An overview of 5 years of research on surrogate modelling in OQUAIDO

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Surrogate Days, Toulouse, 2021 July 1

Outline

Outline

Surrogate models (or metamodels) – Computer experiments

design

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design → **experiment + measurements** → **meas. output**

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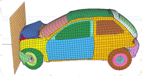


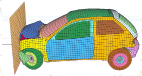
simulator inputs
$\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^n$

→ **simulator**
physical model, numerical methods

→ **simulator output**
$f_{\text{sim}}(\mathbf{x}^1), f_{\text{sim}}(\mathbf{x}^2), \ldots, f_{\text{sim}}(\mathbf{x}^n)$

Surrogate models (or metamodels) – Computer experiments

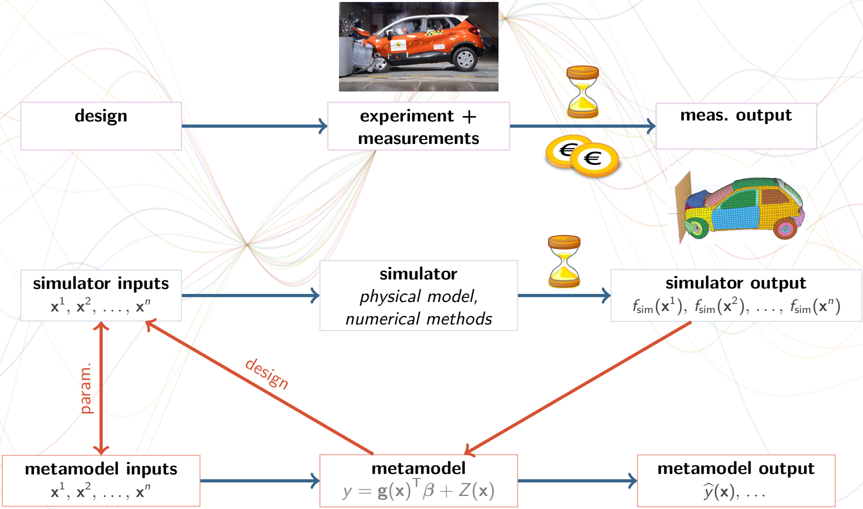
design → **experiment + measurements** → **meas. output**



simulator inputs $\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^n$ → **simulator** *physical model, numerical methods* → **simulator output** $f_{\text{sim}}(\mathbf{x}^1), f_{\text{sim}}(\mathbf{x}^2), \ldots, f_{\text{sim}}(\mathbf{x}^n)$

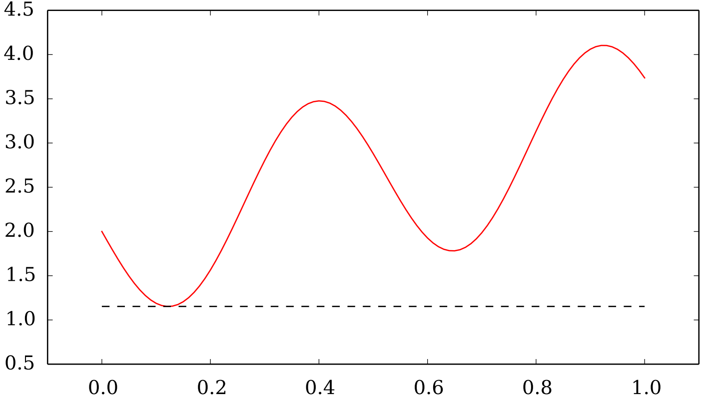
metamodel inputs $\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^n$ → **metamodel** $y = \mathbf{g}(\mathbf{x})^\top \beta + Z(\mathbf{x})$ → **metamodel output** $\widehat{y}(\mathbf{x}), \ldots$

Surrogate models (or metamodels) – Computer experiments



GP-based optimization

How to find the global minimum of a function... when each evaluation is costly ?



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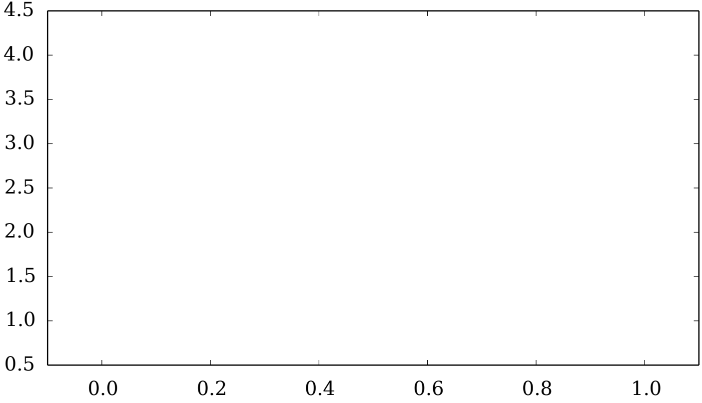

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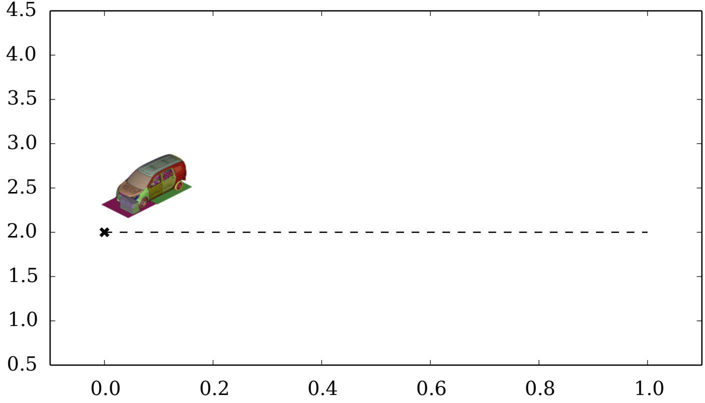

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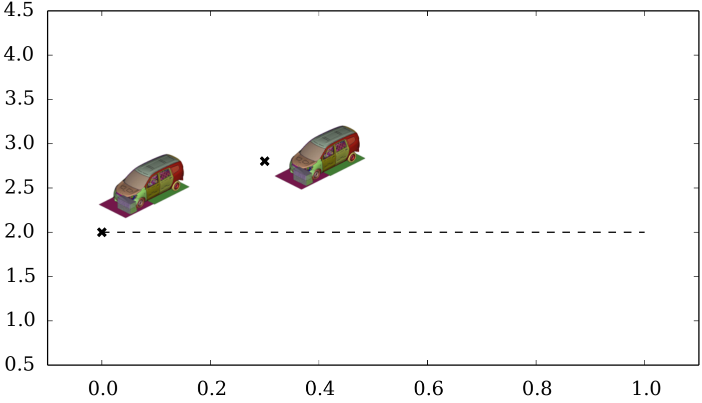

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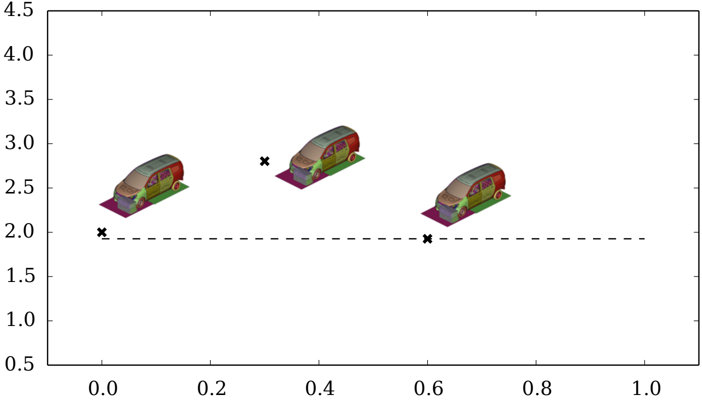

GP-based optimization

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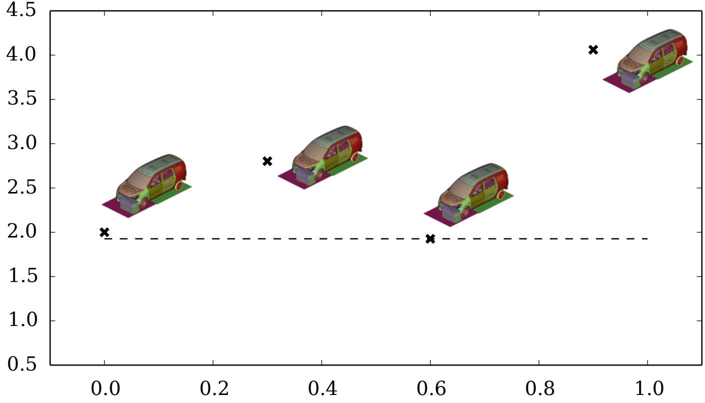
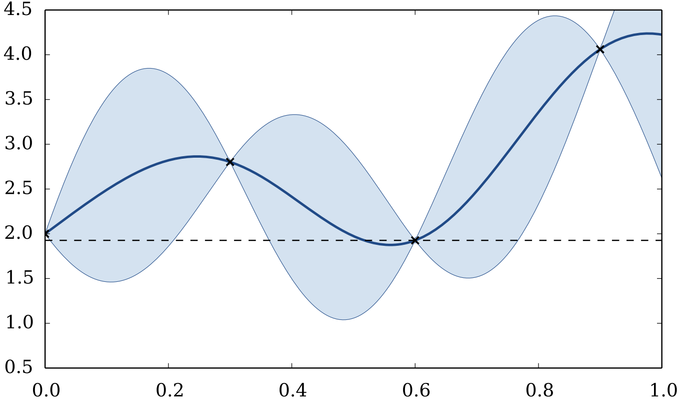


GP-based optimization

A solution : **GP-based (or "Bayesian") optimization** [Močkus, 1975, Jones et al., 1998]

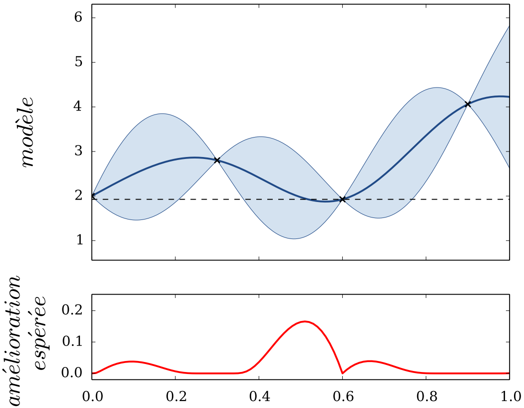
First ingredient : a GP model Y



GP-based optimization

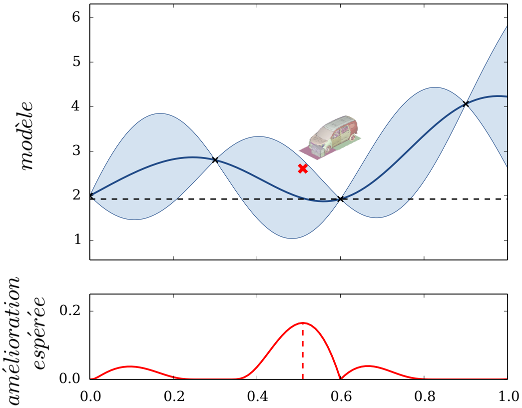
Second ingredient : an **easy-to-compute** criterion **accounting for uncertainty at unknown regions**, e.g. here "expected improvement"

$$EI(x) = \mathrm{E}([f_0 - Y(x)]^+ | Y(x_1), \ldots, Y(x_n)) \qquad f_0 : \textit{ current minimum}$$



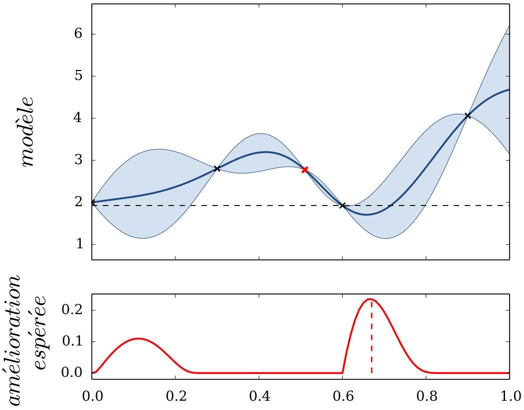
GP-based optimization

The algorithm (here "EGO") : (1) Find the next point by maximizing the criterion $\rightarrow$ (2) Evaluate the function $\rightarrow$ (3) Update the GP model $\uparrow$



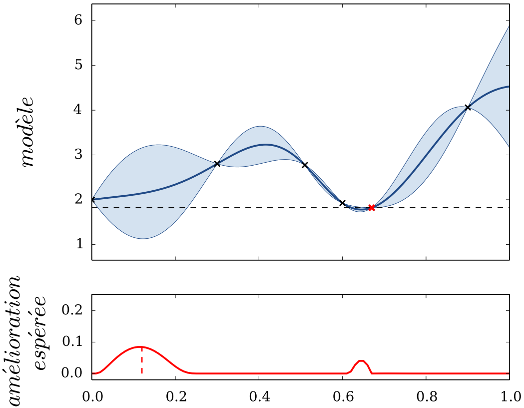
GP-based optimization

Iteration 2 :



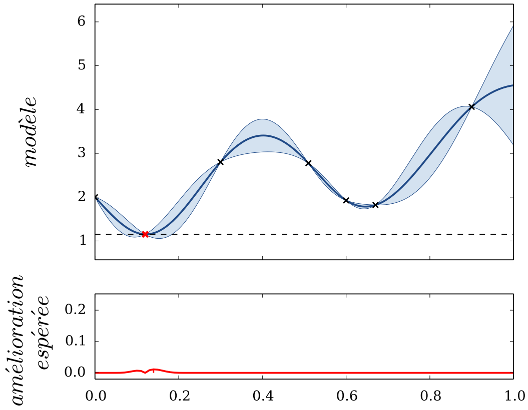
GP-based optimization

Iteration 3 :



GP-based optimization

Theory shows that **EGO algorithm provides a dense sequence of points**, up to a slight condition on the kernel used for GPs [Vazquez and Bect, 2010] .

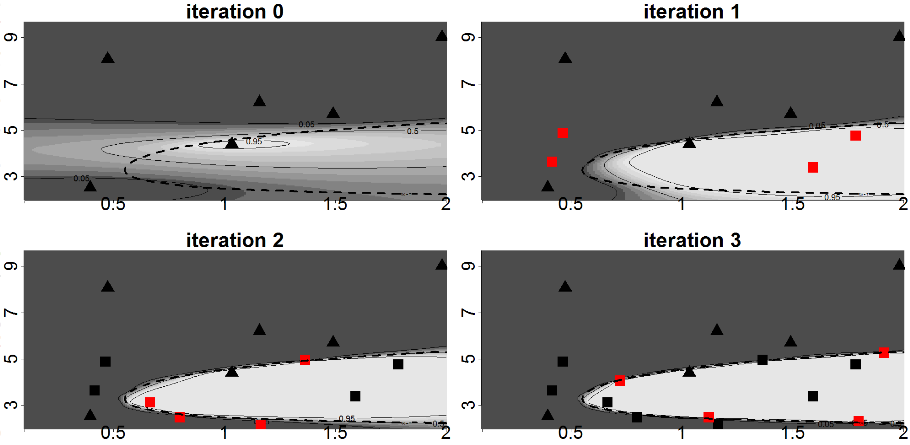


GP-based inversion

Same receipt for estimating a probability of failure ("SUR" strategy).

See [Chevalier et al., 2014] for details and [Bect et al., 2019] for a convergence analysis with supermartingales.

Illustration : Estimation of the nuclear criticity region $k_{\text{eff}} > 0.95$



Gaussian processes

Gaussian processes are stochastic processes (or random fields) s.t. every finite dimensional distribution is Gaussian. → Parameterized by two functions

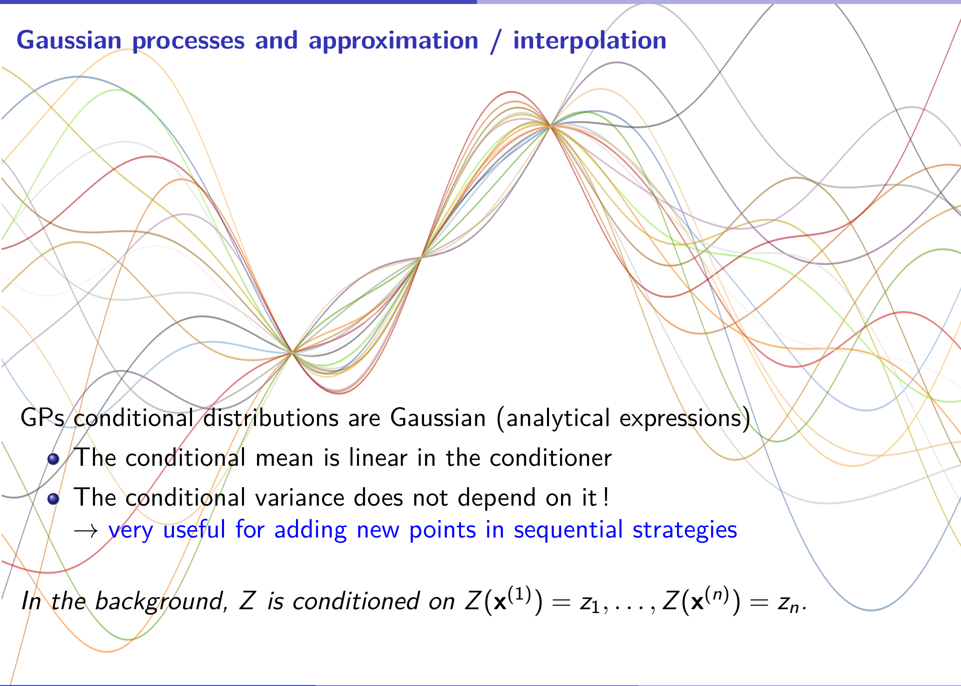
$$Z_{\mathbf{x}} \sim GP(\underbrace{m(\mathbf{x})}_{trend}, \underbrace{k(\mathbf{x}, \mathbf{x}')}_{kernel})$$

- The trend can be any function.
- The kernel is positive semidefinite :

$$\forall n, \alpha_1, \dots, \alpha_n, \mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}, \qquad \sum_{i=1}^{n} \alpha_i \alpha_j k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) \geq 0.$$

It contains the spatial dependence.

Gaussian processes and approximation / interpolation



GPs conditional distributions are Gaussian (analytical expressions)

- The conditional mean is linear in the conditioner
- The conditional variance does not depend on it !
  → very useful for adding new points in sequential strategies

In the background, Z is conditioned on $Z(\mathbf{x}^{(1)}) = z_1, \dots, Z(\mathbf{x}^{(n)}) = z_n$.

Gaussian processes, splines and RKHS

The 3 faces of a kernel

$GP(0, k(\mathbf{x}, \mathbf{x}')) \quad \Leftrightarrow \quad$ p.s.d. functions $k \quad \Leftrightarrow \quad$ RKHS : $\mathcal{H} = \overline{\mathrm{span}\{k(., \mathbf{x}), \mathbf{x} \in D\}}$

where $\mathcal{H}$ is a "Reproducing Kernel" Hilbert Space with dot product :

$$\langle k(\mathbf{x}, .), k(\mathbf{x}', .)\rangle = k(\mathbf{x}, \mathbf{x}') \qquad (*)$$

RKHS can be also defined as Hilbert spaces of functions such that evaluations $f \to f(\mathbf{x})$ are continuous : By Riesz theorem, there exists a unique $k(., \mathbf{x})$ s.t.

$$f(\mathbf{x}) = \langle f, k(., \mathbf{x})\rangle$$

Choosing $f = k(., \mathbf{x}')$ gives the reproducing identity (*).

Ref : [Aronszajn, 1950], [Berlinet and Thomas-Agnan, 2011].

Gaussian processes, splines and RKHS

Correspondence between interpolation spline and GP conditional mean

[Kimeldorf and Wahba, 1971]

The interpolation spline is defined by the functional problem

$$(*) \qquad \min_{h \in \mathcal{H}} \|h\| \qquad s.t. \quad h(\mathbf{x}^{(i)}) = z_i, \; i = 1, \dots, n$$

If $\mathcal{H}$ is the RKHS of kernel k, and if $K = \left(k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})\right)_{1 \leq i,j \leq n}$ is invertible, then (*) has a unique solution in the finite dimensional space spanned by the $k(., \mathbf{x}^{(i)})$:

$$h_{\mathrm{opt}}(\mathbf{x}) = \mathrm{E}\left[Z_{\mathbf{x}} \middle| Z(\mathbf{x}^{(i)}) = z_i, \; i = 1, \dots, n \right]$$

$\rightarrow$ In this sense, GPs are generalizing interpolation splines.

The first part (reduction to finite dimension) is know as Representer theorem.

Playing with kernels

A lot of flexibility can be obtained with kernels !

Building a kernel from other ones (basic examples)

Sum, tensor sum	$k_1 + k_2, \ k_1 \oplus k_2$
Product, tensor product	$k_1 \times k_2, \ k_1 \otimes k_2$
ANOVA	$(1 + k_1) \otimes (1 + k_2)$
Warping	$k(\mathbf{x}, \mathbf{x}') = k_1(f(\mathbf{x}), f(\mathbf{x}'))$
...	...

See examples in [Rasmussen and Williams, 2006]... and in this talk !

Why Gaussian processes are popular in (geo)statistics / machine learning ?

GP strengths

- Probabilistic models that **traduce spatial dependence**
  → provide realistic uncertainty in unvisited area
- **Conditional distributions are analytical**, and the cond. var. is constant
  → Useful for prediction and sequential strategies
- **Parameterized by functions** : mean and covariance **(kernel)**
  → Flexibility
- At the crossing between **rich mathematical theories**
  → Stochastic proc., Reproducing Kernel Hilbert Spaces, Positive Definite Functions

Outline

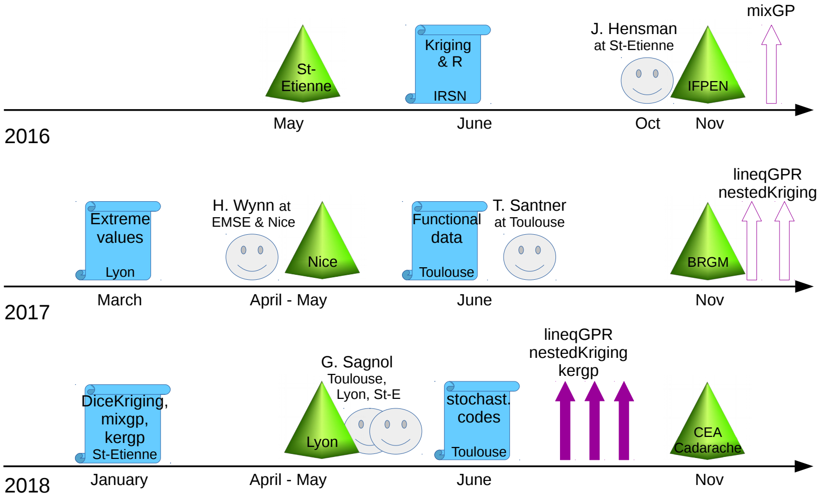
The OQUAIDO Chair

The research Chair OQUAIDO – for "Optimisation et QUAntification d'Incertitudes pour les Données Onéreuses" in French – has gathered academic and technological research partners to work on surrogate modeling and application to optimization and uncertainty quantification.

- Mines Saint-Étienne (that hosts the Chair), École Centrale de Lyon, CNRS, Univ. Grenoble Alpes, Univ. de Nice, Univ. de Toulouse III
- BRGM, CEA, IFPEN, IRSN, Safran, Storengy
- Y. Deville (AlpeStat), J. Garnier (École Polytechnique), D. Ginsbourger (Idiap), L. Polès (XtraFormation), as experts, and L. Carraro, as advisor.

Website : oquaido.emse.fr

OQUAIDO Chair Life



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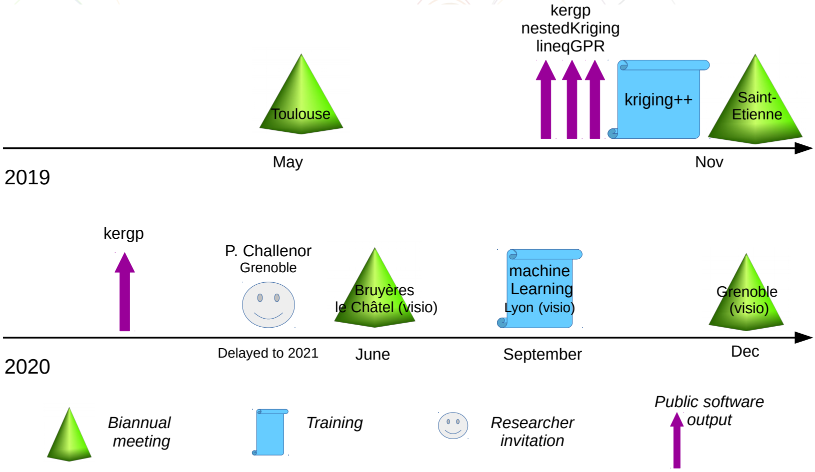


Scientific program and production

\ **Application** **Framework** \	Optimization	Inversion / Calibration	Uncertainty Quantification	Modeling and other
Categorical inputs	PhD 4	Case 2 - Case 2' PhD 4		Post-doc 1
Stochastic codes	Case 4 - Post-doc 2		Case 4 - Post-doc 2	
Functional inputs/outputs High nb of inputs	Case 3 - PhD 1	Case 1 - Case 3 PhD 1, MSc	PhD 1	
Specific constraints			PhD 2	PhD 2
High nb of data				
Other topics				PhD 3

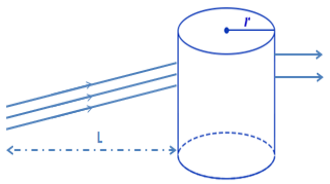
Table – Scientific program, case studies (Case) and extra manpower : post-doc, PhD thesis (PhD), master thesis (MSc).

Outline

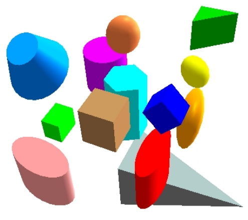
GP for categorical inputs : groups of levels & trees

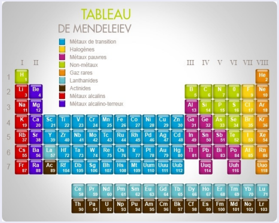
A guiding case study : Nuclear activity quantification

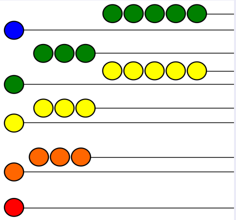
1. Computation using Monte Carlo
2. 4 continuous inputs : L, density, mean width, lateral surface
3. 3 categorical inputs : energy, form, chemical element.



Specific problem : large number of levels





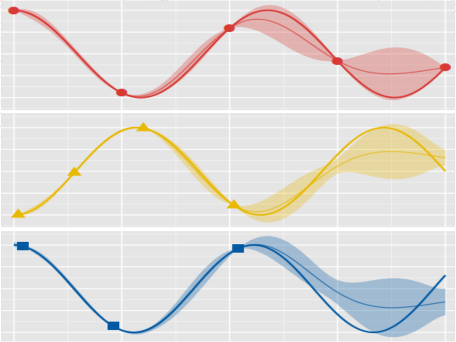


Form (s, c, p) $Z \in \{1, \ldots, 94\}$ $E \in \{E_1, E_2, E_3, E_4, E_5, E_6\}$

GP interpretation when no distance is available

A GP for $(x, u) \in [0, 1] \times \{"red", "yellow", "blue"\}$ can be defined with :

- a kernel on $[0, 1]$, i.e. a **covariance function**
- a kernel on $\{"red", "yellow", "blue"\}$, i.e. a **covariance matrix**
- a valid operation between them, such as *, $+$, ...



Example : $\mathrm{Cov}(Y(x, "blue"), Y(x', "red")) = k(x, x') \times 0.8$

GP for categorical inputs : group kernels for partitioned levels

A group kernel is a block covariance matrix

Block covariance matrix

$$\mathbf{T} = \begin{pmatrix} \mathbf{W}_1 & \mathbf{B}_{1,2} & \cdots & \mathbf{B}_{1,G} \\ \mathbf{B}_{2,1} & \mathbf{W}_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \mathbf{B}_{G-1,G} \\ \mathbf{B}_{G,1} & \cdots & \mathbf{B}_{G,G-1} & \mathbf{W}_G \end{pmatrix}$$

with constant between-group blocks

Hierarchical (group/level) process

$$\eta_{g/\ell} = \mu_g + \lambda_{g/\ell}$$

with :

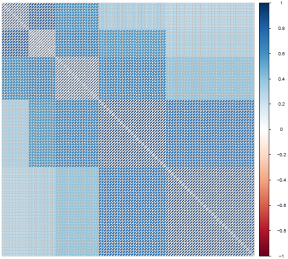
- Gaussian ind. priors for $\boldsymbol{\mu}, \boldsymbol{\lambda}_{g/.}$
- Centering cond. : $\sum_\ell \lambda_{g/\ell} = 0$

Main results [Roustant et al., 2020]

- Connection with hierarchical GPs : $\mathbf{T} = \mathrm{cov}(\boldsymbol{\eta})$.
- Characterization & parameterization of valid group kernels

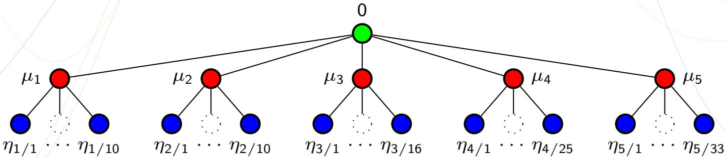
Result on the case study

For the categorical input 'chemical element', 5 groups are identified by experts
$\rightarrow$ Parsimonious parametrization with only 20 parameters (instead of $94 \times 95/2$)

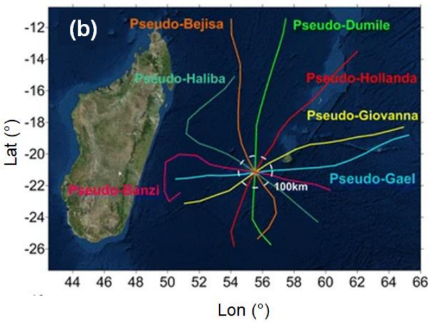


- 10 between-group covariances
- 5 within-group covariances
- 5 within-group variances

With a stratified LHS design of size 3×94, the Q^2 of the whole model is > 0.95

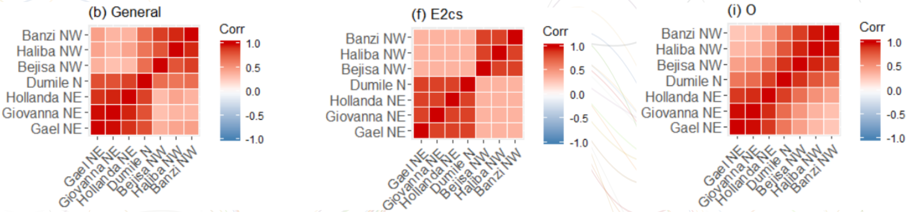


Application to cyclones [Rohmer et al., 2020]



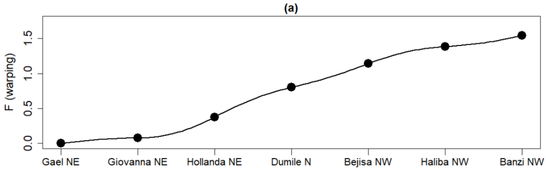
Output : significant wave height (maximum value over time)
Inputs : 5 continuous inputs + 1 categorical (cyclone profile)

Application to cyclones



Here two kernels for the categorical input give a 'good' GP model : a group kernel, or an ordinal kernel. Global kernel used for the second case :

$$k((x,u),(x',u')) = k_{\text{cont}}(x,x')k_{\text{cont2}}(F(u),F(u'))$$



Outline

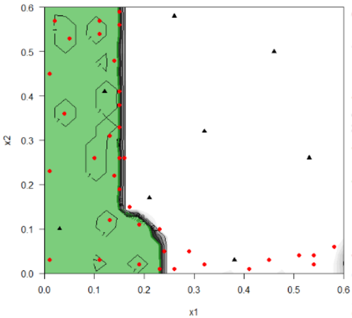
Inversion under uncertainty [El Amri et al., 2020]

Automotive test-case : Estimate

$$\Gamma_{f,V} = \{x, \mathbb{E}_V(f(x, V)) \leq c\},$$

where f is the pollutant concentration, and V represents uncontrolled driving cycles.

Mathematical tools : GP + random sets.



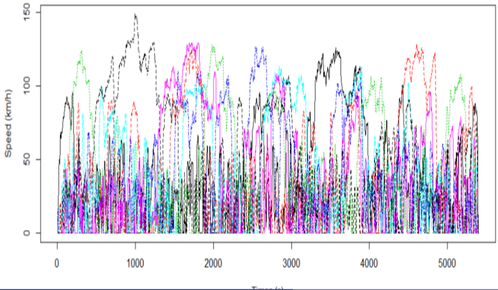
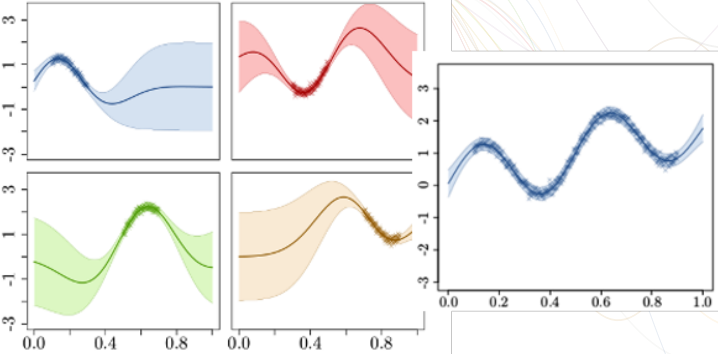


Figure – Left : examples of driving cycles. Top : estimation of $\Gamma_{f,V}$ (green area), after 37 iterations. Black triangles : initial data ; Red points : added data.

Outline

1. Context and motivation
2. The OQUAIDO Chair
3. Categorical inputs
4. Functional inputs/outputs
5. **High nb of data**
6. Specific constraints
7. Other topics and software
8. The CIROQUO consortium

Nested Kriging : Aggregating submodels



Building a GP model on a large dataset is done by linearly aggregating submodels.
Description and proof of consistency can be found in [Rullière et al., 2018].
Tested with 400 000 points in dimension 34 on a Storengy test case.

Outline

GP under linear inequalities : Impact on uncertainty quantification

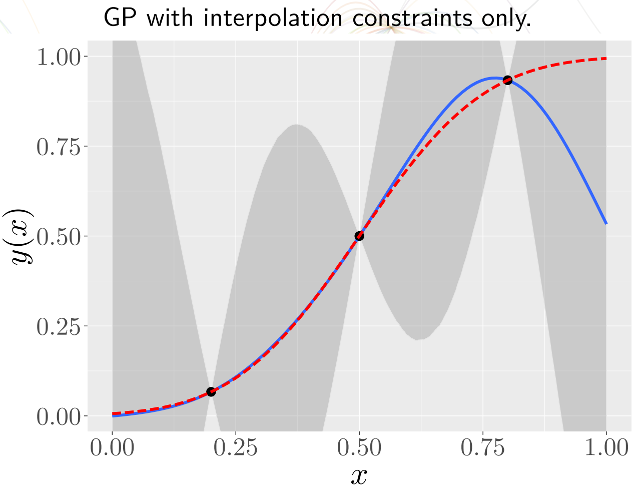


Illustration on a toy example (cdf of a Normal distribution)

GP under linear inequalities : Impact on uncertainty quantification

GP with boundedness + monotonicity additional constraints.

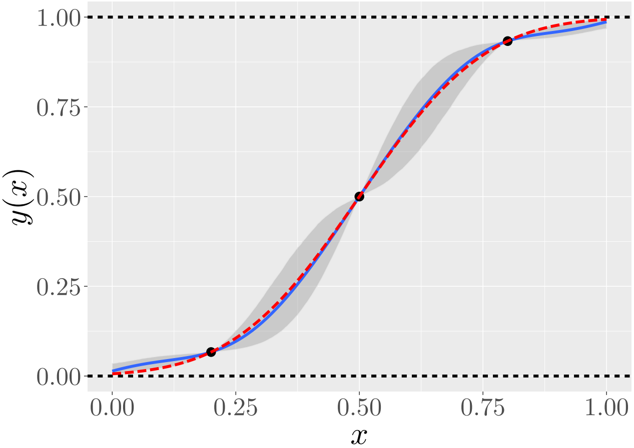


Illustration on a toy example (cdf of a Normal distribution)

GP and linear inequalities : Some theory

A finite elements (P_1) model for 1D GPs

[Maatouk and Bay, 2017, López-Lopera et al., 2018]

Each sample path of a GP Y is approximated by a **piecewise affine function**

$$Y_m(x) = \sum_{j=1}^{m} \xi_j \phi_j(x)$$

where ϕ_j are "hat" functions and $\boldsymbol{\xi}$ is a Gaussian vector extracted from Y

- Key point : Boundedness, monotonicity (and others) for a piecewise affine function can be checked only at knots → finite number of conditions only

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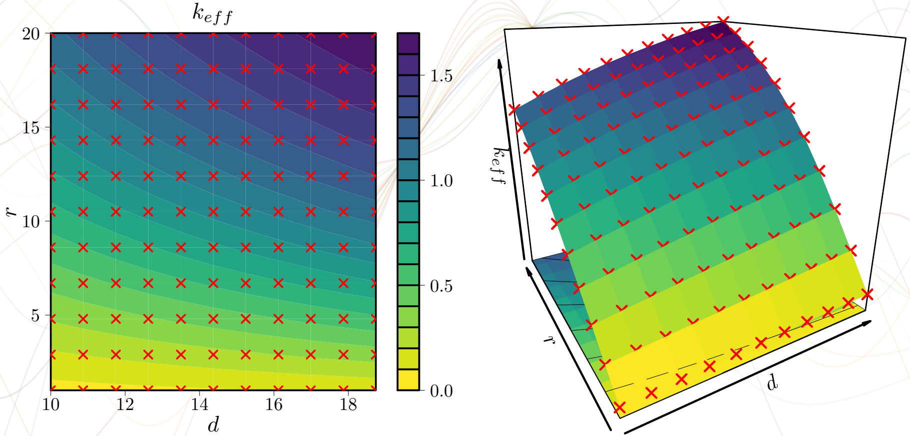
Key feature

All paths / predictions **fullfill inequality constraints everywhere in the space**.

Remark : Immediate extension in 2D (and higher) by using tensors $\phi_{j_1}(x_1)\phi_{j_2}(x_2)$.

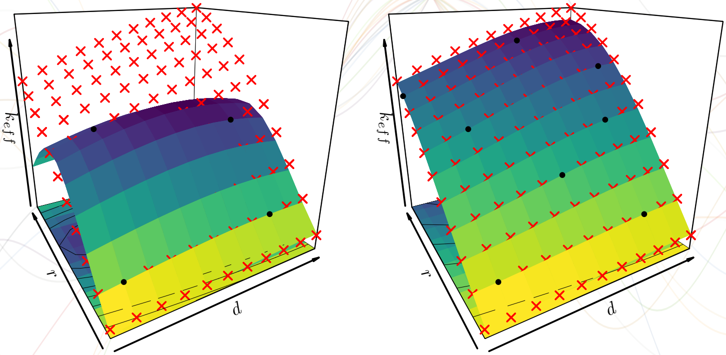
Example of application in 2D



Nuclear criticality safety assessments : IRSN's dataset.

Extra information : k_{eff} is positive and non-decreasing.

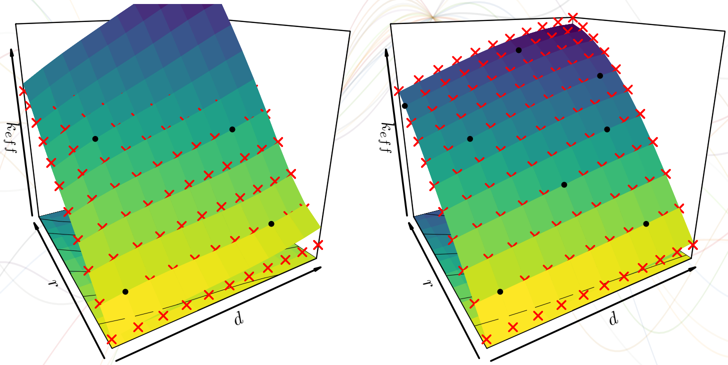
Example of application in 2D



Unconstrained model + MLE.

Monotonicity constraints are nearly learnt with 8 points, but not with 4 points.

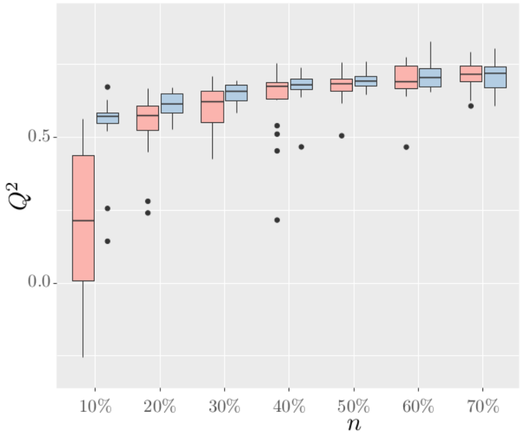
Example of application in 2D



Constrained model + constrained MLE.

Monotonicity constraints are fulfilled everywhere in the space, whatever the size of the training set.

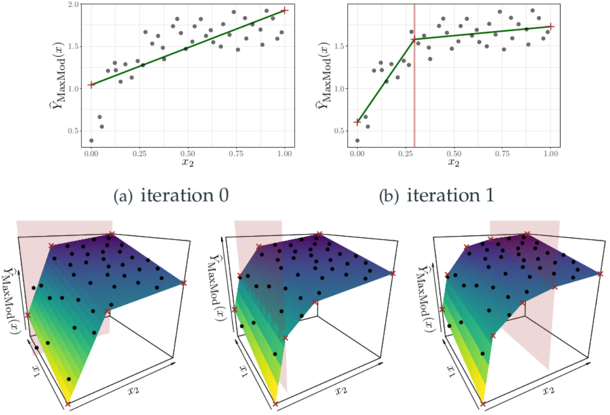
A 5D application (BRGM coastal flooding case study [López-Lopera et al., 2020])



With a fraction (e.g. 10%) of the total budget ($n = 200$), the constrained model (blue boxplots) outperforms the unconstrained one $\Rightarrow$ save budget !

A sequential algorithm to go to higher dimensions [Bachoc et al., 2020]

The MaxMod algorithm adds a knot / variable s.t. the L^2 variation of the mode a posteriori is maximum. Works in dimension 20 when 5 variables are really active.



(a) iteration 0 (b) iteration 1

(c) iteration 2 (d) iteration 3 (e) iteration 4

• training points + knots ■ MAP estimate

Theoretical results

Correspondence with spline under inequality [Bay et al., 2016]

Let $\widehat{Y}_m$ be the mode a posteriori (MAP) of $Y_m(x) = \sum_{j=1}^{m} \xi_j \phi_j(x)$, defined by replacing ξ by the mode of the distribution of ξ conditional on the constraints. Then, when the number of knots m tends to infty,

$$\hat{Y}_m \underset{\text{unif.}}{\longrightarrow} \underset{f \in \mathcal{H} \cap \mathcal{C} \cap \mathcal{I}}{\operatorname{argmin}} \|f\|$$

where $\mathcal{C}$ is a convex set of inequality constraints, $\mathcal{I}$ the set of interpolation constraints $f(x_i) = y_i$ $(i = 1, \dots, n)$, and $\mathcal{H}$ is the RKHS associated to Y.

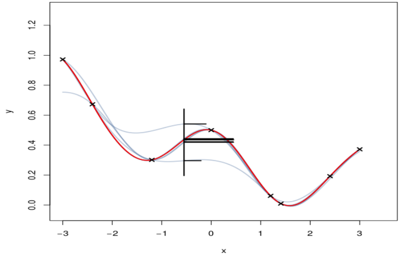
Convergence of the MaxMod algorithm [Bachoc et al., 2020]

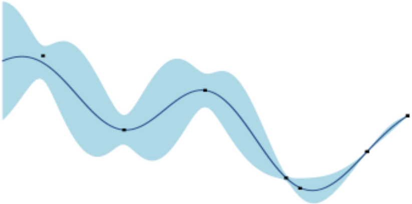
Let $\widehat{Y}_{\text{MaxMod},m}$ be the MAP at iteration m of the MaxMod algorithm. Then,

$$\hat{Y}_{\text{MaxMod},m} \underset{\text{unif.}}{\longrightarrow} \underset{f \in \mathcal{H} \cap \mathcal{C} \cap \mathcal{I}}{\operatorname{argmin}} \|f\|$$

Outline

{General Surrogate}-based optimization [Ben Salem et al., 2017]

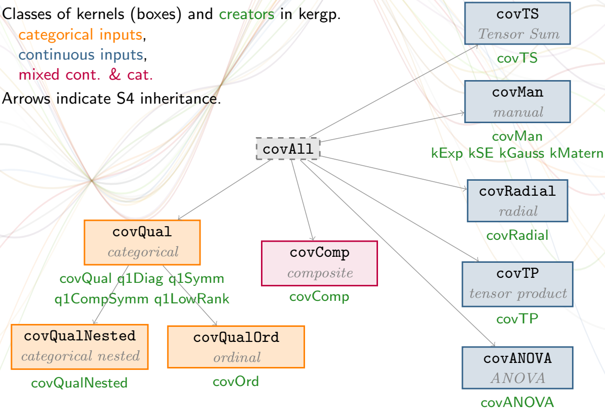




Bayesian optimization can be used with any surrogate model (e.g. SVM) via the Universal Prediction distribution, built by cross-validation.

Open source R packages

- 4 R packages released : *lineqGPR*, *nestedKriging*, *specgp* and *kergp*



Outline

The future of OQUAIDO : CIROQUO

Further information on OQUAIDO (2016 - 2020)

This talk has presented a selection of works done in OQUAIDO.
Read more in our activity report, now on HAL [Roustant et al., 2021]

Next iteration : CIROQUO (2021 - 2025)

- Academics : Centrale Lyon, INRIA, Mines St-Etienne, Univ. Nice & Toulouse
- Technos : IFPEN, BRGM, CEA, IRSN, Storengy
- Experts : M. Mougeot (ENSIIE), P. Havé
- Research lines
  - Calibration, validation and transposition of computer codes
  - Metamodeling for complex environments
  - Optimization and inversion under uncertainty
- New directions
  - more interaction with machine learning
  - wide language software *libKriging*
- Website : ciroquo.ec-lyon.fr

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