

# **A new estimation algorithm for more reliable prediction in Gaussian Process Regression**

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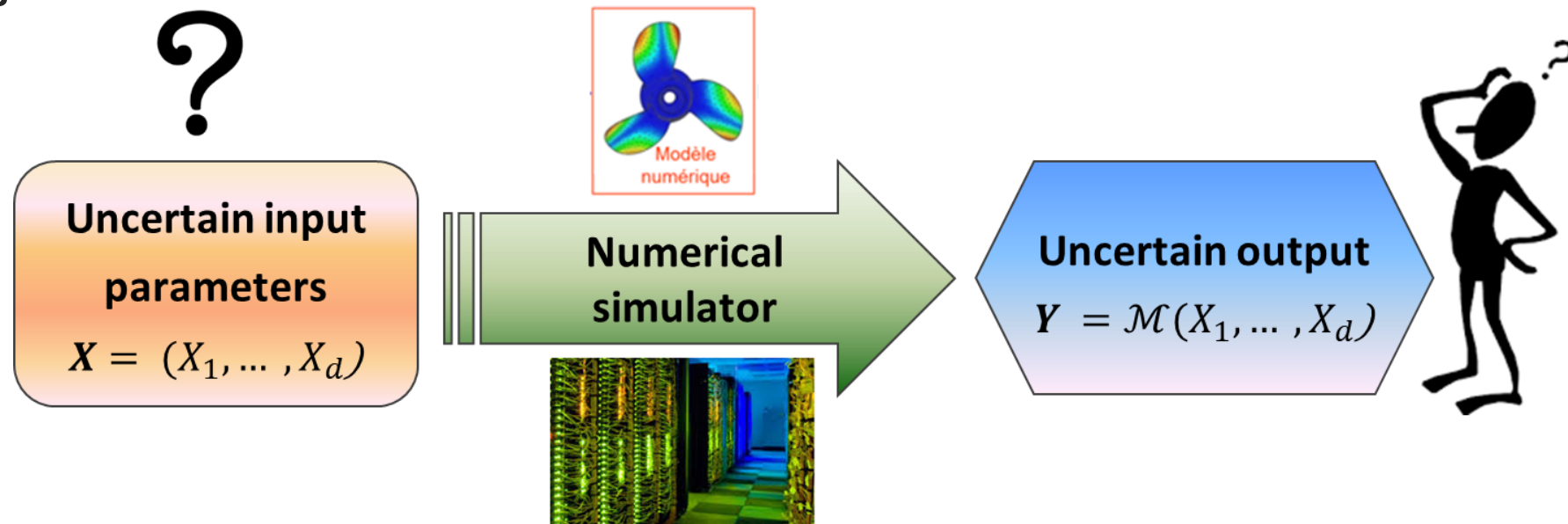
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# Risk assessment in nuclear accident analysis

- **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 mimic the simulator and propagate input uncertainties

→ Applicative constraints/framework:

- ✓ **Given data for training:** a single inputs/output **sample**  $D_S = (x^{(i)}, y^{(i)})_{1 \leq j \leq n}$  where  $y^{(i)} = \mathcal{M}(x^{(i)})$   
→ random or quasi-random sample
- ✓ **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**

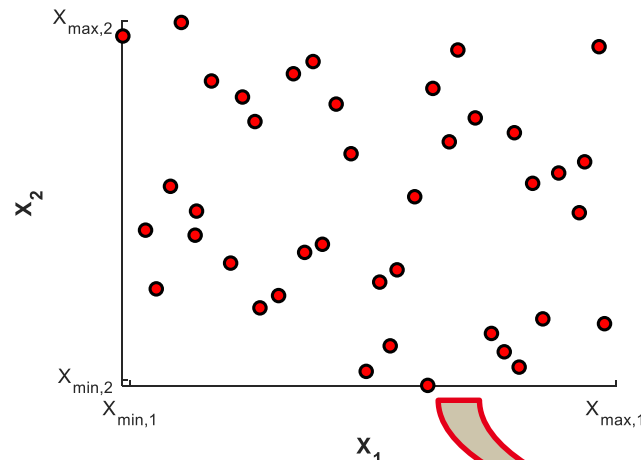
→ Gaussian Process Regression (GPR): particularly well-suited tool ⇒ Very popular

# Crucial use of GPR metamodel

Design of numerical experiments

Numerical simulations

Analysis of simulator outputs



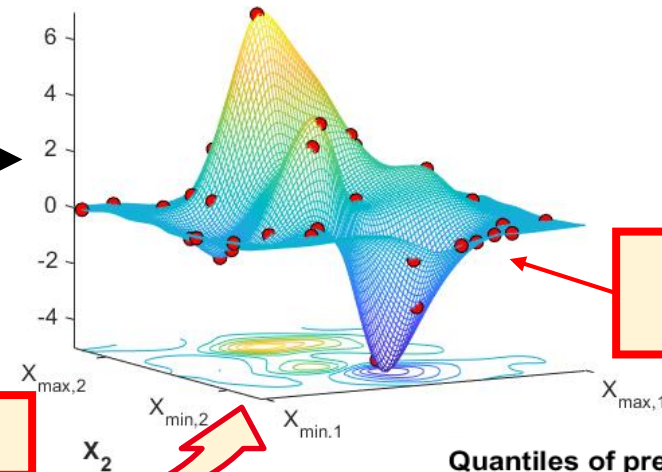
**Uncertain inputs domain**

Simulator  
 $Y = \mathcal{M}(X_1, \dots, X_d)$

**In case of costly  $\mathcal{M}$ :**  
Approximation with GPR

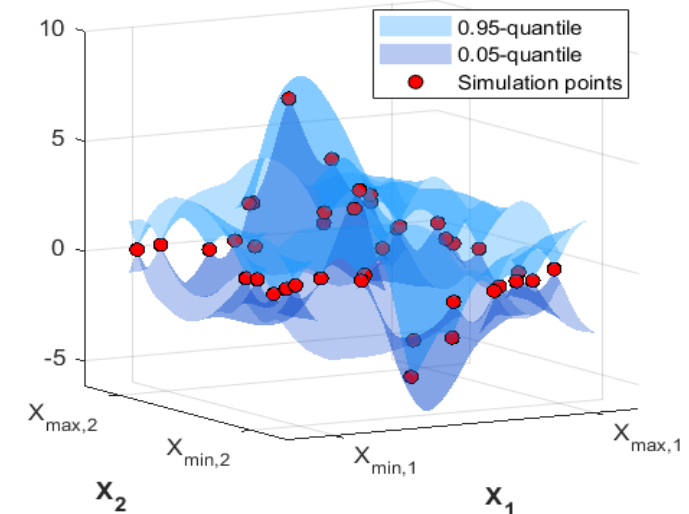
**Metamodel:  $Y_{\text{app}} = \hat{\mathcal{M}}(X) \approx \mathcal{M}(X)$**

Metamodel Predictor



**Probabilistic metamodel**

Quantiles of predictive distribution



- ✓ Build from the dataset, GPR mimics the true model  $\mathcal{M}$ , providing a **GP predictive distribution** for each new evaluation point
  - ⇒ **Intrinsic quantification of prediction error!**
  - ⇒ Very appealing, but **in practice calls for a few good practices!**

# Building 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!



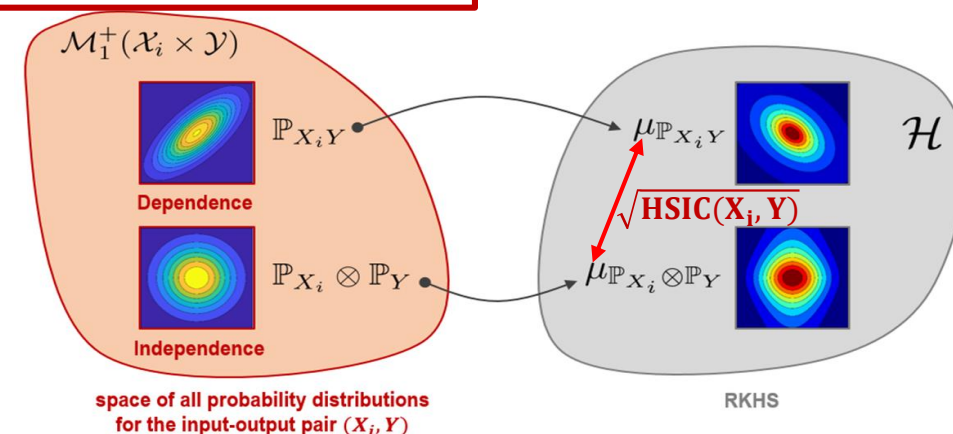
Preliminary SCREENING for input selection (and thus dimension reduction)



**HSIC-based sensitivity measure** [GFT+07]  $\rightarrow$  dependence measure comparing the RKHS embeddings of joint distribution  $\mathbb{P}_{X_i Y}$  and product of marginals  $\mathbb{P}_{X_i} \otimes \mathbb{P}_Y$

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

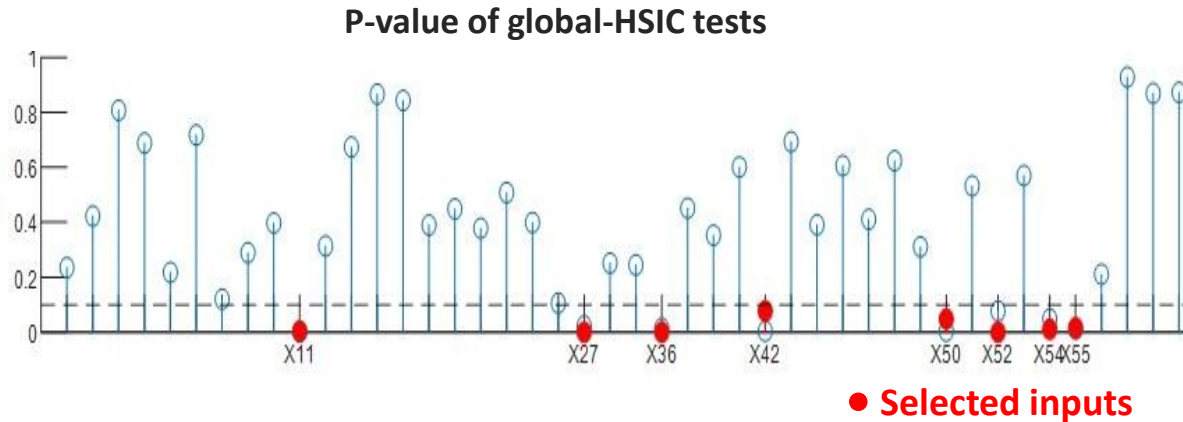
- ✓ HSIC can capture a **large spectrum of input-output relationships** (power of RKHS 😊)
- ✓ **HSIC**: Estimation from a **unique random sample**, robust in practice from  $n \sim 100$



Extract from a presentation by G. Sarazin (CEA)

# Dealing with the large input dimension

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



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

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

- ▶ **HSIC-based ranking with  $R^2HSIC$**  [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 [MIC22]

# Building an efficient GPR in practice

1. Dealing with the large input dimension

2. Estimation of hyperparameters and validation



# 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  $(X_S, Y_S)$ :

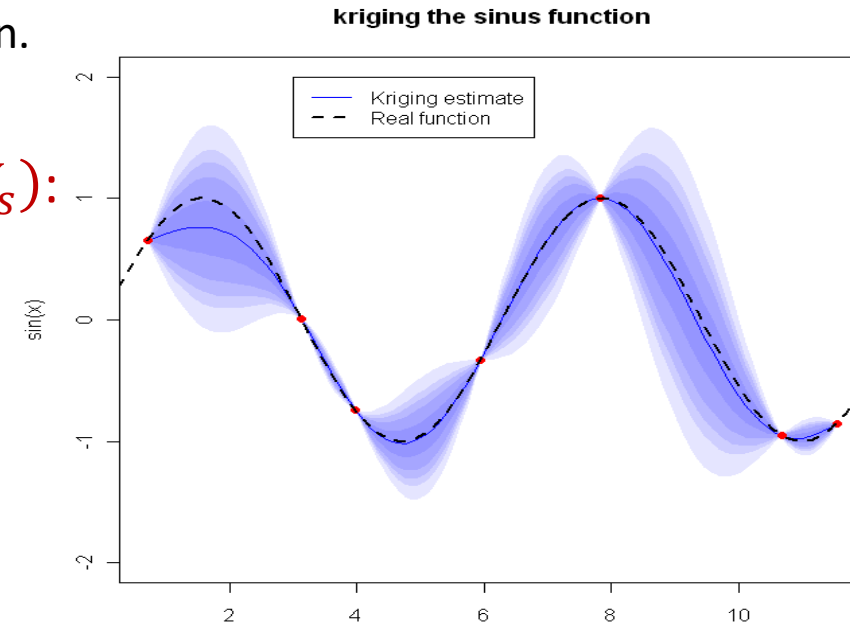
$$Y(\mathbf{x}^*)_{|Y(X_S)=Y_S} \sim GP(\hat{\mu}(\mathbf{x}^*), \hat{s}(\mathbf{x}', \mathbf{x}^*))$$

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  $\mathbf{x}^*$



# Reminders on GPR

► **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

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

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

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

**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	$\mathcal{C}^0$	$\mathcal{C}^1$	$\mathcal{C}^2$	$\mathcal{C}^\infty$

# Estimation of GPR hyperparameters



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



How to ensure that the estimated hyperparameters  $\theta$  yield **good predictivity** but also **reliable GP prediction intervals**?

⇒ Crucial for safety applications



Especially in « **medium** » dimension ( $d \in [10, 20]$ ) and **small dataset** ( $n \in [100, 1000]$ )

# Estimation of GPR hyperparameters

## ► Usual estimation methods [KO22,Mur21,Pet22,PBF+23]

→ **Maximum likelihood (MLE)**  $\Leftrightarrow$  minimization of NLL

→ **Cross-validation and Mean Squared Error** :

$$\text{minimization of RMSE} = \left\{ \frac{1}{n} \sum_{i=1}^n (y^{(i)} - \hat{y}_{-i}(\mathbf{x}^{(i)}))^2 \right\}^{0.5}$$

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.

→ **Bayesian approaches**

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

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

⇒ Could we do better?

⇒ How to **check** that estimated hyperparameters lead to a “**good**” GPR metamodel?

# Validation of GPR

► Validation criteria computed by cross-validation (LOO or K-fold CV) [DIG<sup>+</sup>21, ABG23, MI24a]

→ Accuracy of the GP predictor (only):  $Q^2 = 1 - \frac{RMSE^2}{\frac{1}{n} \sum_{i=1}^n \left( y^{(i)} - \frac{1}{n} \sum_{i=1}^n y^{(i)} \right)^2}$

→ Accuracy of the predictive variance:  $PVA = \left| \log \frac{1}{n} \sum_{i=1}^n \frac{(y^{(i)} - \hat{y}_{-i}(\mathbf{x}^{(i)}))^2}{\hat{s}_{-i}^2} \right|$

→ Accuracy of the whole GP conditional distribution

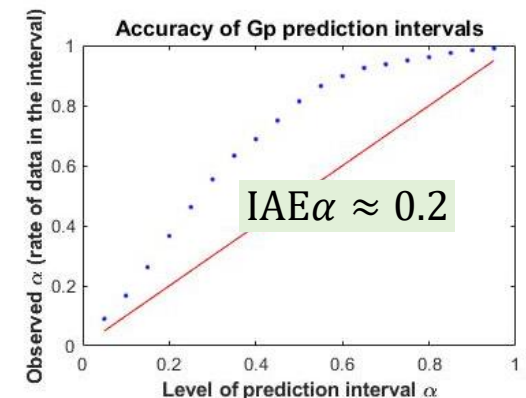
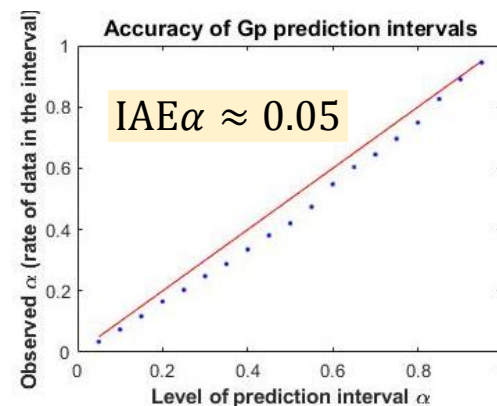
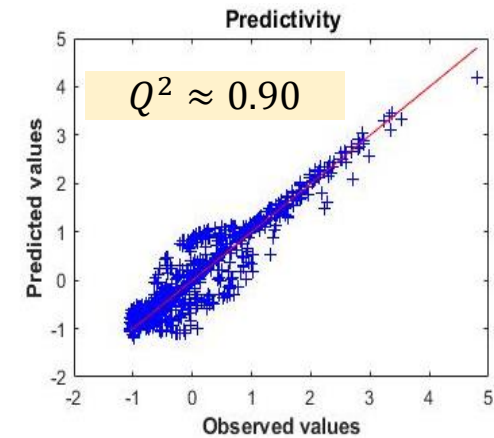
From empirical coverage function for  $\alpha \in [0, 1]$ :  $\hat{\Delta}(\alpha) = \frac{1}{n} \sum_{i=1}^n \mathbf{1}\{y^{(i)} \in PI_{\alpha, -i}(\mathbf{x}^{(i)})\}$

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

⇒  $\alpha$ -PI Plot

⇒ Summarized by Integrated Absolute Error on  $\hat{\Delta}(\alpha)$

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



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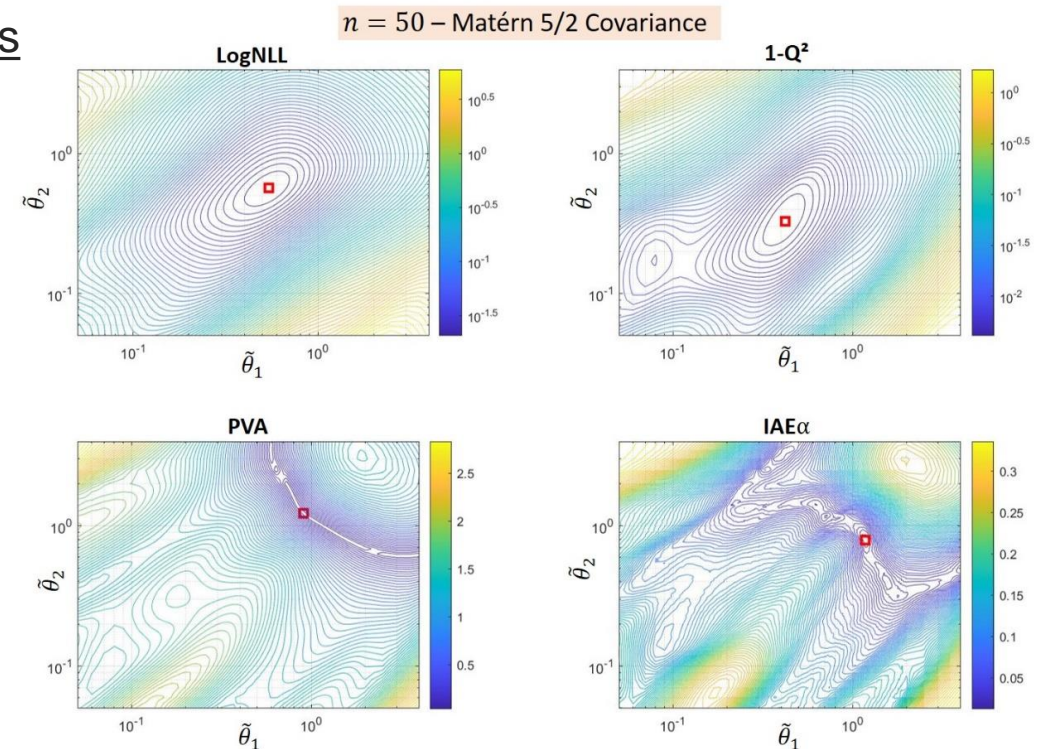
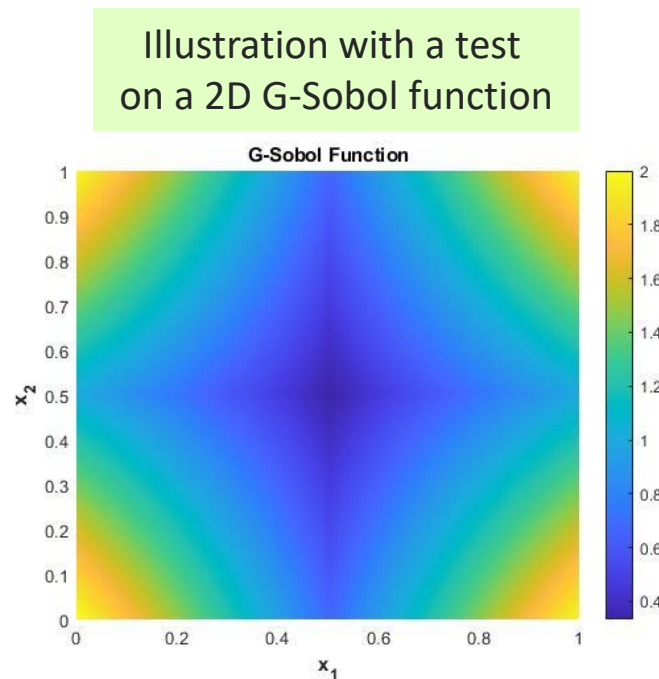
**2. Estimation of hyperparameters and validation**

**3. New hyperparameter estimation algorithm**

# From the analysis of estimation & validation criteria...

## ► Study of criteria NLL, $Q^2$ , PVA and $IAE\alpha$ on a large benchmark of analytical tests

- Close behavior of NLL and  $Q^2 \Rightarrow$  keep NLL as the main estimation objective to ensure predictivity  
→ Consistent with [PBF<sup>+</sup>23, Pet22]
- Similar behavior of PVA and  $IAE\alpha$  but more irregular w.r.t.  $\theta$ 
  - $\Rightarrow$  Some local minima compatible with optimal values of the other criteria
  - $\Rightarrow$  But No to be optimized independently of the others



# To a new estimation algorithm!

## ► Study of criteria NLL, $Q^2$ , PVA and $IAE\alpha$ on a large benchmark of analytical tests

- Close behavior of NLL and  $Q^2$   $\Rightarrow$  keep NLL as the main estimation objective to ensure predictivity
- $IAE\alpha$  more directly related to reliable predictive intervals, than PVA
- In the neighborhood of the optimal NLL point, existence of better points  $\theta$  w.r.t  $IAE\alpha$ , but need to control the possible degradation of  $Q^2$  value, which guarantees the predictivity



$\Rightarrow$  Optimization based on NLL and  $IAE\alpha$  + Control of  $Q^2$

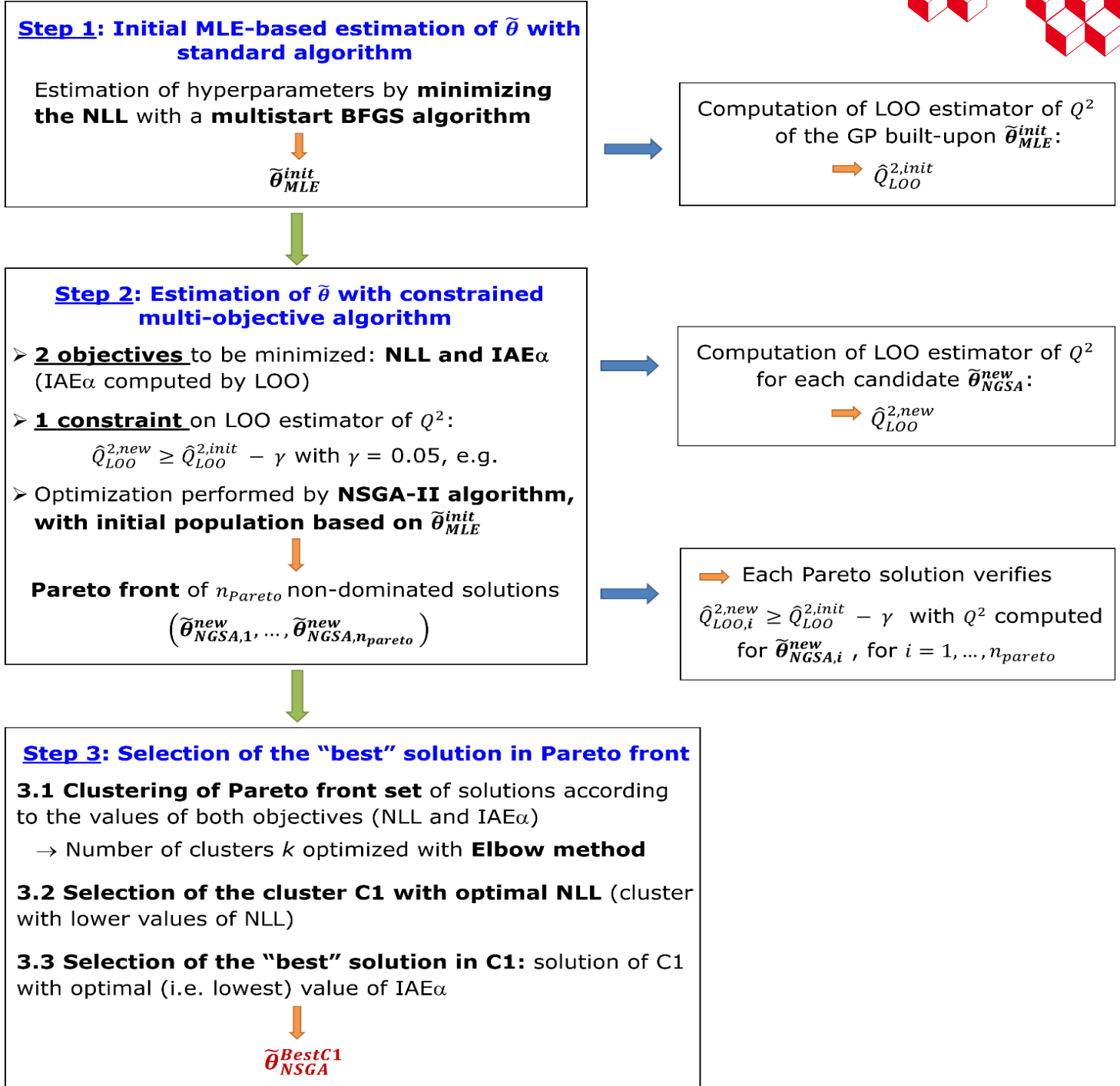
( $IAE\alpha$  and  $Q^2$  estimated by cross validation + use of LOO Dubrule formulas)

$\Rightarrow$  Proposition of a multi-objective NSGA-II algorithm with constraint on  $Q^2$



# Algorithm flowchart

All details in Marrel and B. Iooss, *Probabilistic surrogate modeling by Gaussian process: A new estimation algorithm for more robust prediction*, Reliability Engineering and System Safety, Volume 247, July 2024, 110120.

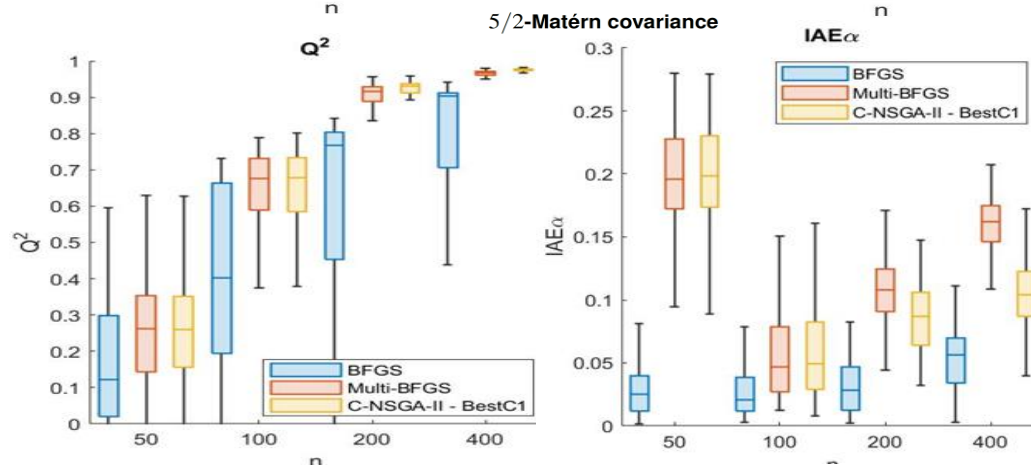
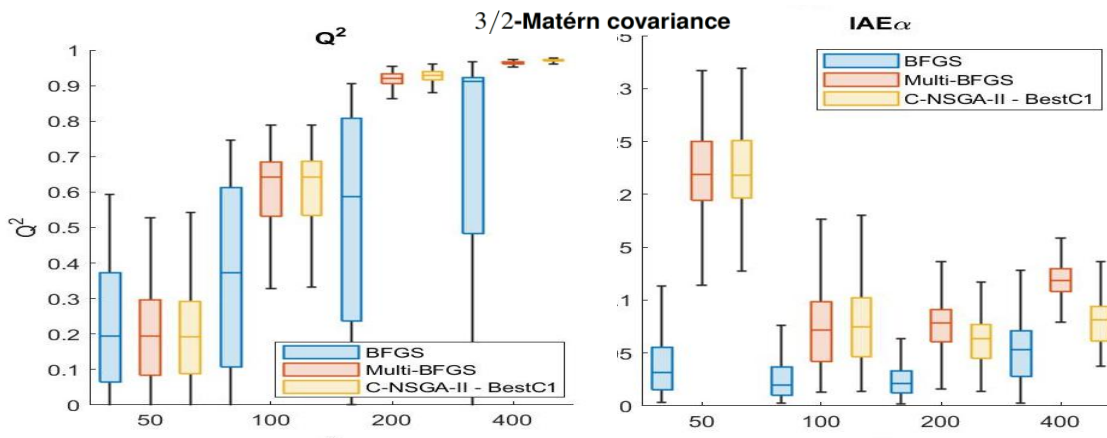
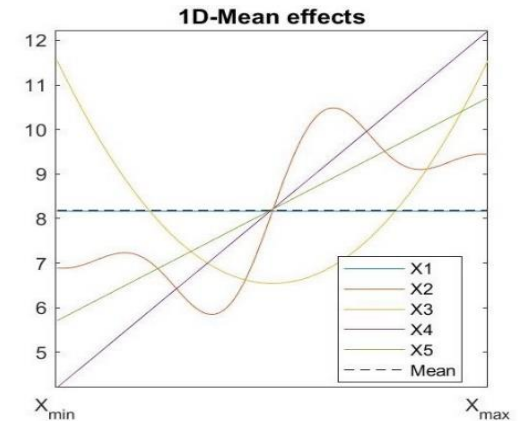


# Intensive benchmark on analytical test functions

## ► Comparison with usual algorithms based on NLL optimization only (BFGS/multistart)

$d = 2$  to  $20$ ,  $\neq$  covariance,  $\neq$  sample sizes,  $\neq$  DoE, with/without nugget effect

Example on Marrel-d20 function :  $Y(X) = a_1 \sin[6\pi X_1^{\frac{5}{2}} (X_2 - \frac{1}{2})] + a_2 (X_3 - \frac{1}{2})^2 + a_3 X_4 + a_4 X_5 + r_{X_6, \dots, X_{15}}$



Results without nugget effect

⇒ **Predictivity with Constr-NSGA-II algorithm at least as good as the simple NLL optimization**

⇒ **Improvement of  $IAE_\alpha$  especially if :**

- The model is misspecified, i.e. if the covariance does not match the regularity of the function
- When the number of hyperparameters is large (e.g. large dimension  $d$  + tensorized anisotropic stationary covariance)

# Building an efficient GPR in practice

1. Dealing with the large input dimension

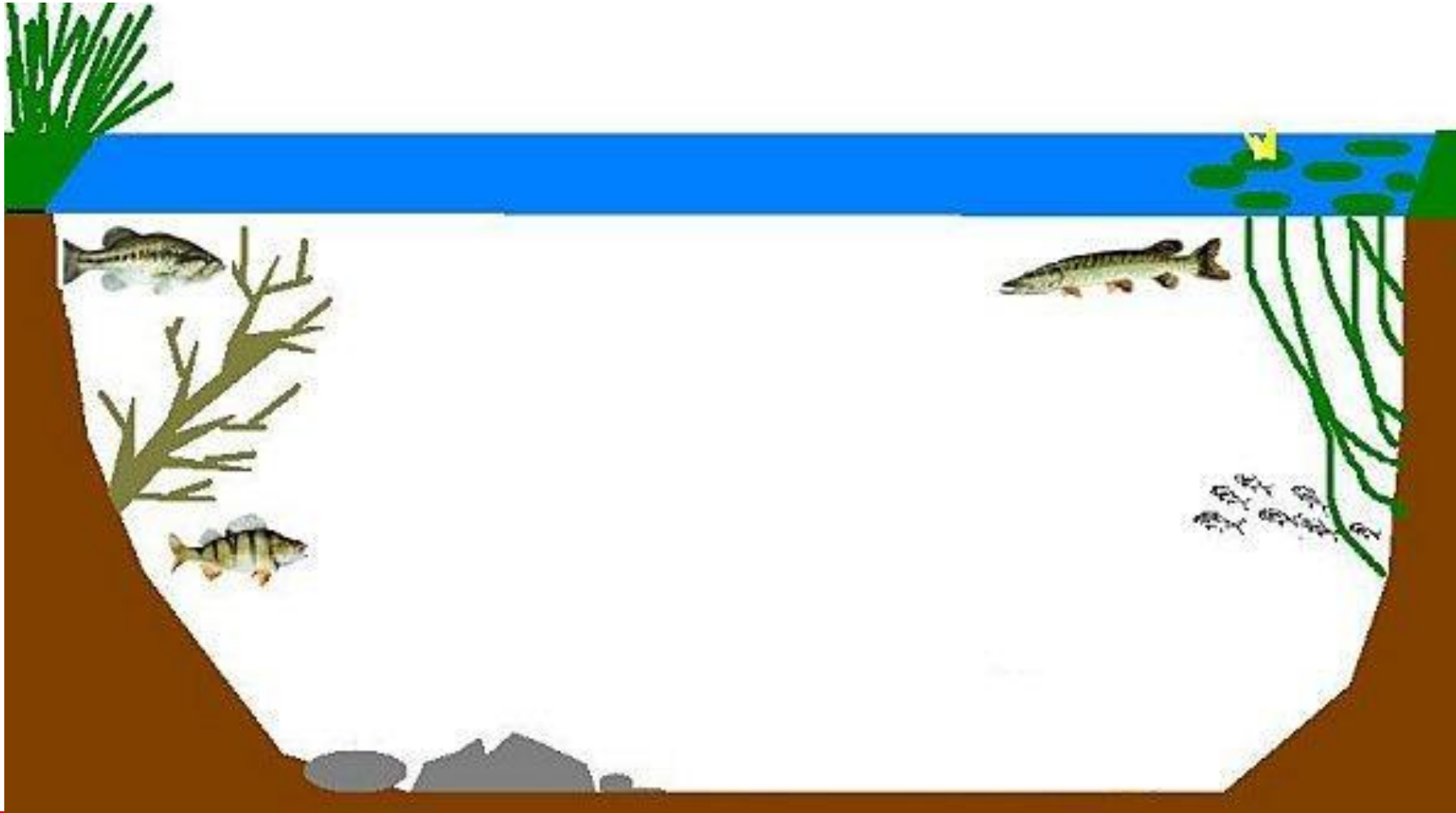
2. Estimation of hyperparameters and validation

3. New hyperparameter estimation algorithm

4. Illustration on aquatic prey-predator chain model

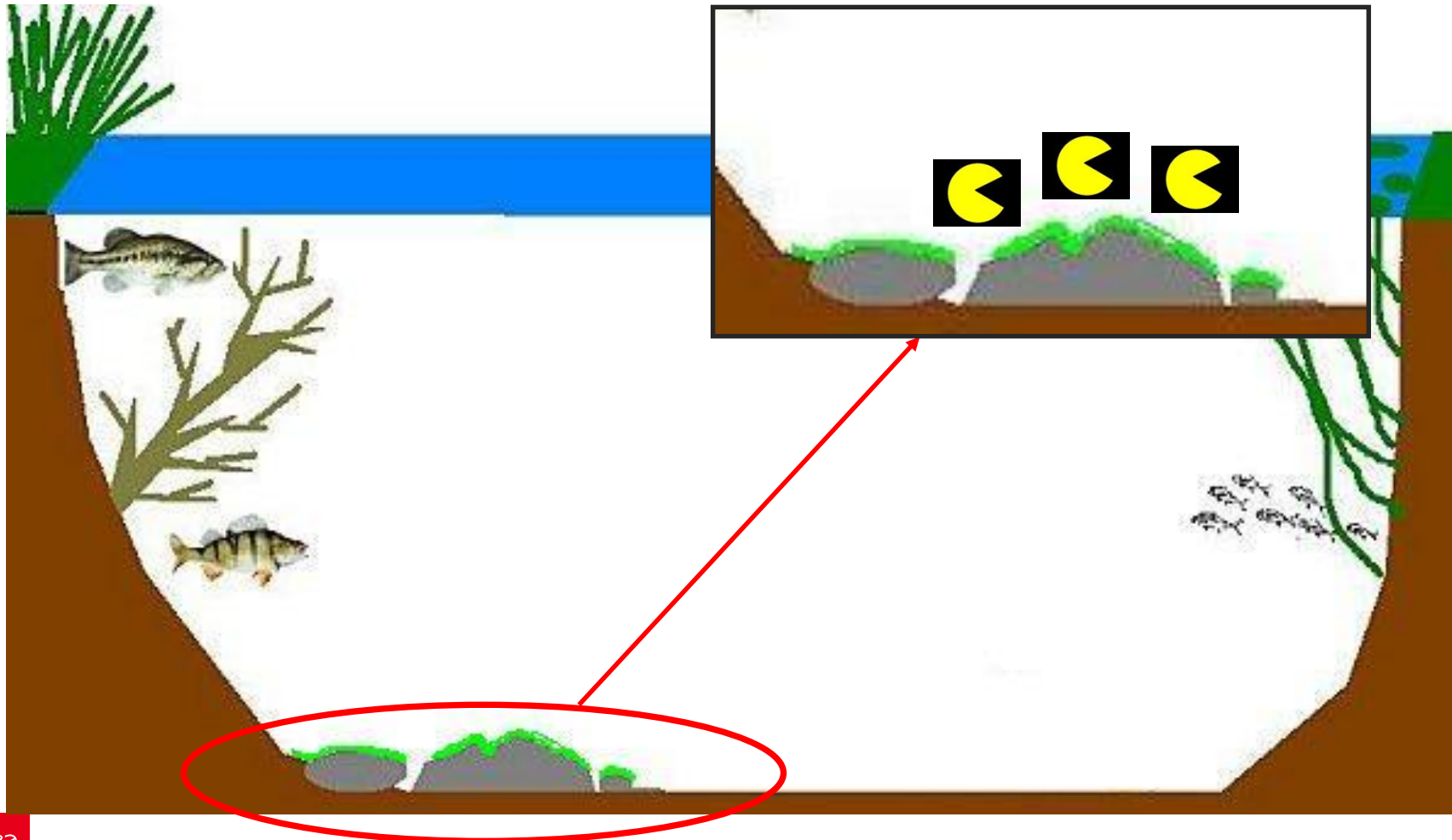
# Application: aquatic prey-predator chain model

Studies of biological contamination of rivers



# Application: aquatic prey-predator chain model

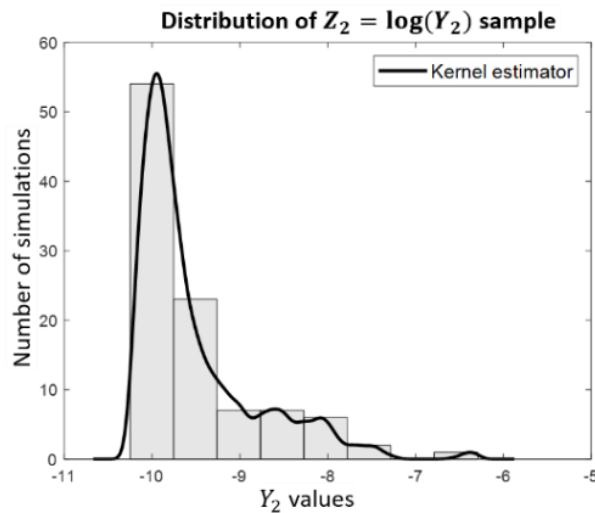
EDO-type equations describing the growth of microorganisms, grazing and prey-predator interactions



# Application: aquatic prey-predator chain model

## ► Simulator: MELODY with $d = 20$ uncertain inputs:

- Periphyton: photosynthesis/mortality/excretion rates, survival temperature, saturation constants, ...
- Grazers: consumption/assimilation/ mortality/excretion rate, survival temperature, ...
- **2 outputs of interest:** Periphyton ( $Y_1$ ) and Grazers ( $Y_2$ ) biomasses at day 60
- Sample of  $n = 100$  simulations of the model MELODY (from space-filling design)
- Need of **preliminar logarithmic transformation**



## ⇒ Lognormal-kriging modeling:

- Emulation of  $Z_i = \log(Y_i)$  with GP regression
- Lognormal-kriging back-transformations to obtain metamodel for  $Y_i$

$$\hat{y}_i(\mathbf{x}) = e^{(\hat{z}_i(\mathbf{x}) + 0.5\hat{s}_{z_i}^2(\mathbf{x}))}$$
$$\hat{s}_Y^2(\mathbf{x}) = \left( e^{\hat{s}_{z_i}^2(\mathbf{x})} - 1 \right) e^{(2\hat{z}_i(\mathbf{x}) + \hat{s}_{z_i}^2(\mathbf{x}))}$$

- Additional comparison with **Bayesian RobustGaSP approach** [GWB18]

# Application: aquatic prey-predator chain model

⇒ **With** nugget effect (included in the set of GP hyperparameters to be estimated)

Data	Covariance	Predictivity Coefficient $Q^2$			IAE $\alpha$		
		Multi-BFGS	C-NSGA-II-BestC1	RobustGaSP	Multi BFGS	C-NSGA-II-BestC1	RobustGaSP
Y <sub>2</sub>	Matern3/2	0,70	0,74	0,25	0,10	0,07	0,04
	Matern5/2	0,77	<b>0,82</b>	0,66	0,09	<b>0,02</b>	0,07
	Gaussian	0,75	<b>0,79</b>	0,66	0,08	<b>0,02</b>	0,06

⇒ Best results with **Constr-NSGA-II algorithm**: better  $Q^2$  and IAE $\alpha$

⇒ **Without** nugget effect

Data	Covariance	Predictivity Coefficient $Q^2$			IAE $\alpha$		
		Multi-BFGS	C-NSGA-II-BestC1	RobustGaSP	Multi BFGS	C-NSGA-II-BestC1	RobustGaSP
Y <sub>2</sub>	Matern3/2	0,70	<b>0,75</b>	0,47	0,10	0,06	0,03
	Matern5/2	0,78	<b>0,84</b>	<b>0,83</b>	0,08	<b>0,02</b>	0,07
	Gaussian	0,70	<b>0,72</b>	<b>0,89</b>	0,06	<b>0,03</b>	0,06

⇒ Better behavior of RobustGasp without nugget : best  $Q^2$  but not IAE $\alpha$

⇒ **Constr-NSGA-II algorithm is more robust to modeling choices** (prior choice of GPR covariance)

# Conclusions and remaining challenges

- ✓ GPR benefits greatly from **preliminary HSIC-based screening**
- ✓ GPR calls for **robust estimation of hyperparameters**: considering validation criteria of the whole GP distribution when estimating hyperparameters  $\Rightarrow$  enables more robust estimation !
- ✓ Particular attention must be paid to **GP validation**
  - $\Rightarrow$  Part of a more general effort to **ensure confidence in machine learning for UQ**

## ► Some interesting challenges for UQ applications

- ✓ Use **more powerful tests** based on SupHSIC [EM24] and HSIC-ANOVA indices [SMD+23]
- ✓ **Screening-free approaches for high dimensional problems** (e.g. beyond 30 to 50 inputs)
- ✓ Learning **outputs with highly irregular**, or even **chaotic behavior** (due to physical threshold phenomena and phenomenological bifurcations, for instance)



# References 1/2

## Reference of this work

[MI24a] A. Marrel and B. Iooss, Probabilistic surrogate modeling by Gaussian process: A review on recent insights in estimation and validation, *Reliability Engineering and System Safety*, Volume 247, July 2024, 110120.

[MI24b] A. Marrel and B. Iooss, Probabilistic surrogate modeling by Gaussian process: A new estimation algorithm for more robust prediction, - *Reliability Engineering and System Safety*, Volume 247, July 2024, 110094.

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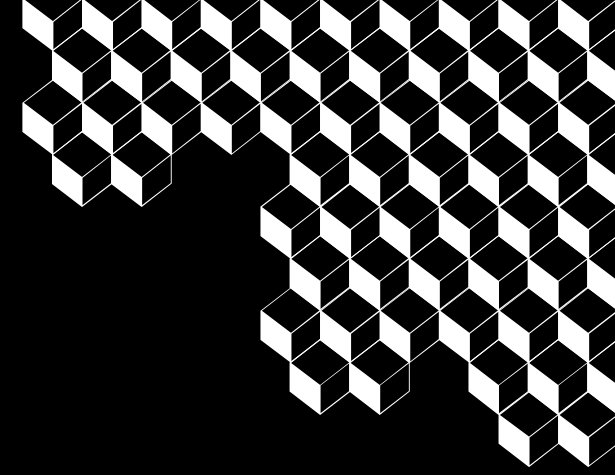
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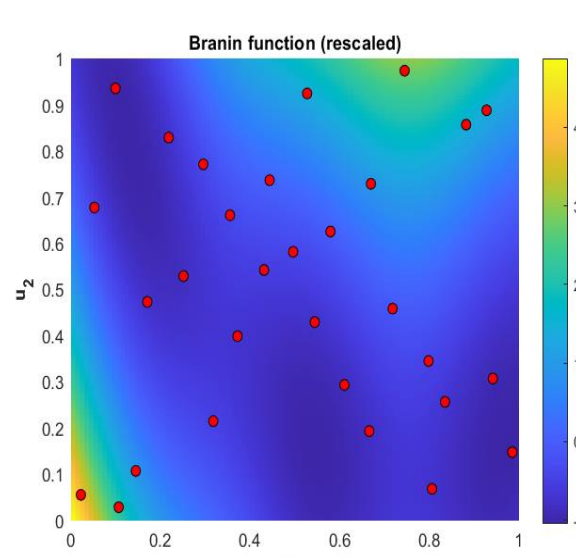
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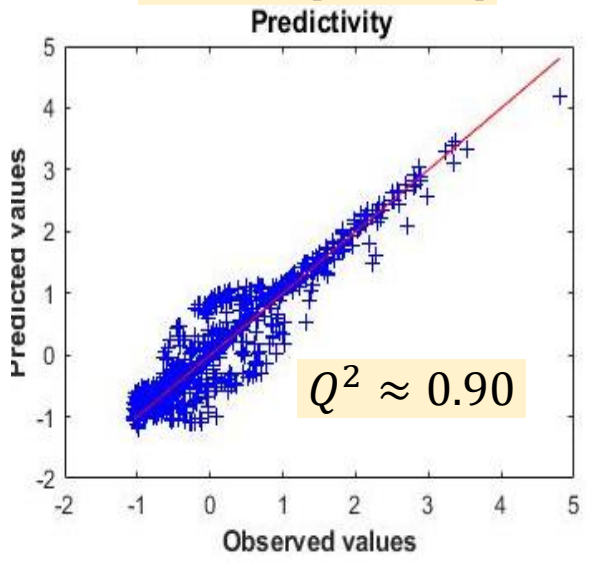


# Appendix

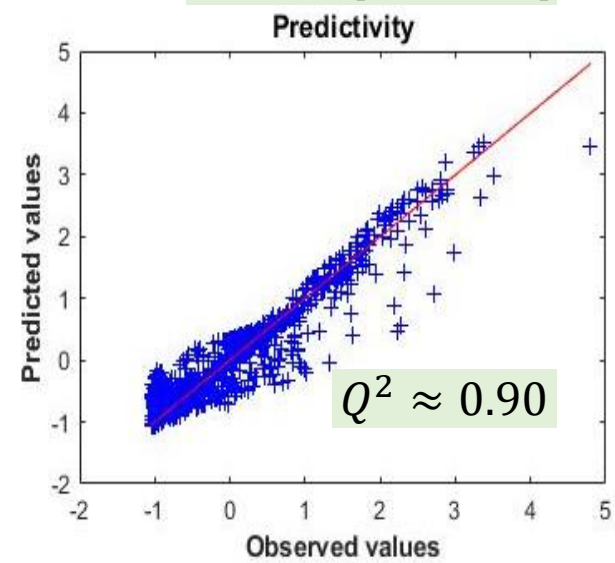
# Illustration of criteria for GPR validation [MI24a]



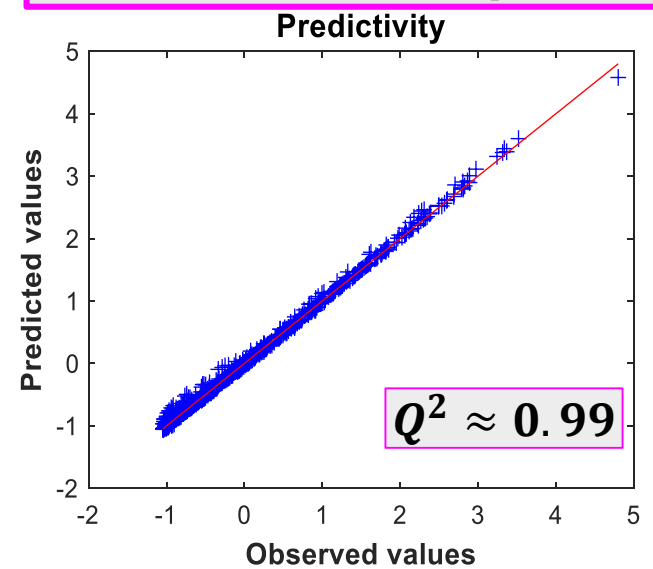
$[\theta_1, \theta_2] = [1.12 \ 0.8]$



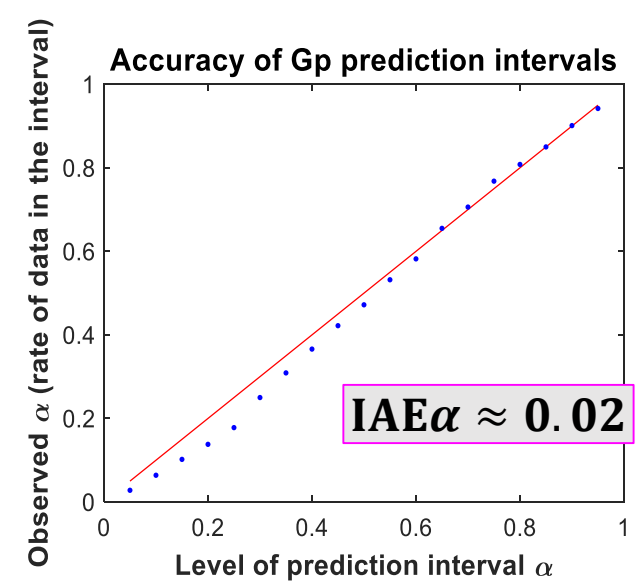
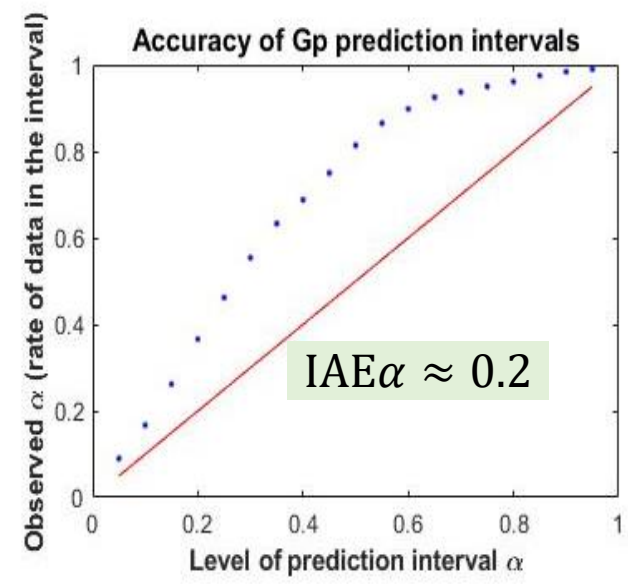
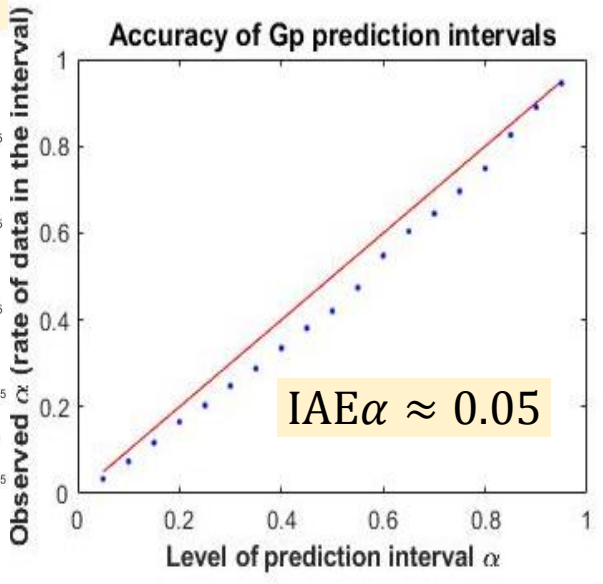
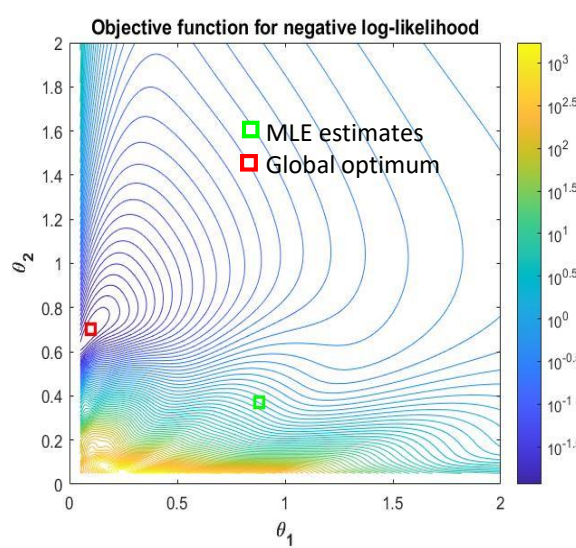
$[\theta_1, \theta_2] = [0.78 \ 0.52]$



MLE estimates:  $[\theta_1, \theta_2] = [0.88 \ 0.37]$



$n=30$ , GPR with constant mean and Gaussian covariance



# Dealing with the large input dimension

## ► HSIC-based ranking [Dav15] :

$$R_{HSIC}^2 = \frac{HSIC(X,Y)}{\sqrt{HSIC(X,X)HSIC(Y,Y)}} \Rightarrow R_{HSIC}^2 \in [0,1] \text{ for easier interpretation}$$

$$\text{Influence}(X_{[1]}) > \text{Influence}(X_{[2]}) > \dots > \text{Influence}(X_{[d]})$$

Where order  $[\cdot]$  is such that  $\hat{R}_{H,X_{[1]}}^2 > \hat{R}_{H,X_{[2]}}^2 > \dots > \hat{R}_{H,X_{[d]}}^2$

⇒ Use for ranking of inputs

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

# HSIC review: a kernel-based GSA method

►  $MMD^2$  applied between  $P_{X_i Y}$  and  $P_{X_i} \otimes P_Y \Rightarrow HSIC(X_i, Y)_{\mathcal{H}_{X_i}, \mathcal{H}_Y}$

$\mathcal{H}_{X_i}$  and  $\mathcal{H}_Y$  **RKHS** associated to  $X_i$  and  $Y$ , resp :

Kernel  $k_{X_i}: \mathcal{X}_i \times \mathcal{X}_i \rightarrow \mathbb{R}$  with feature space  $\mathcal{H}_{X_i}$  and feature map  $\varphi_{X_i}$

Kernel  $k_Y: \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$  with feature space  $\mathcal{H}_Y$  and feature map  $\varphi_Y$

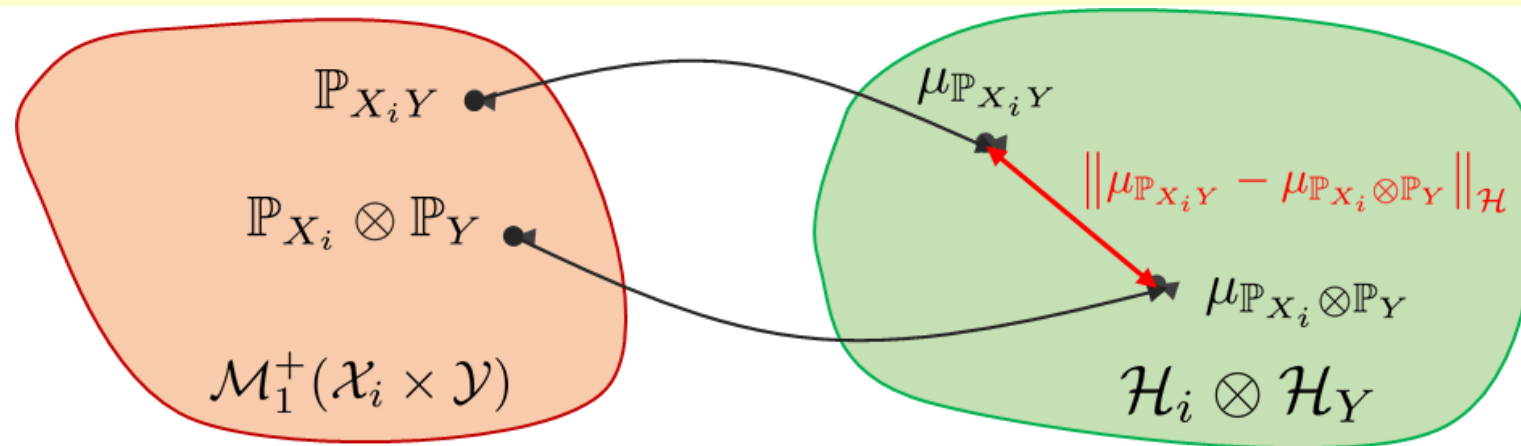
$$K_{X_i}(x, x') = \langle \varphi_{X_i}(x), \varphi_{X_i}(x') \rangle_{\mathcal{H}_{X_i}} \text{ and } K_Y(y, y') = \langle \varphi_Y(y), \varphi_Y(y') \rangle_{\mathcal{H}_Y}$$

kernel defines the inner product in the RKHS

**HSIC** = distance in the RKHS between the images of the two distributions of interest

Gretton et al. [2005]

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



Space of all probability distributions  
for the input-output pair

Tensorized RKHS

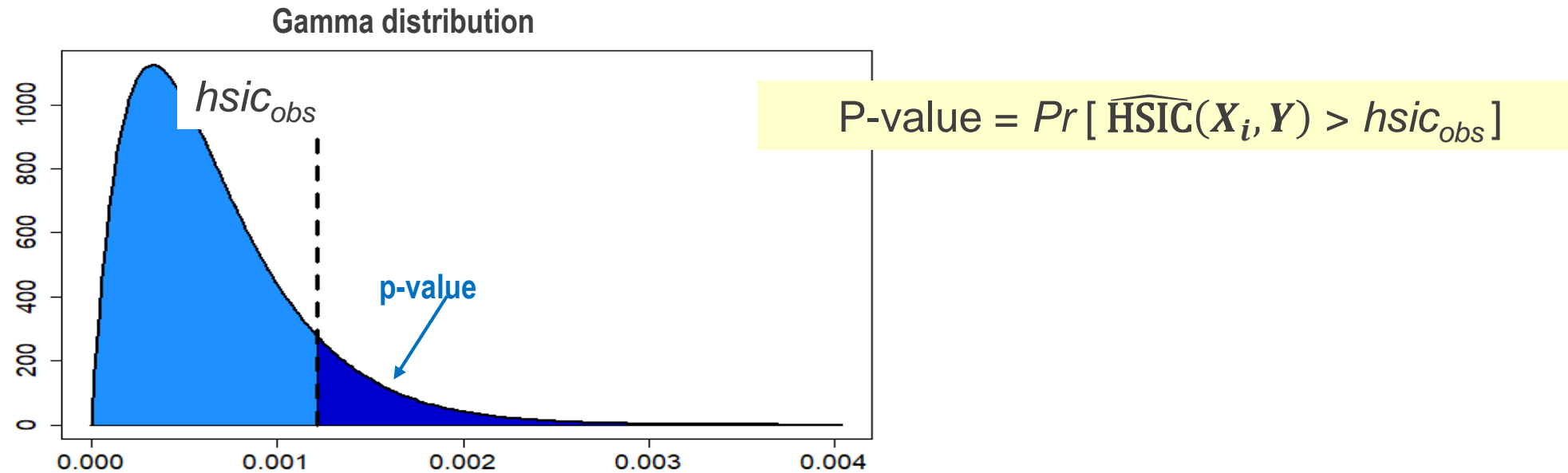
Extracted from G. Sarazin's (CEA) slides

# HSIC review: a kernel-based GSA method

## HSIC-based independence tests for screening

How to have the distribution  $n\widehat{\text{HSIC}}(X_i, Y)$  under  $\mathcal{H}_0$  to compute  $p$ -value?

- ▶ If  $n$  large: asymptotic test based on approximation with Gamma law (Gretton et al. (2008))
- ▶ If  $n$  small: Permutation-based approximation (De Lozzo & Marrel [2016a], Meynaoui [2019], El Amri & Marrel [2021a])



Interpretation of  $p$ -value for a level  $\alpha$  ( $\alpha = 5\%$  or  $10\%$ ) for screening:

- $pval < \alpha$   $\Rightarrow H_0$  (Independence) rejected  $\Rightarrow X_i$  is significantly influential