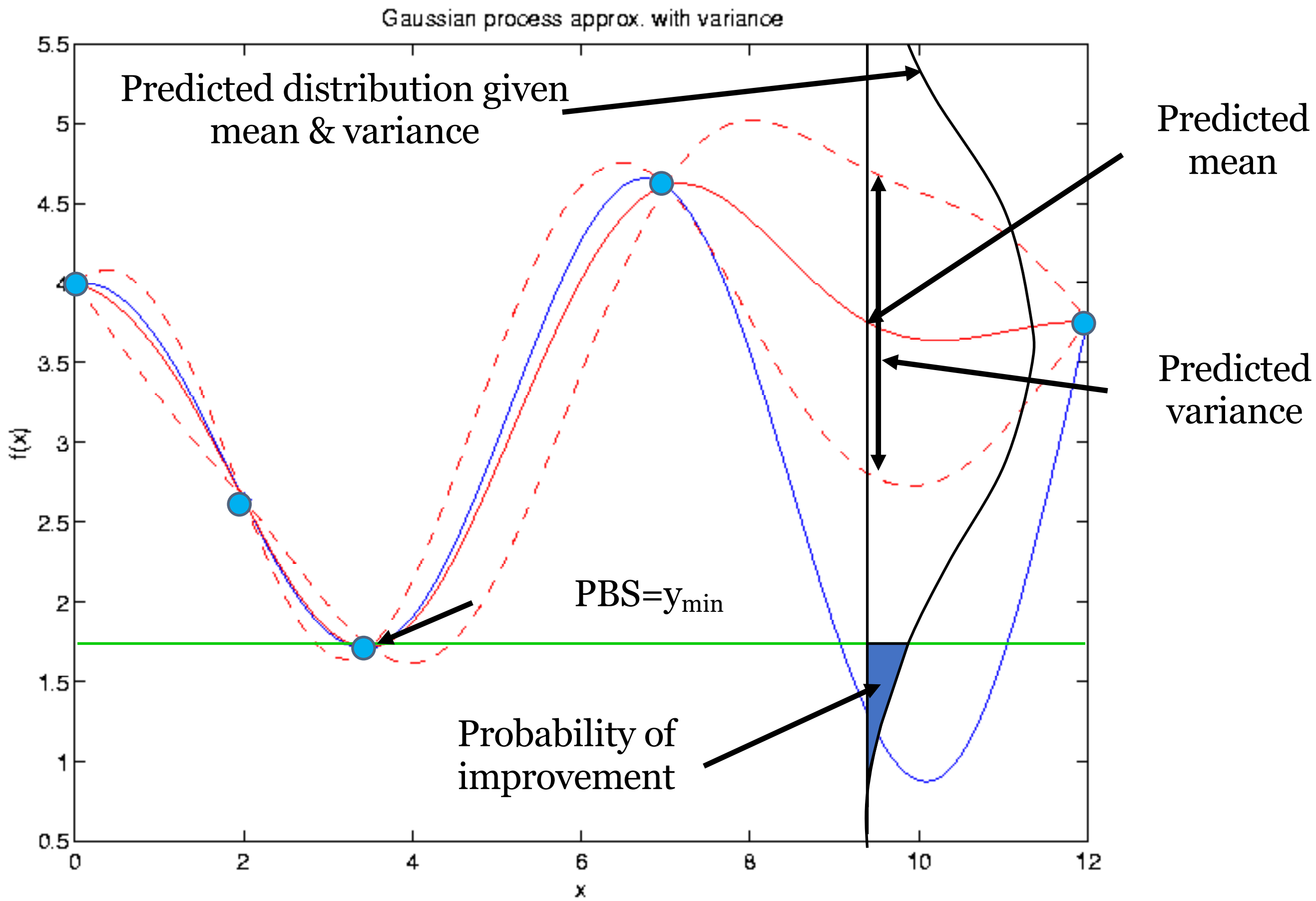


$\hat{y}$ is the kriging prediction of y

$\hat{s}$ is the estimation error (standard deviation) of the prediction (often noted σ_y)

PBS=y_{min}

Probability of improvement



Improvement … explicitely

- *Improvement* : $I(\mathbf{x}) = \max\left(y_{min} - \hat{Y}(\mathbf{x}), 0\right)$
- *Expected Improvement* :

$$\boxed{\mathrm{EI}(x) = \mathrm{E}[\max(0, y_{\min} - \hat{y}(x))]}$$

$$E[I(\mathbf{x})] = \int_{-\infty}^{y_{min}} (y_{min} - \hat{y})\varphi\left(\frac{y_{min} - \mu_{\hat{Y}}(\mathbf{x})}{\sigma_{\hat{Y}}(\mathbf{x})}\right) d\hat{y}$$

$$E[I(\mathbf{x})] = (y_{min} - \mu_{\hat{Y}}(\mathbf{x}))\Phi\left(\frac{y_{min} - \mu_{\hat{Y}}(\mathbf{x})}{\sigma_{\hat{Y}}(\mathbf{x})}\right) + \sigma_{\hat{Y}}(\mathbf{x})\varphi\left(\frac{y_{min} - \mu_{\hat{Y}}(\mathbf{x})}{\sigma_{\hat{Y}}(\mathbf{x})}\right)$$

Exploitation

Exploration

global optimum can be found because *P[I(x)] = 0 when s = 0 so that there is no probability of improvement* at a point which has already been sampled → guarantees global convergence

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

*Jones, D. R., Schonlau, M., & Welch, W. J. (1998). Efficient global optimization of expensive black-box functions. Journal of Global optimization, 13(4), 455-492.

Infill Criteria : max(Expected improvement)

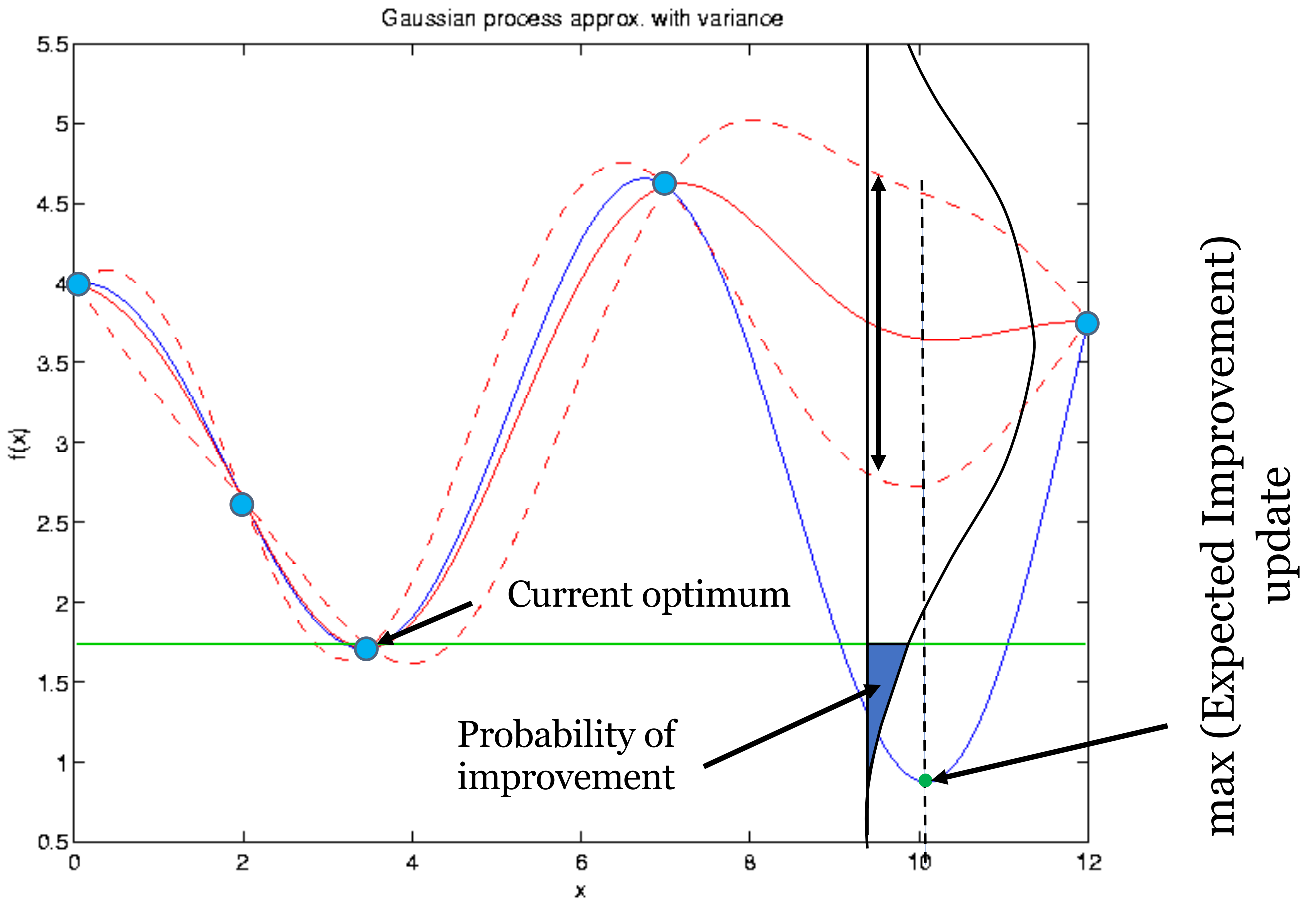
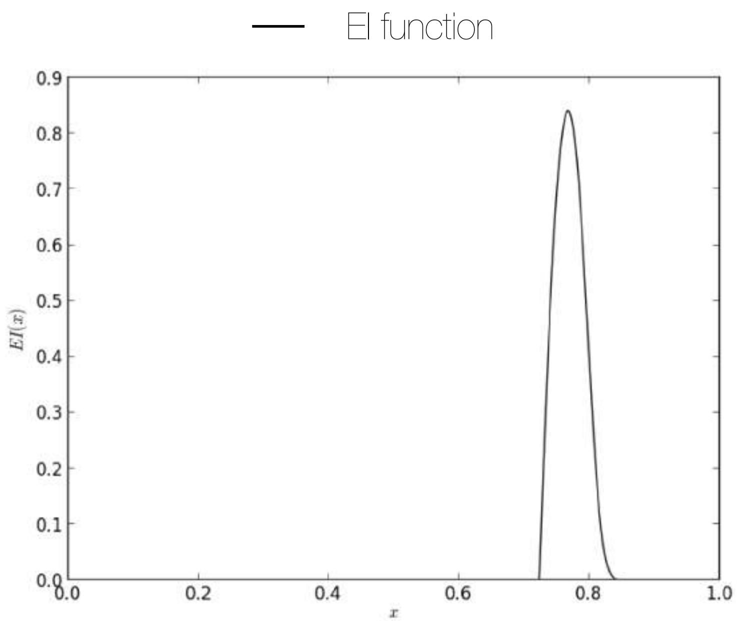
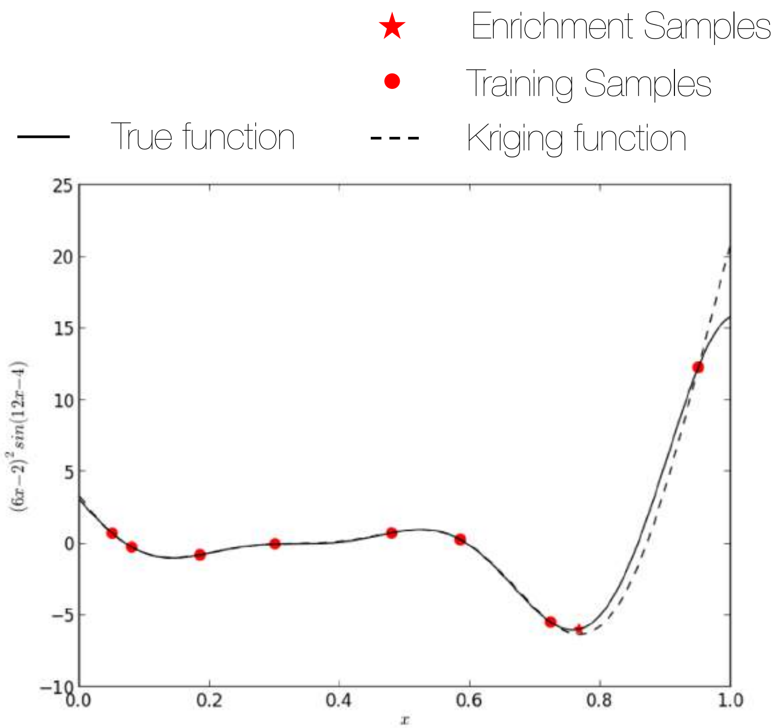


Illustration on 1D example

$$
\begin{cases}
\min \ (6x-2)^2 \sin(12x-4) \\
s.t. \\
0 \le x \le 1
\end{cases}
$$





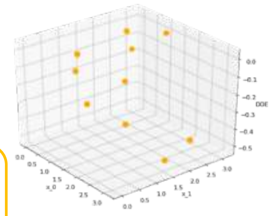
SEGOMOE algorithm

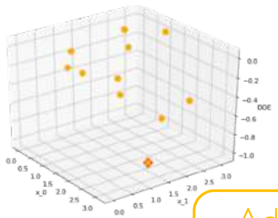
N. Bartoli, T. Lefebvre, S. Dubreuil, R. Olivanti, N. Bons, J.R.R.A. Martins, M.-A. Bouhlel, J. Morlier, " An adaptive optimization strategy based on mixture of experts for wing aerodynamic design optimization", 18th AIAA/ISSMO Multidisciplinary Analysis Optimization Conference, AIAA-2017-4433,Denver, USA, June 2017

$$\begin{cases} \min f(x) \\ c_1(x) \geq 0 \\ \cdot \\ c_i(x) = 0 \\ \cdot \\ c_n(x) \geq 0 \end{cases}$$

Problem definition

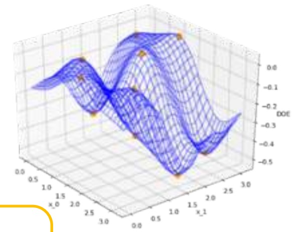
Initial DOE building



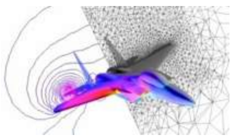


Adding new point to DOE

Building / Training
Surrogate models

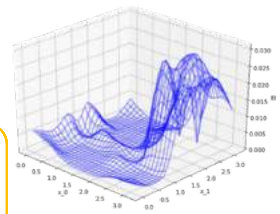


MOE



Evaluation of problem true functions

Optimization criteria



New formulation

N. Bartoli, T. Lefebvre, S. Dubreuil, R. Olivanti, N. Bons, J.R.R.A. Martins, M.-A. Bouhlel, J. Morlier, " An adaptive optimization strategy based on mixture of experts for wing aerodynamic design optimization", 18th AIAA/ISSMO Multidisciplinary Analysis Optimization Conference, AIAA-2017-4433,Denver, USA, June 2017

Adapted from Super EGO

Costly initial problem

$$\begin{cases} \min f(x) \\ c_1(x) \geq 0 \\ \cdot \\ c_i(x) = 0 \\ \cdot \\ c_n(x) \geq 0 \end{cases}$$

Cheap enrichment problem

$$\begin{cases} \max\limits_{x \in \mathbb{R}^d} \quad \mathrm{EI}(x)/\mathrm{WB2}(x)/\mathrm{WB2s}(x) \\ \text{s.t.} \\ \hat{c}_1(x) \geq 0 \\ \cdot \\ \hat{c}_i(x) = 0 \\ \cdot \\ \hat{c}_n(x) \geq 0 \end{cases}$$

n +1 metamodels

Possibly Multimodal

Multimodal

Global optimization method

ADODG6 * testcase (R. Olivanti, R. Priem MsC)

CFD guys know very well the multimodality of this problem...

Wing drag minimization problem (subsonic, Euler equations)

	Function/variable	Description	Quantity	Range
minimize	C_D	Drag coefficient	1	
with respect to	α	Angle of attack	1	$[-3.0, 6.0]$ (°)
	θ	Twist	8	$[-3.12, 3.12]$ (°)
	δ	Dihedral	8	$[-0.25, 0.25]$ (unit of chord)
		Total variables	17	
subject to	$C_L = 0.2625$	Lift coefficient	1	
		Total constraints	1	

Can SEGOMOE help us to reach the global optimum ?
Is it less dependant on X_0 compared to SNOPT £?

*AIAA, Aerodynamic Design Optimization Discussion Group
http://mdolab.engin.umich.edu/content/aerodynamic-design-optimization-workshop

£ https://web.stanford.edu/group/SOL/snopt.htm

ADODG* 6 TOOLS

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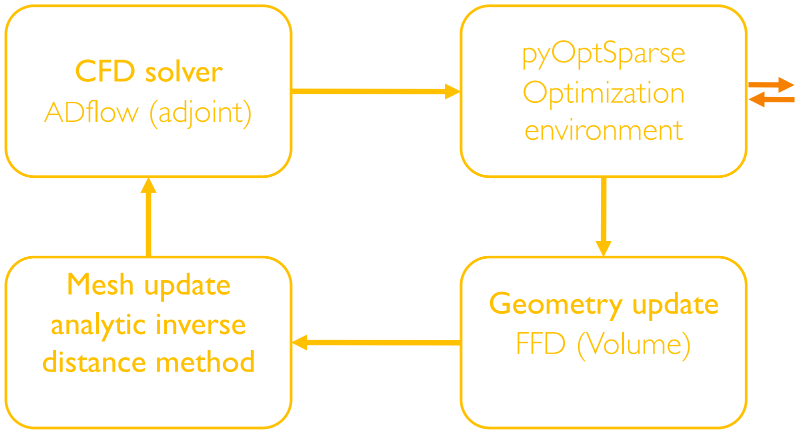

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Stanford

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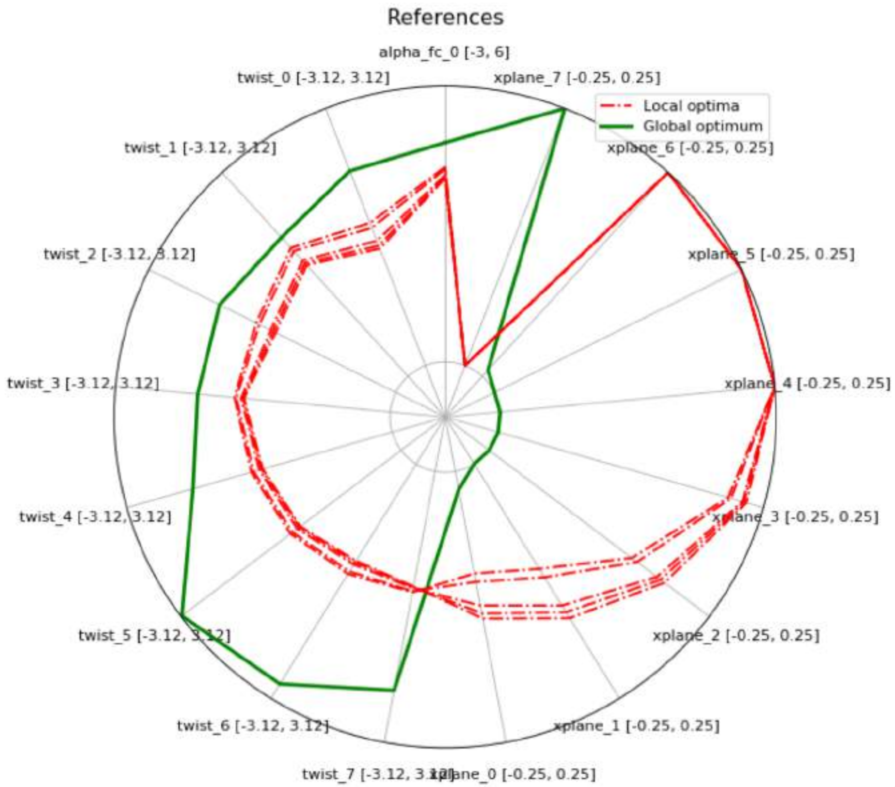
SNOPT | SEGOMOE

GOAL: Bench our SBO method with a reference SNOPT
→ Compare the robustness of the solution with respect to X_0

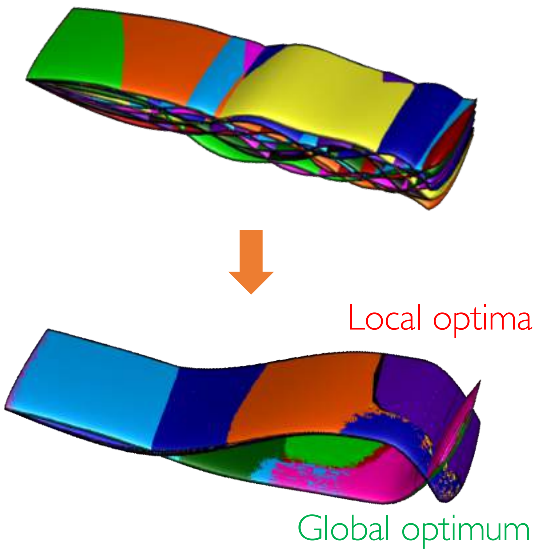
Multimodal optimization problem (SNOPT Benchmark)

Wing drag minimization problem (subsonic, Euler equations with ADFlow solver) (Mesh 180K cells)



→ 5/15 runs found the global optimum

X_0:Multi start with DOE of 15 (LHS)



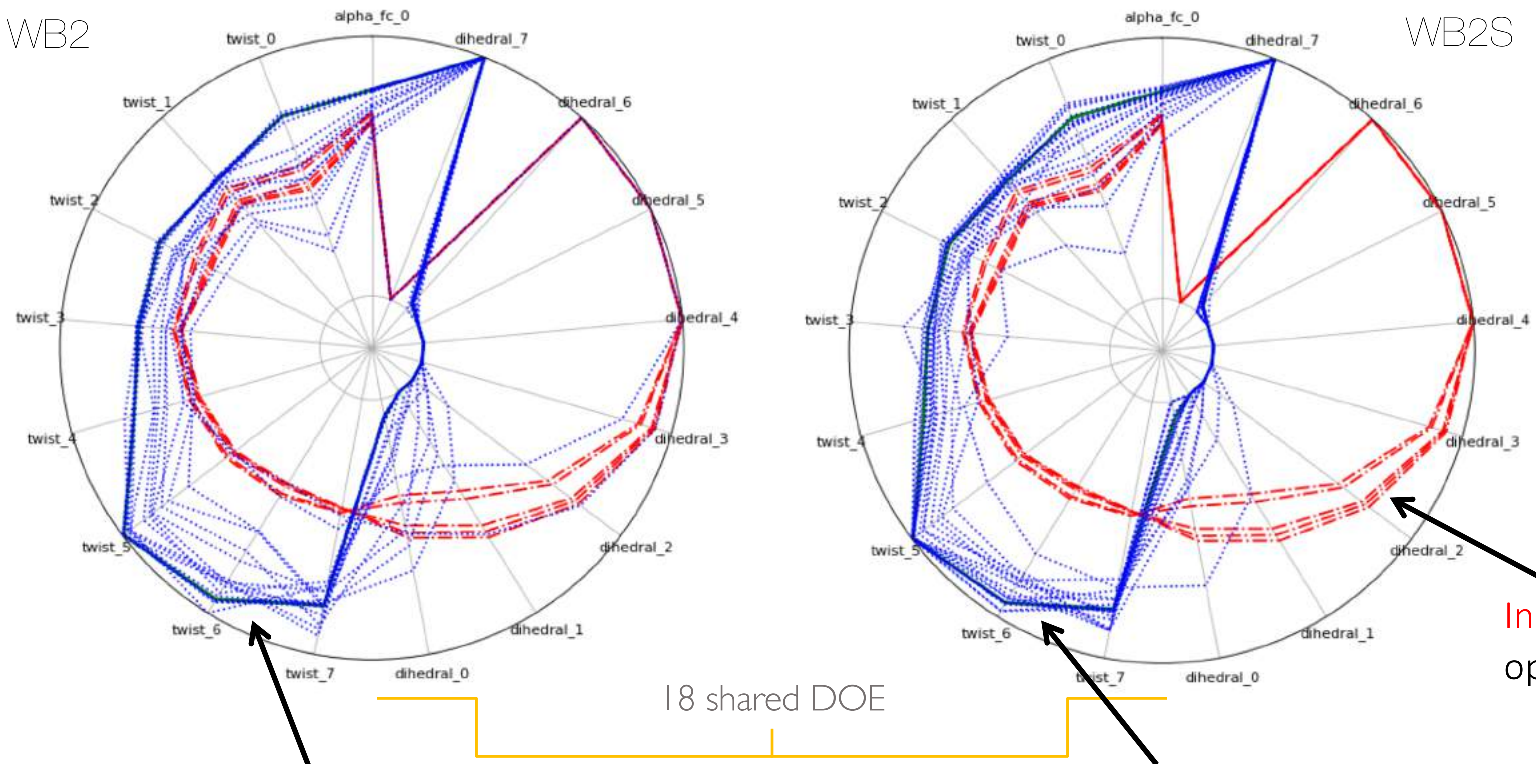
67% Local optimum

Accuracy Cz ~$1e^{-10}$ – 300 calls to ADflow

Multimodal optimization problem (SEGOMOE 2)

Initial DOE= 68 points (4xd)

Frozen budget: 500 evaluations   Surrogate models : KPLSK



In red: Local optima of SNOPT

➡ Global optimum 16 / 18

Best point ~ 409 evaluations   Accuracy Cz ~ 2.97e-6

➡ Global optimum 18 / 18

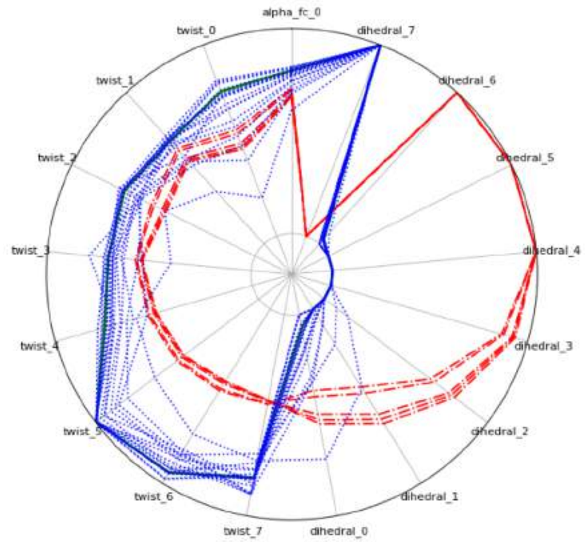
Best point ~ 477 evaluations

Accuracy Cz ~ 3.24e-6

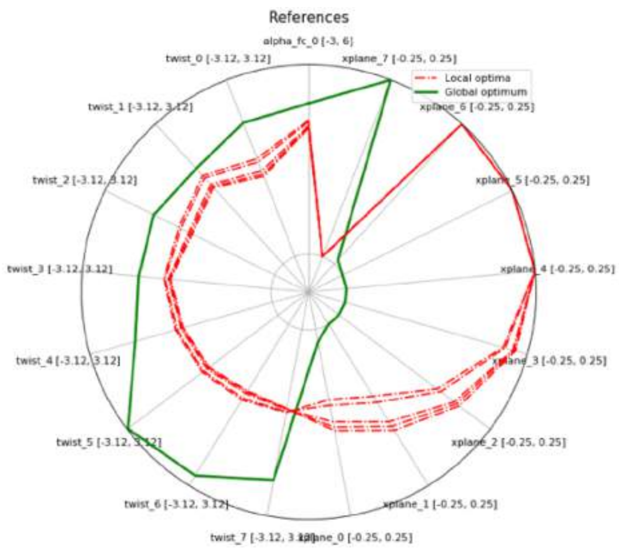
Idea: 2 steps method

1. Start with SEGOMOE, stop with maxiter

x° with high confidence near x^{*} (so we avoid to get stuck in local minima !)



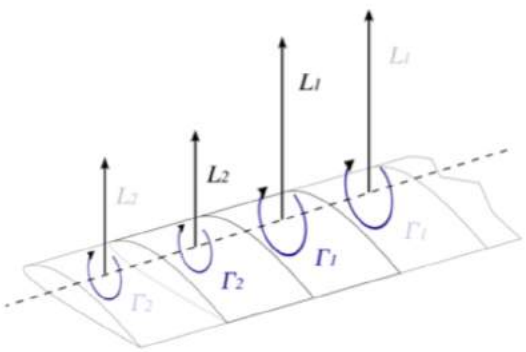
2. Use x° as x_0 in SNOPT to reach rapidly the Global Optimum x^{*}

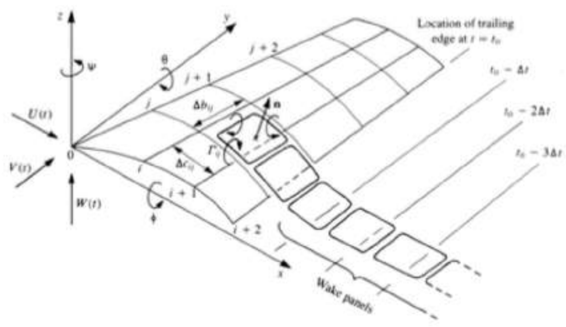


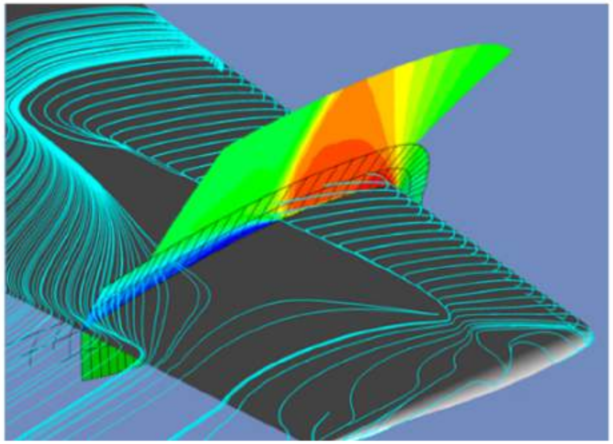
What if ?

- Several levels of fidelity of the same simulation are available

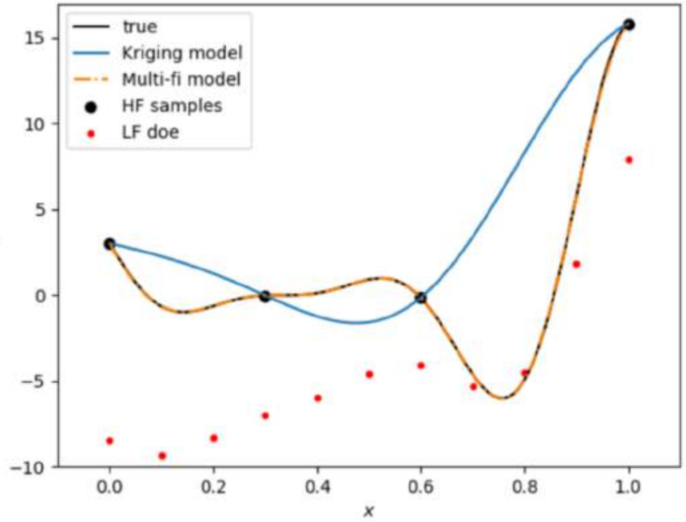
→ For example, in aerodynamics: Liflting line theory, Vortex lattice method, and RANS CFD code

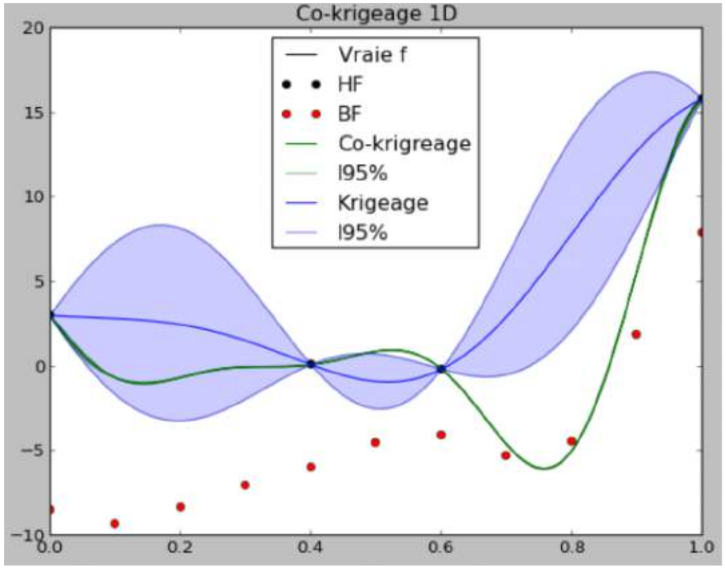






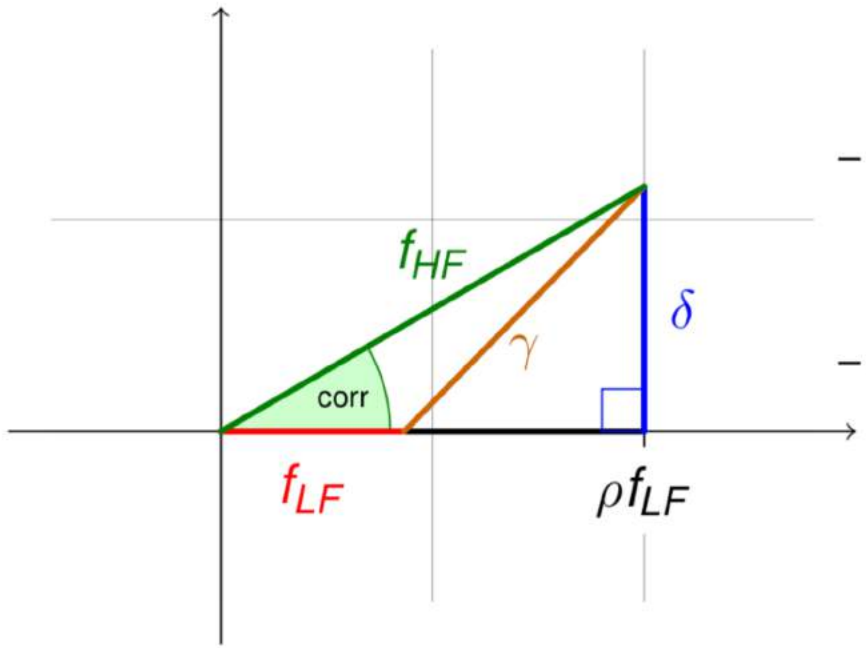
How to use low-fidelity information to speed up the optimization?





→ It is also away to learn the difference between HF & LF …

Co Kriging



– Additive formulation [Lewis 2000]

$$f_{HF}(x) = f_{LF}(x) + \gamma(x)$$

– Kennedy-O'Hagan [Kennedy 2001]

$$\begin{cases} f_{HF}(x) = \rho f_{LF}(x) + \delta(x) \\ f_{LF}(\cdot) \perp \delta(\cdot) \end{cases}$$

The addition of the term ρ makes the multi-fidelity learning more robust to poor correlation as well as differences in modelization.

$Alexandrov, N., Lewis, R., Gumbert, C., Green, L., & Newman, P. (2000, January). Optimization with variable-fidelity models applied to wing design. In 38th Aerospace Sciences Meeting and Exhibit (p. 841).

Kennedy, M. C., & O'Hagan, A. (2001). Bayesian calibration of computer models. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 63(3), 425-464.

MFEGO

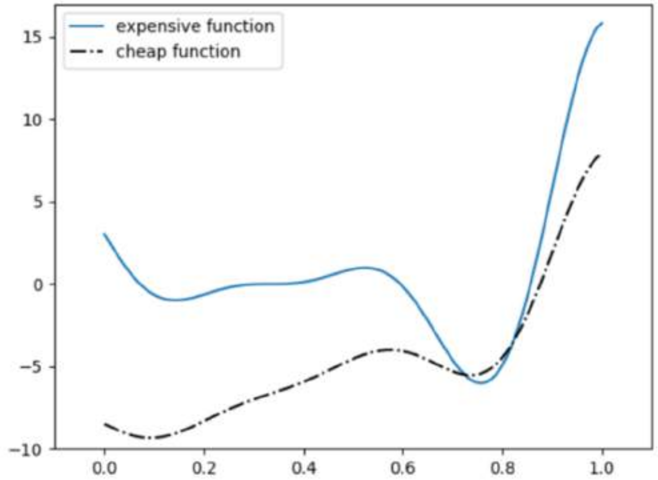
2 step approach

- Most promising point: EI-based criterion

$$\mathbf{x}^* = \arg\max_{\mathbf{x}} \left(\mathrm{EI}(\mathbf{x})\right)$$

- Choice of levels of enrichment: trade off information gain/cost

$$k^* = \arg \max_{k \in (0,\ldots,\ell)} \frac{\sigma^2_{\mathrm{red}}(k, \mathbf{x}^*)}{\mathrm{cost}_{\mathrm{total}}(k)^2}$$

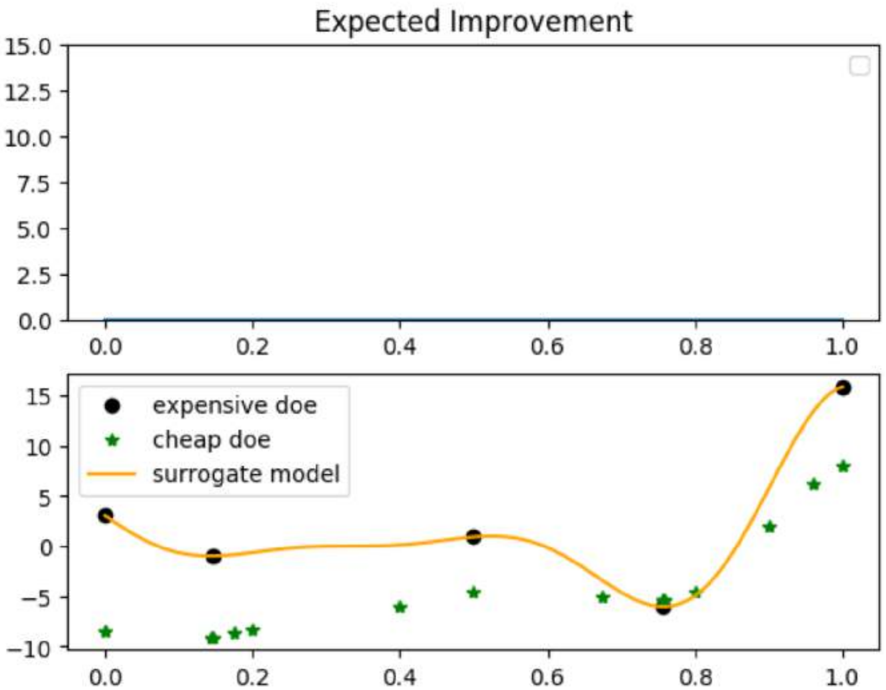


$\Rightarrow$ By using low-fidelity to reduce the uncertainty we reduce the Exploration contribution to the EI criterion

$$f_{HF}(x) = (6x-2)^2 \times \sin(2(6x-2))$$
$$f_{LF}(x) = 0.5 f_{HF} + 10(x-0.5) - 5$$

$\Rightarrow$ High-fidelity is used for Exploitation and model enhancement

Results (Toy problem)

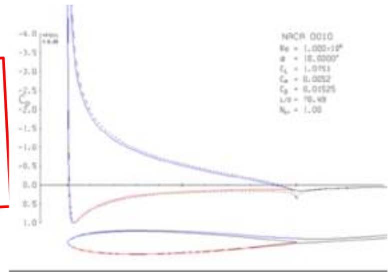


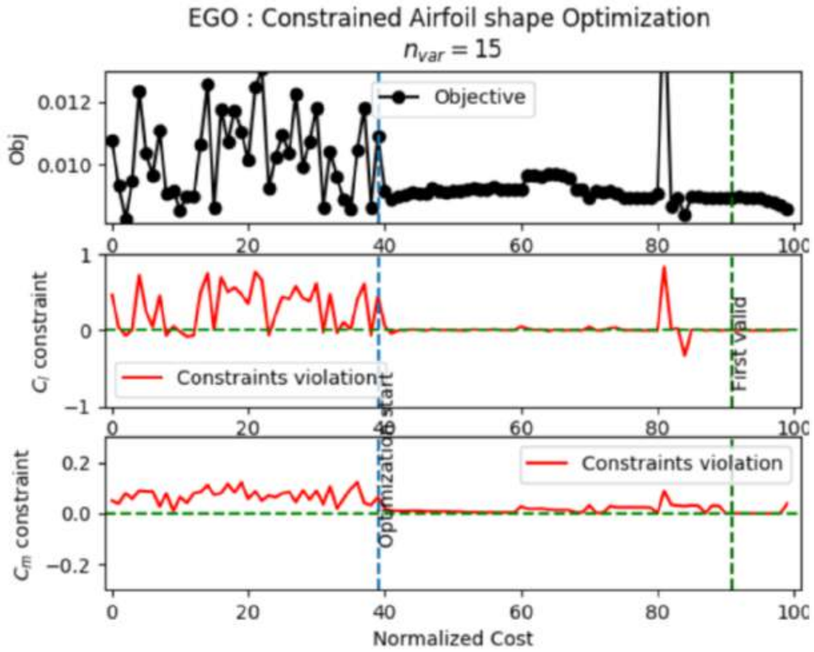
Cost ratio: 1/1000

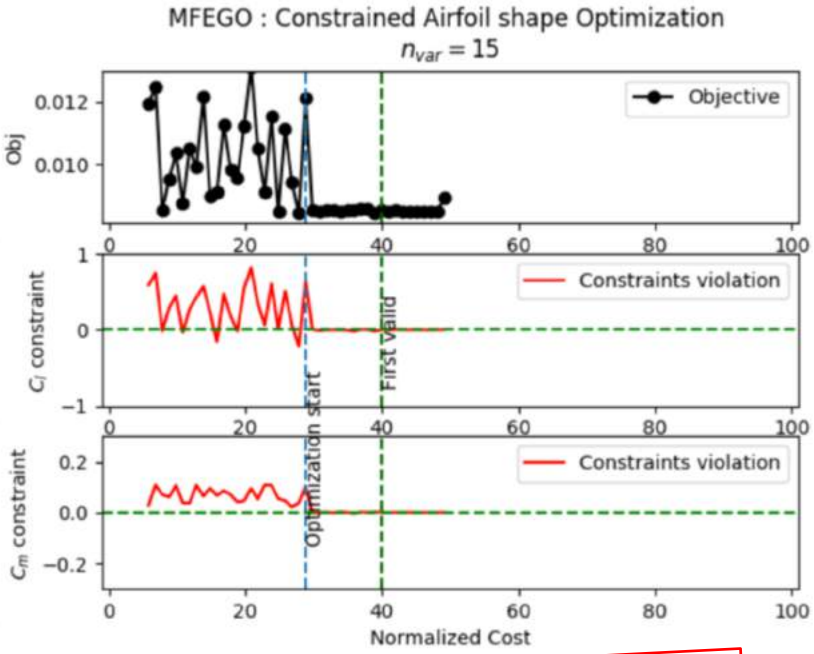
	HF	LF	Cost
MFEGO	3+2	6+9	5.015
EGO	4+11	-	15

Second application: Constrained Optimization

Estimated COST RATIO: 1/200







*https://web.mit.edu/drela/Public/web/xfoil/
$ http://mdolab.engin.umich.edu

MFEGO can speed up the Optimization process by reducing the calls to HF expensive code !

Conclusions

- Our new Bayesian Optimization offers about the same efficiency than standard Gradient Based Method even for HD problems wlithout the influence of starting point (Exploration-Exploitation trade off) on a pure aerodynamic shape optimization problem

EGO on SMT

- The multifidelity / Mixture of experts (MOE) options help us to speed the process (ongoing work)

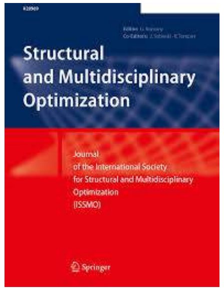
MFK, MOE on SMT

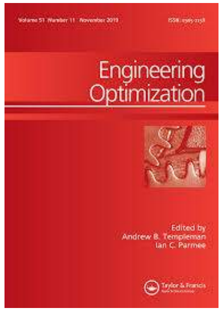
- Still have some Matlab codes to translate in python such as Sparse Physics-Based GP (AIRBUS Flight Physics)

- SBO widely used in collaborative projects (A CFD group can work with a CSM group independently) …the Global optimizer is asking the good point to be computed for each group
- A good example:

AGILE AIRCRAFT 3RD GENERATION MDO FOR INNOVATIVE COLLABORATION OF HETEROGENEOUS TEAMS OF EXPERTS

Recent Papers on this topic





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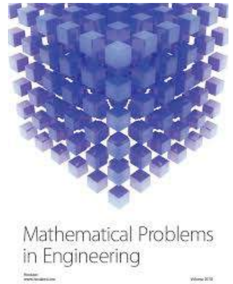

MDO courses & seminars

- NB: Since 2013 new course at SUPAERO : MDO [Structural&Multidisciplinary Design Optimization, 2*30H] (MsC level] with ONERA/AIRBUS. Since 2016 one MDO seminar per year (open to PhDs and researchers)

- Since 2017 we offer some fund to SUPAERO students to do research with us in order to be « PhD ready ». Part of this presentation has been made by SUPAERO MsC Students

Thanks

to My co-workers:

Joaquim Martins, Nathalie Bartoli, Thierry Lefevbre, Mohamed Bouhlel,
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MID2 https://github.com/mid2SUPAERO

Multidisciplinary optimization for Innovation : Design and Data

SUPAERO

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40+ Students In MDO Courses At Master Level

In 2019 We Developed New Methodologies (or Applications) In :

Computational Structural Mechanics

#Gaussian Processes For Linear Elasticity
#Geometric Projection In Topology Optimization (AIRBUS and ICA)
#Topology Optimization For 3Dprinting (AIRBUS and ICA)
#High Resolution Topology Optimization (AIRBUS and ICA)
#Levet Set For Automatic Fiber Placement
#Eco Material Selection
#1D Refined FE Model In Dynamics
#IsoGeometric Analysis (LAMCOS and IMT)

Multidisciplinary Design Optimization

#HALE Ecodesign (CEDAR Chair)
#Reusable Launchers (SACLAB Chair)
#Multifidelity Method with Gaussian Processes (ONERA and MDOlab)*
#MDA Acceleration
#Codesign For Robust Flutter (AIRBUS)
#Trajectory Control
#Gaussian Processes and POD for coupled problem (ONERA)
#Aeroelastic for Scaled Aircraft (CEDAR Chair, ONERA and MDOlab)
#Hybrid Optimization (AIRBUS And IRT)
#BWB (CEDAR Chair, ONERA)

Thanks To All Supaero's Students (MAE, PIR, PhDs And Postdoc)

* https://smt.readthedocs.io/en/latest/