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# Hidden But Essential Recipes for Successful Gaussian Process Metamodeling to Support Uncertainty Quantification in Numerical Simulation

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**Speaker: Amandine Marrel**

**Part of MS194 Gaussian Process Modeling for Inverse Problems**

# **Hidden But Essential Recipes for Successful Gaussian Process Metamodeling to Support Uncertainty Quantification in Numerical Simulation**

*Amandine Marrel*

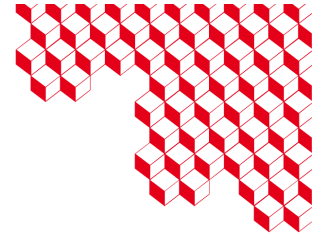
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The value of using Gaussian Process (GP) regression to emulate costly computational codes for uncertainty management is now widely established. The probabilistic metamodel provided by GP-regression, in the sense that it provides a predictive distribution for each new evaluation point, offers great added value, particularly for safety, reliability or risk assessment studies. However, guaranteeing confidence in the use of this metamodel requires two crucial steps: its training on the available learning data and its validation (often by cross-validation process in our application context). We are particularly interested here in the context of given data, small data (number of model simulations limited to a few hundred) and large numbers of uncertain inputs (from a few dozen to a hundred). In this context, building a successful GP metamodel often calls for a preliminary variable selection. Kernel-based methods (HSIC) and associated independence tests are especially appropriate, for screening but also ranking the inputs. Then, particular care is required when estimating GP hyperparameters: going beyond simple maximum likelihood approaches may be wise. Finally, GP validation must include various criteria to assess the predictivity and reliability of the metamodel's entire predictive law.

The presentation will focus on recent advances in these three topics, with the aim of providing guidelines and recipes for successful GP metamodeling in the considered application context.



## Hidden But Essential Recipes for Successful Gaussian Process Metamodeling to Support UQ in Numerical Simulation

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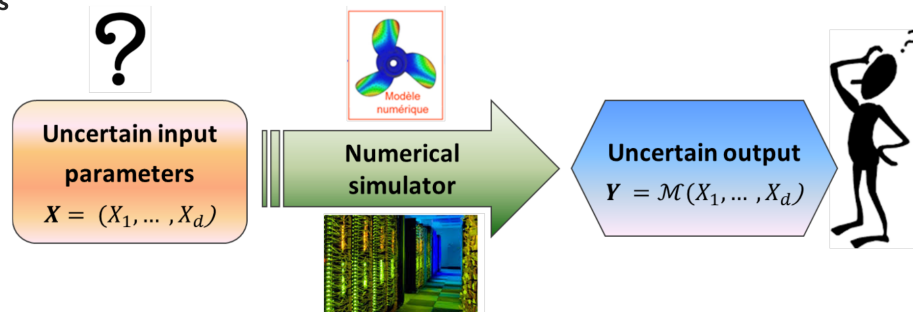
‡EDF R&D, Chatou, France

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## Risk assessment in nuclear accident analysis



- **Safety studies:** compute a failure risk (margins, rare events) with validated computer/numerical models
- **Numerical simulators:** fundamental tools to understand, model & predict physical phenomena
- **Large number of input parameters**, related to physical and numerical modelling
- **Uncertainty on some inputs** → **uncertainty on output & safety margins**
- **BEPU (Best-Estimate-Plus-Uncertainties):** realistic models + uncertain inputs → **Better assessment of the real margins**



# Risk assessment in nuclear accident analysis

## How to deal with uncertainties in numerical simulation?

→ Probabilistic framework and Monte Carlo-based methods

→ **CPU-expensive simulator** ⇒ Use of **machine learning to propagate input uncertainties**

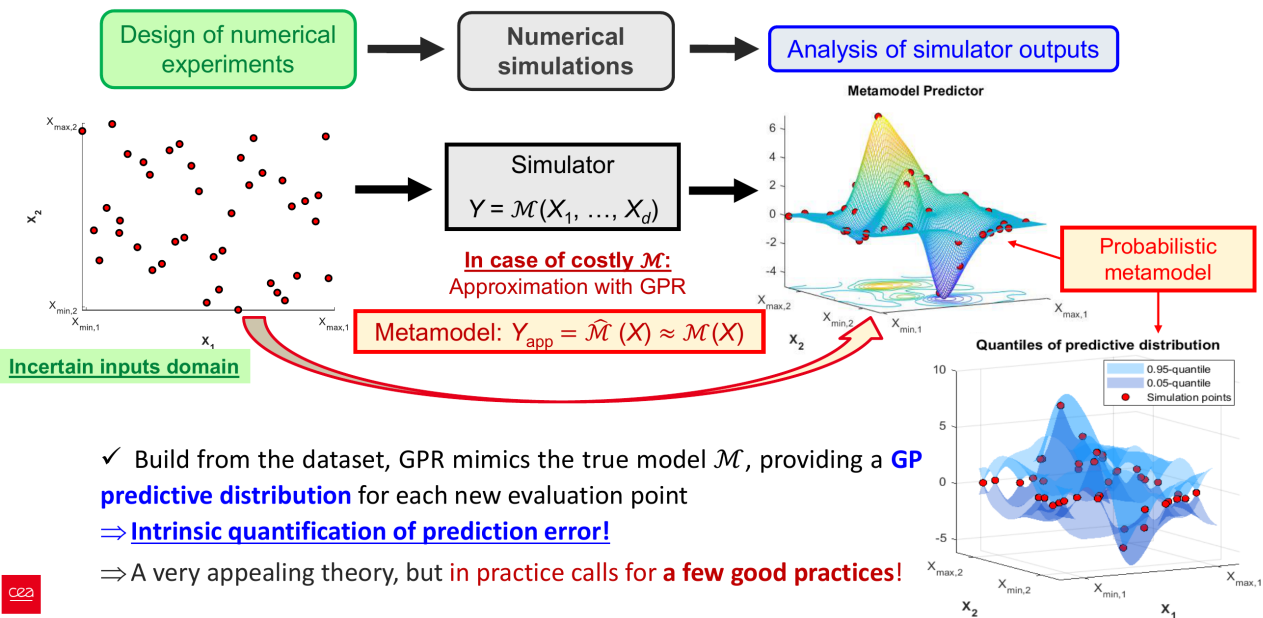
### → Applicative constraints/framework:

- ✓ **Given data:** a single inputs/output sample  $(x^{(i)}, y_i)_{1 \leq i \leq n}$  where  $y_j = \mathcal{M}(x^{(i)})$  to be used for multi-purpose (sensitivity analysis, uncertainty propagation... And **training a metamodel**)
- ✓ **Small sample size:**  $n \approx 100$  to 1000 simulations
- ✓ **Large number of uncertain inputs:**  $d \approx 10$  to 100 inputs
- ✓ **Required UQ associated to each prediction**

→ Gaussian Process Regression (GPR): particularly well-suited tool ⇒ Very popular



## Crucial use of GPR metamodel



# Challenges for an efficient GPR in practice

## 1. Dealing with the **large input dimension**



### Dealing with the large input dimension

→ How to train the GP in large dimension? ( $d \sim 10$  to 100, e.g.)

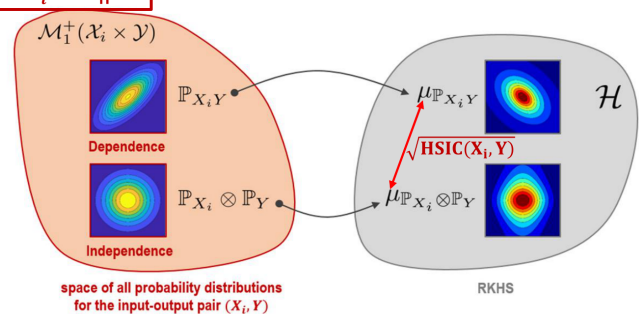
► **Curse of dimensionality**  $\Rightarrow$  too many GP hyperparameters have to be optimized!

→ Use of **preliminary SCREENING** for input selection (and thus dimension reduction).

► **Sensitivity measure from HSIC** (Hilbert-Schmidt Independence Criterion [GFT+07]), built-upon RKHS embeddings

$$HSIC(X_i, Y) = MMD^2(P_{X_i Y}, P_{X_i} \otimes P_Y) = \left\| \mu_{P_{X_i Y}} - \mu_{P_{X_i} \otimes P_Y} \right\|^2$$

- ✓ **HSIC**: Estimation of from a **unique random sample**, efficient in practice from  $n \sim 100$
- ✓ HSIC "summarizes" the cross-cov between feature maps  $\Rightarrow$  Large panel of input-output dependency captured



MMD: Maximum Mean Discrepancy

Extract from a presentation by G. Sarazin (CEA)

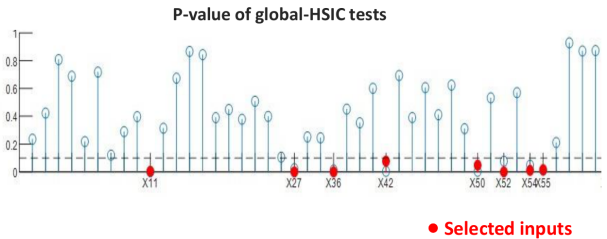


## Dealing with the large input dimension

► **HSIC-based independence tests** [GFT+07]:  $HSIC(X_i, Y) = 0 \Leftrightarrow X_i \perp Y$  (with characteristic kernels!)

- ✓ Null hypothesis:  $\mathcal{H}_0 : X_i \perp Y$  against  $\mathcal{H}_1 : X_i \not\perp Y$
- ✓ Test statistics:  $n\widehat{HSIC}(X_i, Y)$
- ✓ Decision rule:  $\mathcal{H}_0$  rejected iff  $n\widehat{HSIC}(X_i, Y) > q_{1-\alpha}$  where  $q_{1-\alpha}$  is the  $(1 - \alpha)$  quantile of  $n\widehat{HSIC}(X_i, Y)$  under  $\mathcal{H}_0$  (several available procedures to estimate  $q_{1-\alpha}$  [GFT+07, EM24])

⇒ Use for screening of inputs



Selection of **significant inputs** (<20)

- ✓ **Explicative inputs** of GPR
- ✓ Non-significant influential inputs captured by an additional variance in GPR (**nugget effect**)



## Dealing with the large input dimension

► **HSIC-based ranking** [Dav15]

Inputs ordered by degree of influence

Can be used for **more robust sequential GPR estimation**

⇒ “forward” estimation of GPR hyperparameters: successive inclusion of ordered inputs

See the “**ICSCREAM**” methodology [MIC21]



# Dealing with the large input dimension



- ▶ HSIC can capture **a large spectrum of relationships** (power of RKHS ☺)
- ▶ Able to deal with **many types of variables and purposes**:
  - Goal-oriented for safety studies** [MC21], to measure the influence in a restricted domain:  $Y \in \mathcal{C}$
  - Functional output**  $\Rightarrow$  definition of specific kernels [EM24]
- ▶ More powerful tests based on SupHSIC [EM24] and HSIC-ANOVA indices [SMD+23]



More robust selection of inputs



Efficiency demonstrated in **numerous industrial applications**, especially with small sample size  $n$  and large dimension  $d$



## Challenges for an efficient GPR in practice

### 1. Dealing with the large input dimension

### 2. Reliable estimation of GPR hyperparameters





## Reminders on GPR

- **Probabilistic surrogate model:** response is considered as a realization of a random GP field [RW05,Gra21]:

$$Y(\mathbf{x}) \sim GP(\mu(\mathbf{x}), k(\mathbf{x}', \mathbf{x}))$$

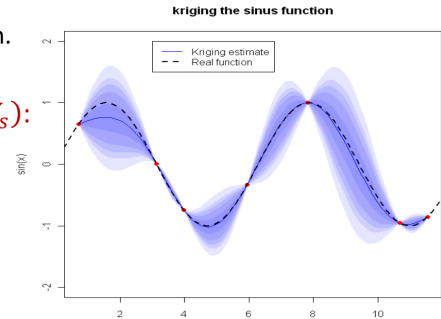
With  $\mu(\mathbf{x})$  the mean and  $k(\mathbf{x}', \mathbf{x})$  the covariance function.

⇒ **Predictive GP** is the GP conditioned by the observations  $(X_S, Y_S)$ :

$$Y(\mathbf{x}^*) | Y(X_S) = Y_S \sim GP(\hat{\mu}(\mathbf{x}^*), \hat{s}(\mathbf{x}', \mathbf{x}^*))$$

With analytical formulations for  $\hat{\mu}(\mathbf{x}^*)$  and  $\hat{s}(\mathbf{x}', \mathbf{x}^*)$

- ⇒ **Conditional mean**  $\hat{\mu}(\mathbf{x}^*)$  serves as the **predictor** at location  $\mathbf{x}^*$
- ⇒ **Prediction variance** (i.e. mean squared error) is given by **conditional covariance**  $\hat{s}(\mathbf{x}^*, \mathbf{x}^*)$
- ⇒ **Prediction interval** of any level  $\alpha$  can be built at any location  $\mathbf{x}^*$



C22



## Recommendations for parametric choices

- **In practice:** parametric choices for trend function  $\mu$  and covariance function  $k$

$$Y(\mathbf{x}) \sim GP(\mu(\mathbf{x}), k(\mathbf{x}', \mathbf{x}))$$

⇒ For  $\mu$ : either **constant** or linear basis

⇒ For  $k$ : stationary covariance built-upon tensorized 1-D covariance functions of  $\nu$ -Matérn

$$1\text{-Dim} \rightarrow k_{\sigma, \nu, \theta}(x, \tilde{x}) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left( \frac{\sqrt{2\nu}h}{\theta} \right)^\nu K_\nu \left( \frac{\sqrt{2\nu}h}{\theta} \right)$$

**3/2 or 5/2 Matérn covariances**  
offer good properties and  
« intermediate » regularity

$$d\text{-Dim} \rightarrow k_{\sigma, \nu, \theta}(\mathbf{x}, \tilde{\mathbf{x}}) = \sigma^2 \prod_{i=1}^d k_{1, \nu, \theta_i}(x_i - \tilde{x}_i) \quad \text{with } h = |\mathbf{x} - \tilde{\mathbf{x}}|$$

**Hyperparameters**  
 $\theta \in \mathbb{R}^{+, d}$

⇒ **Additional variance** (nugget effect → nugget hyperparameter  $\lambda \in \mathbb{R}^+$ )

	$\nu = \frac{1}{2}$	$\nu = \frac{3}{2}$	$\nu = \frac{5}{2}$	$\nu = +\infty$
Usual name	exponential	3/2-Matérn	5/2-Matérn	Gaussian
$k_{\sigma, \nu, \theta}(x, \tilde{x})$	$\sigma^2 e^{-\frac{h}{\theta}}$	$\sigma^2 (1 + \sqrt{3}\frac{h}{\theta}) e^{-\sqrt{3}\frac{h}{\theta}}$	$\sigma^2 \left( 1 + \sqrt{5}\frac{h}{\theta} + \frac{5}{3} \left( \frac{h}{\theta} \right)^2 \right) e^{-\sqrt{5}\frac{h}{\theta}}$	$\sigma^2 e^{-\frac{1}{2} \left( \frac{h}{\theta} \right)^2}$
Differentiability of GP trajectories	$\mathcal{C}^0$	$\mathcal{C}^1$	$\mathcal{C}^2$	$\mathcal{C}^\infty$

C22



# Estimation of GP hyperparameters



⇒ How to robustly estimate the **hyperparameters**  $\theta \in \mathbb{R}^{+,d}$  from the learning sample ?



For good **predictivity + reliable GP prediction intervals**  
⇒ Crucial for safety applications



# Estimation of GP hyperparameters



► Usual estimation methods [KO22,Mur21,Pet22,PBF+22]

→ Maximum likelihood

→ Cross-validation Mean Squared Error

→ Bayesian approaches



Ill-posedness of MLE, problem of **flatness** of functions to be minimized

CPU ++, delicate choice of priors  
Except RobustGAsp method of [GWB18]

Proposition of a new multi-objective estimation algorithm for more reliable GP prediction intervals in [MI24b]



Bertrand Iooss' talk on Wednesday, MS 120:  
"Gaussian process regression: new hyperparameter estimation algorithm for more reliable prediction - Application to an aquatic ecosystem model"

Work supported by French ANR SAMOURAI Project



# Challenges for an efficient GPR in practice

## 1. Dealing with the large input dimension

## 2. Reliable estimation of GPR hyperparameters

## 3. Careful GPR **validation** for confident use



## GPR validation

► Validation criteria computed by cross-validation (LOO or K-fold CV) [DIG+21]

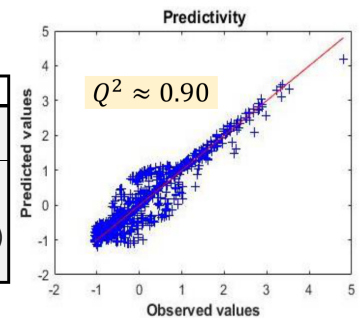
→ Accuracy of the GP predictor (only):

$$Q^2 = 1 - \frac{MSE}{\frac{1}{n} \sum_{i=1}^n (y_i - \frac{1}{n} \sum_{i=1}^n y_i)^2} \text{ with } MSE = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_{-i}(\mathbf{x}^{(i)}))^2$$

where  $\hat{y}_{-i}(\mathbf{x}^{(i)})$  is the metamodel predictor in  $\mathbf{x}^{(i)}$  when  $(\mathbf{x}^{(i)}, y_i)$  is removed from the learning sample.

The closer to one the  $Q^2$ , the better the accuracy of the metamodel predictor.

Values	Interpretation
High value, close to 1	Good predictive capability of metamodel predictor for unobserved points.
Low value ( $Q^2 \leq 0.5$ , e.g.)	Poor predictive capability. Some possible reasons: <ul style="list-style-type: none"><li>- unsuitable or poorly estimated model;</li><li>- very poorly predicted areas (<math>Q^2</math> sensitive to highest or extreme errors)</li><li>- Insufficient learning sample to properly explore the space of input</li></ul>





# GPR validation

► Validation criteria computed by cross-validation (LOO or K-fold CV) [DIG+21]

→ Accuracy of the whole GP conditional distribution [DIG+21,ABG23]

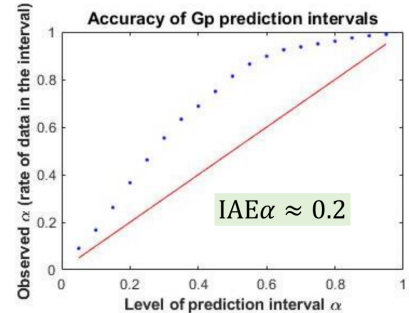
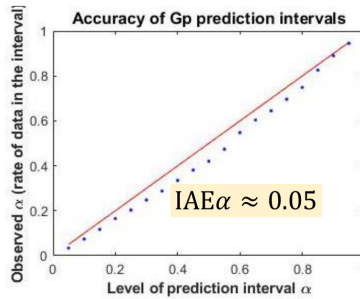
From empirical coverage function for  $\alpha \in [0,1]$ :  $\hat{\Delta}(\alpha) = \frac{1}{n} \sum_{i=1}^n \mathbf{1}\{y_i \in PI_{\alpha,-i}(\mathbf{x}^{(i)})\}$

with  $PI_{\alpha,-i}(\mathbf{x}^{(i)})$  the  $\alpha$ -level GP prediction interval for  $\mathbf{x}^{(i)}$  when  $(\mathbf{x}^{(i)}, y_i)$  is removed from learning sample

⇒  $\alpha$ -PI Plot

⇒ Integrated Absolute Error on  $\hat{\Delta}(\alpha)$  [MI24a]

$$IAE\alpha = \int_0^1 |\hat{\Delta}(\alpha) - \alpha|$$



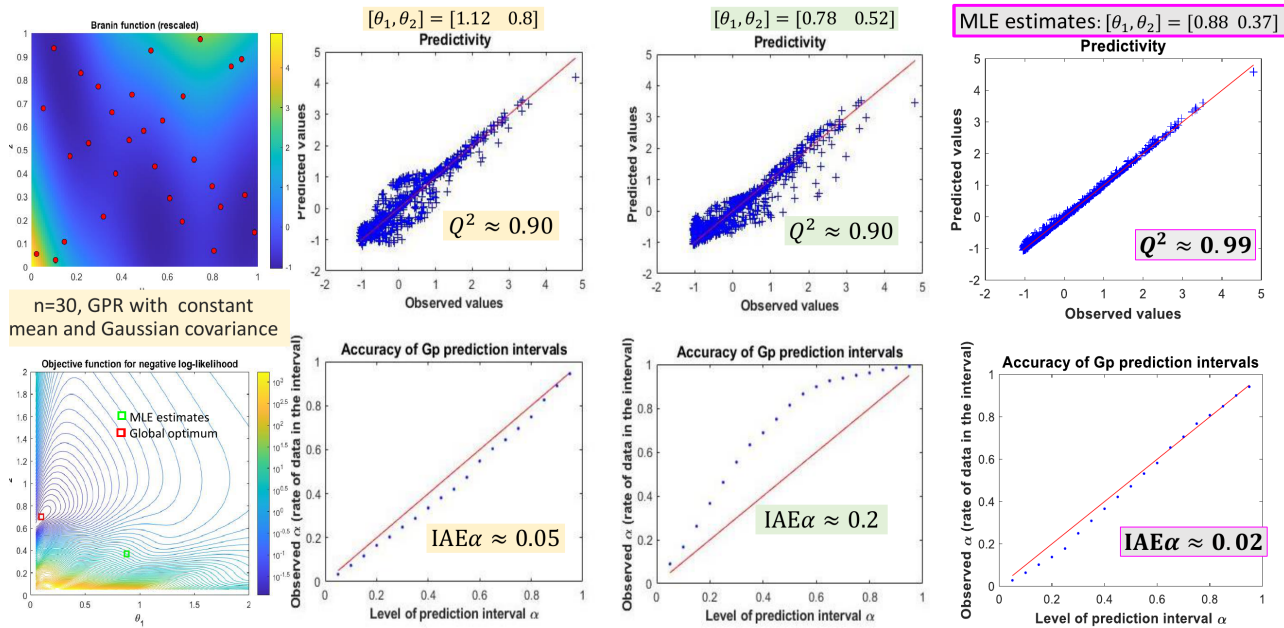
# GPR validation

► One message: Joint interpretation of  $Q^2$  and  $IAE\alpha$  ! [MI24a]

Criterion	Values	Interpretation
<b><math>IAE\alpha</math></b>	Value close to 0	<u>Only if <math>Q^2</math> is also high</u> , reliable predicted confidence intervals
	High values, close to 0.5 e.g.	Unreliable predicted prediction intervals ("underconfident" or "overconfident" model) ⇒ <b>Explanation from cross-interpretation with <math>Q^2</math> and <math>\alpha</math>-PI plot</b>



# Illustration of criteria for GPR validation [MI24a]



## Conclusions and remaining challenges



# Conclusions

## ► Recommendations for an efficient GP Regression:

- ✓ GPR benefits greatly from **preliminary HSIC-based screening**
- ✓ GPR calls for **robust estimation of hyperparameters**
- ✓ Particular attention must be paid to **GP validation**

⇒ All these recipes are integrated in **ICSCREAM methodology** [MIC21]

⇒ Part of a more general effort to **ensure confidence in machine learning for UQ**

## ► Interesting challenges for UQ applications

- ✓ **High dimensional** problems (for example beyond 30 to 50 inputs and screening-free)
- ✓ Extension to **more complex inputs** (graph structure, e.g.)
- ✓ Learning **outputs with highly irregular**, or even **chaotic behavior** (due to physical threshold phenomena and phenomenological bifurcations, for instance)



# References 1/2

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[MI24b] A. Marrel and B. Iooss, Probabilistic surrogate modeling by Gaussian process: A new estimation algorithm for more robust prediction, Preprint <https://hal.science/cea-04322818>

Work partly funded by ANR SAMOURAI research project



Simulation Analytics and Meta-model-based solutions for Optimization, Uncertainty and Reliability Analysis

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