Introduction to Gaussian-process based Kriging models for metamodeling and validation of computer codes

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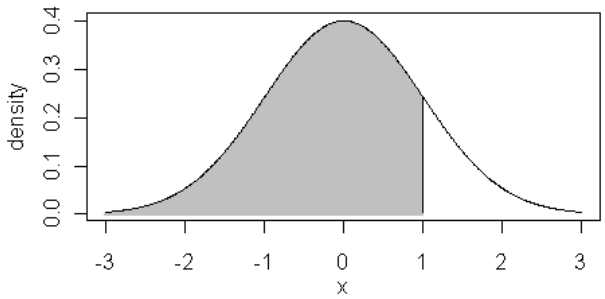
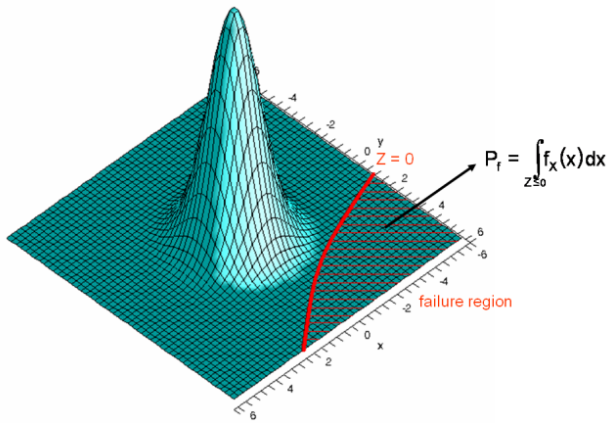
- A random Variable X is a random number, defined by a probability density function $f_X : \mathbb{R} \to \mathbb{R}^+$ for which, for $a, b \in \mathbb{R}$:

  "probability of $a \leq X \leq b$" $= \int_a^b f_X(x)dx$



- Similarly a random Vector $V = (V_1, ..., V_n)^t$ is a vector of random variables. It is also defined by a probability density function $f_V : \mathbb{R}^n \to \mathbb{R}^+$ for which, for $E \in \mathbb{R}^n$:

  "probability of $V \in E$" $= \int_E f_V(v)dv$



Remark

Naturally we have $\int_{-\infty}^{+\infty} f_X(x)dx = \int_{\mathbb{R}^n} f_V(v)dv = 1$

Mean, variance and covariance

- The mean of a random variable X with density f_X is denoted $\mathbb{E}(X)$ and is

$$\mathbb{E}(X) = \int_{-\infty}^{+\infty} x f_X(x) dx$$

- Let X be a random variable. The variance of X is denoted $var(X)$ and is

$$var(X) = \mathbb{E}\left\{(X - \mathbb{E}(X))^2\right\}$$

  - $var(X)$ is large $\rightarrow$ X can be far from its mean $\rightarrow$ more uncertainty.
  - $var(X)$ is small $\rightarrow$ X is close to its mean $\rightarrow$ less uncertainty.

- Let X, Y be two random variables. The covariance between X and Y is denoted $cov(X, Y)$ and is

$$cov(X, Y) = \mathbb{E}\left\{(X - \mathbb{E}(X))(Y - \mathbb{E}(Y))\right\}$$

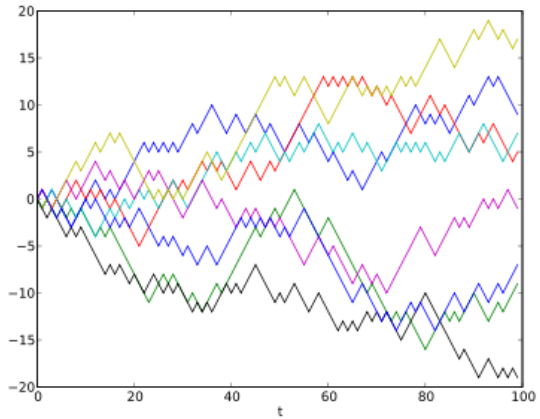
  - $|cov(X, Y)| \approx \sqrt{var(X)var(Y)} \rightarrow$ X and Y are almost proportional to one another.
  - $|cov(X, Y)| << \sqrt{var(X)var(Y)} \rightarrow$ X and Y are almost independent (when they are Gaussian).

Mean vector and covariance matrix

- Let $V = (V_1, ..., V_n)^t$ be a random vector. The mean vector of V is denoted $\mathbb{E}(V)$ and is the $n \times 1$ vector defined by
$$(\mathbb{E}(V))_i = \mathbb{E}(V_i)$$
- Let $V = (V_1, ..., V_n)^t$ be a random vector. The covariance matrix of V is denoted $cov(V)$ and is the $n \times n$ matrix defined by
$$(cov(V))_{i,j} = cov(V_i, V_j)$$
  - The diagonal terms show which components are the most uncertain.
  - The non-diagonal terms show the dependence between the components.

Stochastic processes

A stochastic process is a function $Z : \mathbb{R}^n \to \mathbb{R}$ such that $Z(x)$ is a random variable. Alternatively a stochastic process is a function on $\mathbb{R}^n$ that is unknown, or that depends of underlying random phenomena.



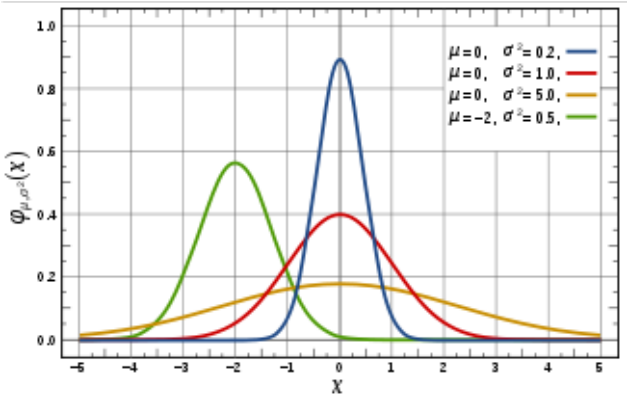
We explicit the randomness of $Z(x)$ by writing it $Z(\omega, x)$ with ω in a probability space Ω. For a given ω_0, we call the function $x \to Z(\omega_0, x)$ a realization of the stochastic process Z.

Mean function $M : x \to M(x) = \mathbb{E}(Z(x))$
Covariance function $C : (x_1, x_2) \to C(x_1, x_2) = cov(Z(x_1), Z(x_2))$

Gaussian variables and vectors

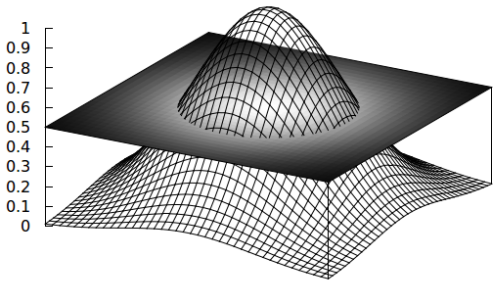
A random variable X is a Gaussian variable with mean μ and variance $\sigma^2 > 0$ when its probability density function is

$$f_{\mu,\sigma^2}(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$$



A n-dimensional random vector V is a Gaussian vector with mean vector m and invertible covariance matrix R when its multidimensional probability density function is

$$f_{m,R}(v) = \frac{1}{(2\pi)^{\frac{n}{2}}\sqrt{det(R)}} \exp\left(-\frac{1}{2}(v-m)^t R^{-1}(v-m)\right)$$



E.g. for Gaussian variables : μ and σ^2 are both parameters of the probability density function and the mean and variances of it. That is $\int_{-\infty}^{+\infty} x f_{\mu,\sigma^2}(x)dx = \mu$ and $\int_{-\infty}^{+\infty}(x-\mu)^2 f_{\mu,\sigma^2}(x)dx = \sigma^2$

Gaussian processes

A stochastic process Z on $\mathbb{R}^d$ is a Gaussian process when for all $x_1, ..., x_n$, the random vector $(Z(x_1), ..., Z(x_n))$ is Gaussian.

- A Gaussian process is characterized by its mean and covariance functions.

Why are Gaussian processes convenient ?

- Gaussian distribution is reasonable for modeling a large variety of random variables
- Gaussian processes are simple to define and simulate
- They are characterized by their mean and covariance functions
- As we will see, Gaussian properties simplify the resolution of problems
- Gaussian processes have been the most studied theoretically

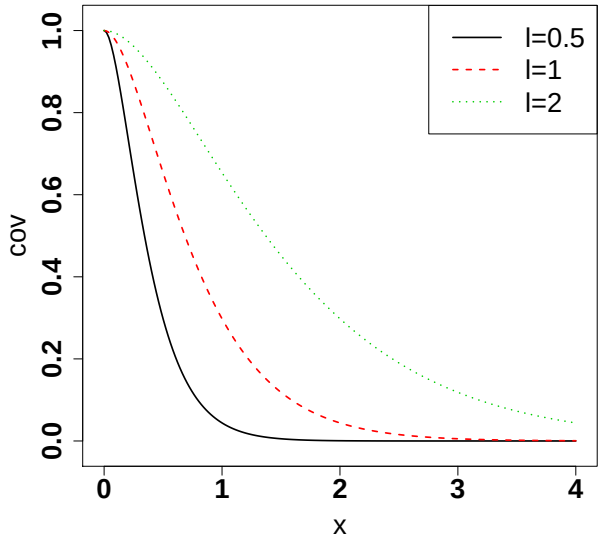
Example of the Matérn $\frac{3}{2}$ covariance function on $\mathbb{R}$

The Matérn $\frac{3}{2}$ covariance function, for a Gaussian process on $\mathbb{R}$ is parameterized by

- A variance parameter $\sigma^2 > 0$
- A correlation length parameter $\ell > 0$

It is defined as

$$C(x_1, x_2) = \left(1 + \sqrt{6}\frac{|x_1 - x_2|}{\ell}\right) e^{-\sqrt{6}\frac{|x_1 - x_2|}{\ell}}$$

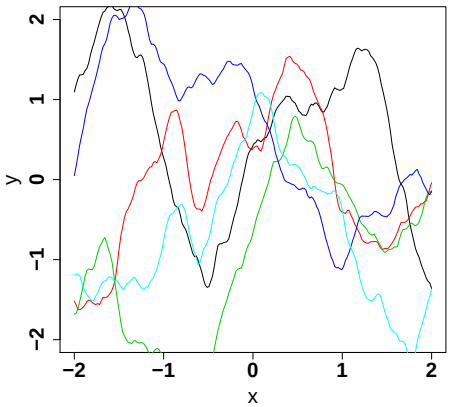


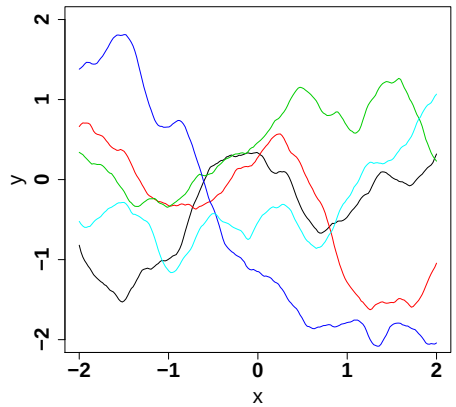
Interpretation

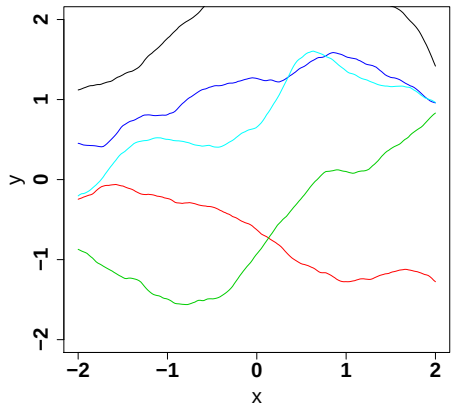
- The Matérn $\frac{3}{2}$ function is stationary : $C(x_1 + h, x_2 + h) = c(x_1, x_2) \Rightarrow$ The behavior of the corresponding Gaussian process is invariant by translation.
- σ^2 corresponds to the order of magnitude of the functions that are realizations of the Gaussian process
- ℓ corresponds to the speed of variation of the functions that are realizations of the Gaussian process

The Matérn $\frac{3}{2}$ convariance function on $\mathbb{R}$: illustration of ℓ

Plot of realizations of a Gaussian process having the Matérn $\frac{3}{2}$ covariance function for $\sigma^2 = 1$ and $\ell = 0,5, 1, 2$ from left to right







The Matérn $\frac{3}{2}$ convariance function : generalization to $\mathbb{R}^d$

We now consider a Gaussian process on $\mathbb{R}^d$.
The corresponding multidimensional Matérn $\frac{3}{2}$ convariance function is parameterized by

- A variance parameter $\sigma^2 > 0$
- d correlation length parameters $\ell_1 > 0, ..., \ell_d > 0$

It is defined as

$$C(x,y) = \left(1 + \sqrt{6}||x-y||_{\ell_1,...,\ell_d}\right) e^{-\sqrt{6}||x-y||_{\ell_1,...,\ell_d}}$$

with

$$||x-y||_{\ell_1,...,\ell_d} = \sqrt{\sum_{i=1}^{d} \frac{(x_i - y_i)^2}{\ell_i^2}}$$

Interpretation

- Still stationary
- σ^2 still drives the order of magnitudes of the realizations
- $\ell_1, ..., \ell_d$ correspond to the speed of variation of the realizations $x \to Z(\omega, x)$ when only the corresponding variable $x_1, ..., x_d$ varies.
- $\Rightarrow$ when ℓ_i is particularly small, then the variable x_i is particularly important $\Rightarrow$ hierarchy of the input variables $x_1, ...x_d$ according to their correlation lengths $\ell_1, ..., \ell_d$

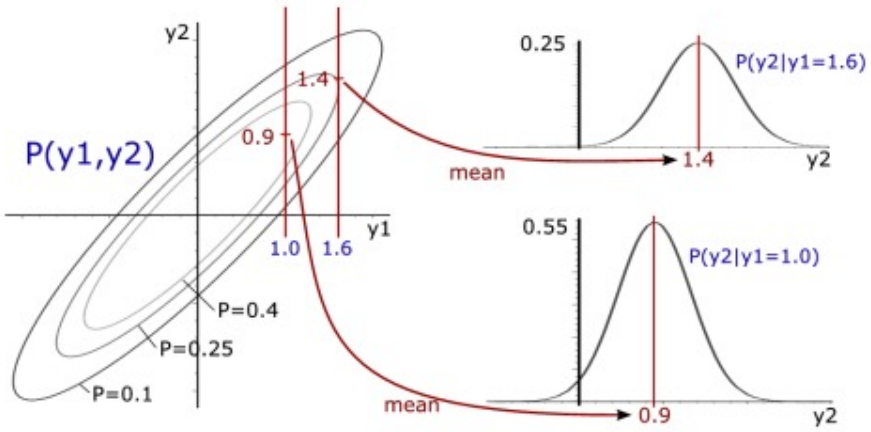
Summary

- A Gaussian process can be seen as a random phenomenon yielding realizations, i.e. specific functions $\mathbb{R}^d \to \mathbb{R}$
- The standard probability tools enable to model and quantify the uncertainty we have on these realizations
- The choice of the covariance function (e.g. Matérn $\frac{3}{2}$) enables to synthesize the information we have (get) on the nature of the realizations with a small number of parameters

Conditional probability density function

Consider a partitioned random vector $(Y_1, Y_2)^t$ of size $(n_1 + 1) \times 1$, with probability density function $f_{Y_1,Y_2} : \mathbb{R}^{n_1+1} \to \mathbb{R}^+$. Then, Y_1 has the probability density function
$f_{Y_1}(y_1) = \int_{\mathbb{R}} f_{Y_1,Y_2}(y_1, y_2) dy_2$.
The conditional probability density function of Y_2 given $Y_1 = y_1$ is then

$$f_{Y_2|Y_1=y_1}(y_2) = \frac{f_{Y_1,Y_2}(y_1, y_2)}{f_{Y_1}(y_1)}$$



Interpretation

It is the continuous generalization of the Bayes formula

$$P(A|B) = \frac{P(A, B)}{P(B)}$$

Conditional mean

Consider a partitioned random vector $(Y_1, Y_2)^t$ of size $(n_1 + 1) \times 1$, with conditional probability density function of Y_2 given $Y_1 = y_1$ given by $f_{Y_2|Y_1=y_1}(y_2)$.
Then the conditional mean of Y_2 given $Y_1 = y_1$ is

$$\mathbb{E}(Y_2|Y_1 = y_1) = \int_{\mathbb{R}} y_2 f_{Y_2|Y_1=y_1}(y_2) dy_2$$

$\mathbb{E}(Y_2|Y_1 = y_1)$ is in fact a function of Y_1. Thus it is also a random variable. We emphasize this by writing $\mathbb{E}(Y_2|Y_1)$. Thus $\mathbb{E}(Y_2|Y_1 = y_1)$ is a realization of $\mathbb{E}(Y_2|Y_1)$.

Optimality

The function $y_1 \to \mathbb{E}(Y_2|Y_1 = y_1)$ is the best prediction of Y_2 we can make, when observing only Y_1. That is, for any function $f : \mathbb{R}^{n_1} \to \mathbb{R}$:

$$\mathbb{E}\left\{(Y_2 - f(Y_1))^2\right\} \geq \mathbb{E}\left\{(Y_2 - \mathbb{E}(Y_2|Y_1))^2\right\}$$

Conditional variance

Consider a partitioned random vector $(Y_1, Y_2)^t$ of size $(n_1 + 1) \times 1$, with conditional probability density function of Y_2 given $Y_1 = y_1$ given by $f_{Y_2|Y_1=y_1}(y_2)$.
Then the conditional variance of Y_2 given $Y_1 = y_1$ is

$$var(Y_2|Y_1 = y_1) = \int_{\mathbb{R}} (y_2 - \mathbb{E}(Y_2|Y_1 = y_1))^2 f_{Y_2|Y_1=y_1}(y_2) dy_2$$

Summary

- The conditional mean $\mathbb{E}(Y_2|Y_1)$ is the best possible prediction of Y_2 given Y_1
- The conditional probability density function $y_2 \to f_{Y_2|Y_1=y_1}(y_2)$ can give the probability density function of the corresponding error ($\Rightarrow$ most probable value, probability of threshold exceedance...)
- The conditional variance $var(Y_2|Y_1 = y_1)$ summarizes the order of magnitude of the prediction error

Gaussian conditioning theorem

Theorem

Let $(Y_1, Y_2)^t$ be a $(n_1 + 1) \times 1$ Gaussian vector with mean vector $(m_1^t, \mu_2)^t$ and covariance matrix

$$\begin{pmatrix} R_1 & r_{1,2} \\ r_{1,2}^t & \sigma_2^2 \end{pmatrix}$$

Then, conditionaly on $Y_1 = y_1$, Y_2 is a Gaussian vector with mean

$$\mathbb{E}(Y_2|Y_1 = y_1) = \mu_2 + r_{1,2}^t R_1^{-1}(y_1 - m_1)$$

and variance

$$var(Y_2|Y_1 = y_1) = \sigma_2^2 - r_{1,2}^t R_1^{-1} r_{1,2}$$

Illustration

When $(Y_1, Y_2)^t$ be a 2×1 Gaussian vector with mean vector $(\mu_1, \mu_2)^t$ and covariance matrix

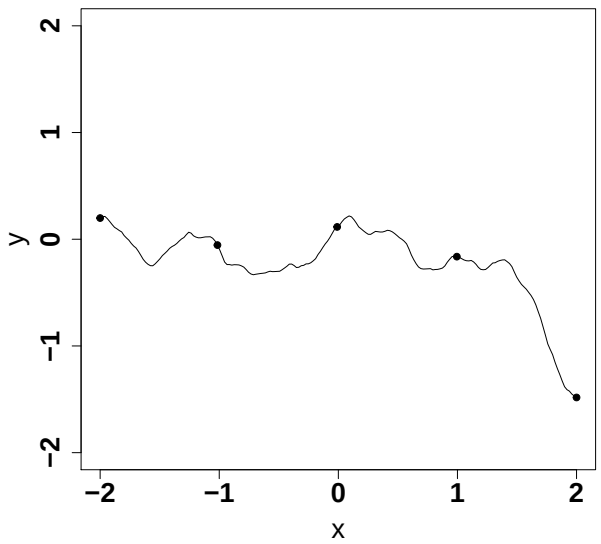
$$\begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}$$

Then

$$\mathbb{E}(Y_2|Y_1 = y_1) = \mu_2 + \rho(y_1 - \mu_1) \quad \text{and} \quad var(Y_2|Y_1 = y_1) = 1 - \rho^2$$

A problem of function approximation

We want to approximate a deterministic function, from a finite number of observed values of it.



A possibility : deterministic approximation : polynomial regression, neural networks, splines, RKHS, ...

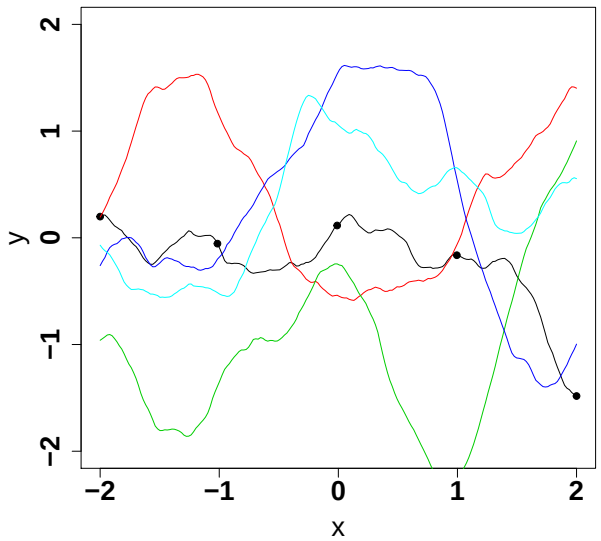
$\longrightarrow$ we can have a deterministic error bound

With a Kriging model : stochastic method

$\longrightarrow$ gives a stochastic error bound

Kriging model with Gaussian process realizations

Kriging model : representing the deterministic and unknown function by a realization of a Gaussian process.



Bayesian interpretation

In statistics, a Bayesian model generally consists in representing a deterministic and unknown number by the realization of a random variable ($\Rightarrow$ enables to incorporate expert knowledge, gives access to Bayes formula...). Here, we do the same with functions

Kriging prediction

We let Y be the Gaussian process, on $\mathbb{R}^d$. Y is observed at $x_1, ..., x_n \in \mathbb{R}^d$. We consider here that we know the covariance function C of Y, and that the mean function of Y is zero

Notations

- Let $Y_n = (Y(x_1), ..., Y(x_n))^t$ be the observation vector. It is a Gaussian vector
- Let R be the $n \times n$ covariance matrix of Y_n : $(R)_{i,j} = C(x_i, x_j)$.
- Let $x_{new} \in \mathbb{R}^d$ be a new input point for the Gaussian process Y. We want to predict $Y(x_{new})$.
- Let r be the $n \times 1$ covariance vector between y and $Y(x_{new})$: $r_i = C(x_i, x_{new})$

Then the Gaussian conditioning theorem gives the conditional mean of $Y(x_{new})$ given the observed values in Y_n :

$$\hat{y}(x_{new}) := \mathbb{E}(Y(x_{new})|Y_n) = r^t R^{-1} Y_n$$

We also have the conditional variance :

$$\hat{\sigma}^2(x_{new}) := var(Y(x_{new})|Y_n) = C(x_{new}, x_{new}) - r^t R^{-1} r$$

Exact reproduction of known values

Assume, $x_{new} = x_1$. Then , $R_{i,1} = C(x_i, x_1) = C(x_i, x_{new}) = r_i$. Thus

$$r^t R^{-1} Y_n = r^t \times \begin{pmatrix} r^t \\ * \\ \vdots \\ * \end{pmatrix}^{-1} \times \begin{pmatrix} Y(x_1) \\ \vdots \\ Y(x_n) \end{pmatrix} = (1, 0, \ldots, 0) \begin{pmatrix} Y(x_1) \\ \vdots \\ Y(x_n) \end{pmatrix} = Y(x_1)$$

Conservative extrapolation

Let x_{new} be far from $x_1, ..., x_n$. Then, we generally have $r_i = C(x_i, x_{new}) \approx 0$. Thus

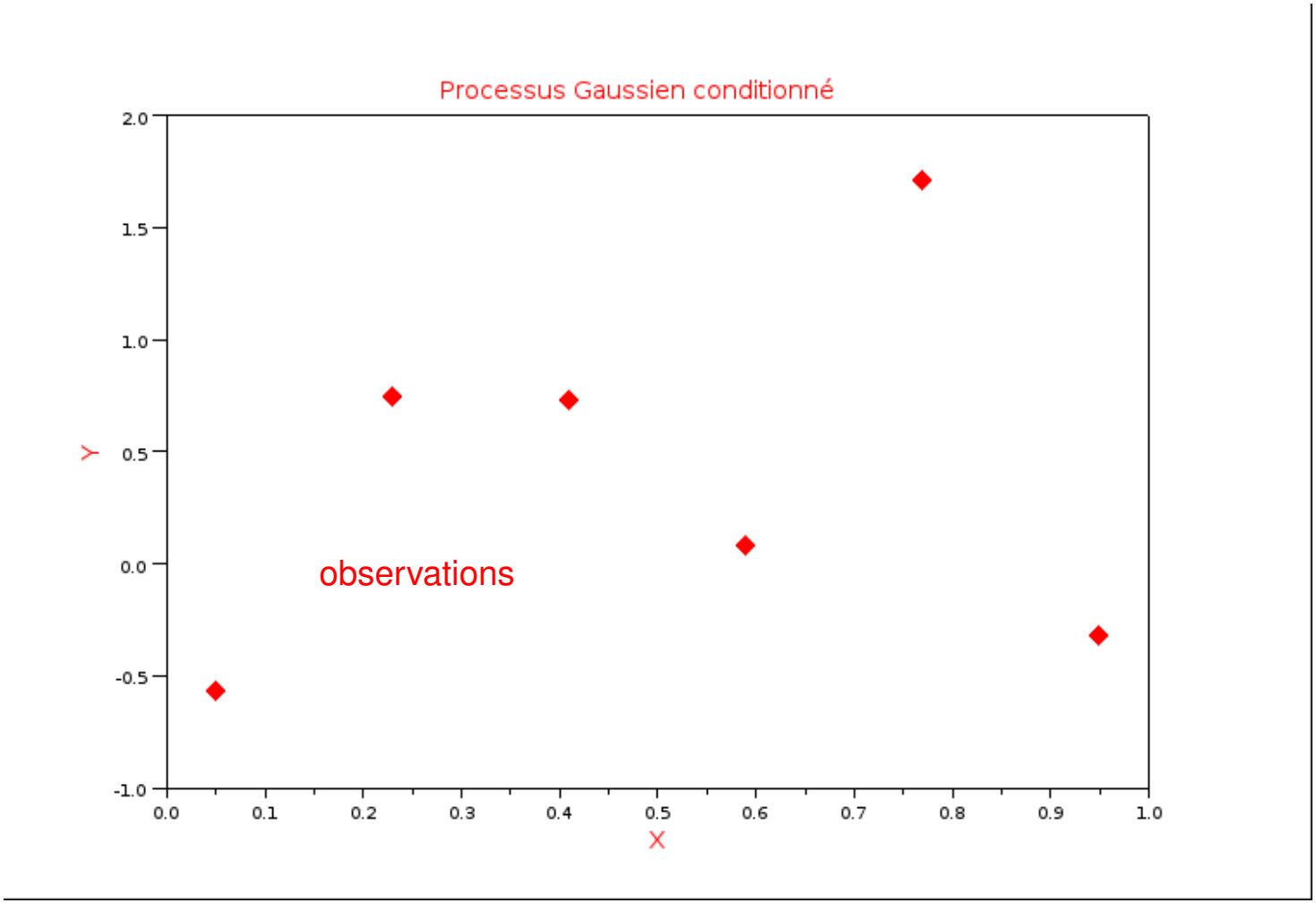
$$\hat{y}(x_{new}) = r^t R^{-1} Y_n \approx 0$$

and

$$\hat{\sigma}^2(x_{new}) = C(x_{new}, x_{new}) - r^t R^{-1} r \approx C(x_{new}, x_{new})$$

$\Rightarrow$ conservative

Illustration of Kriging prediction



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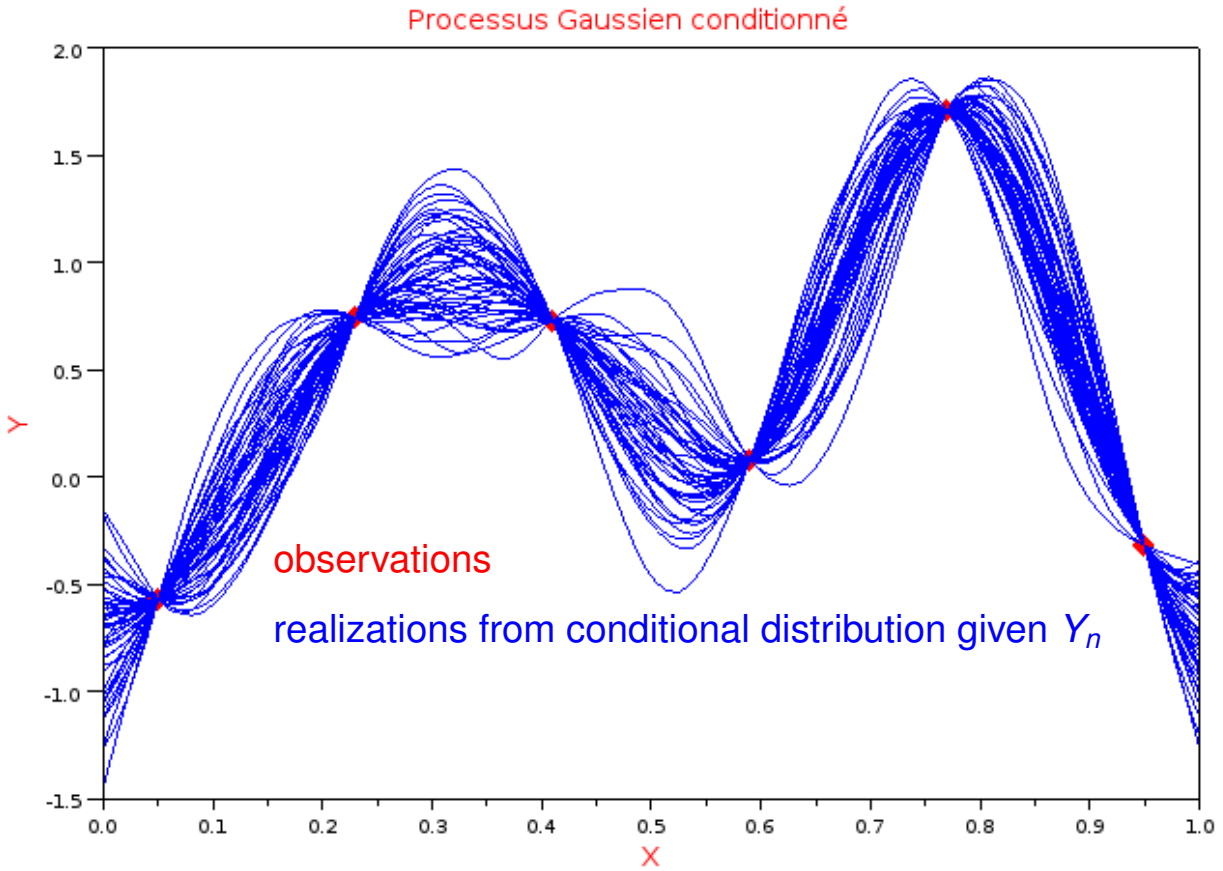

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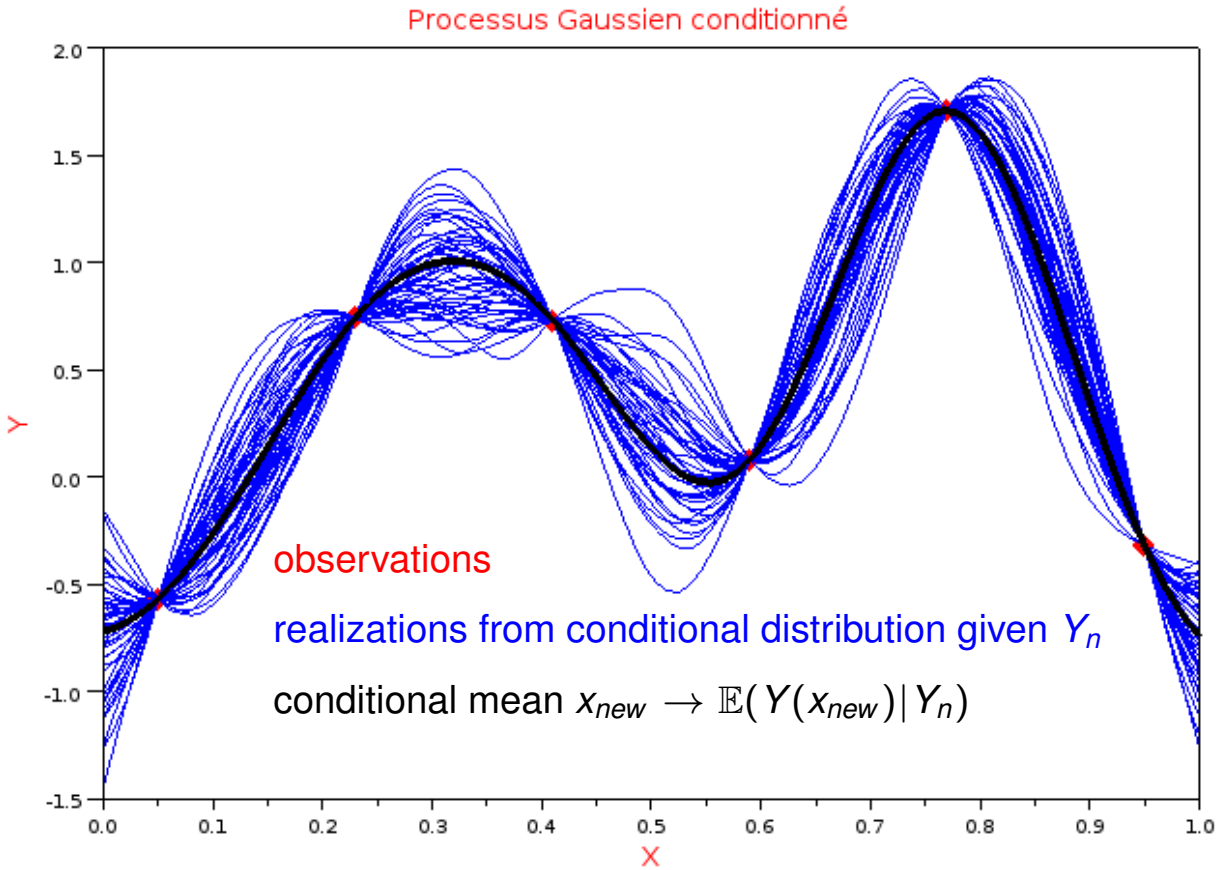

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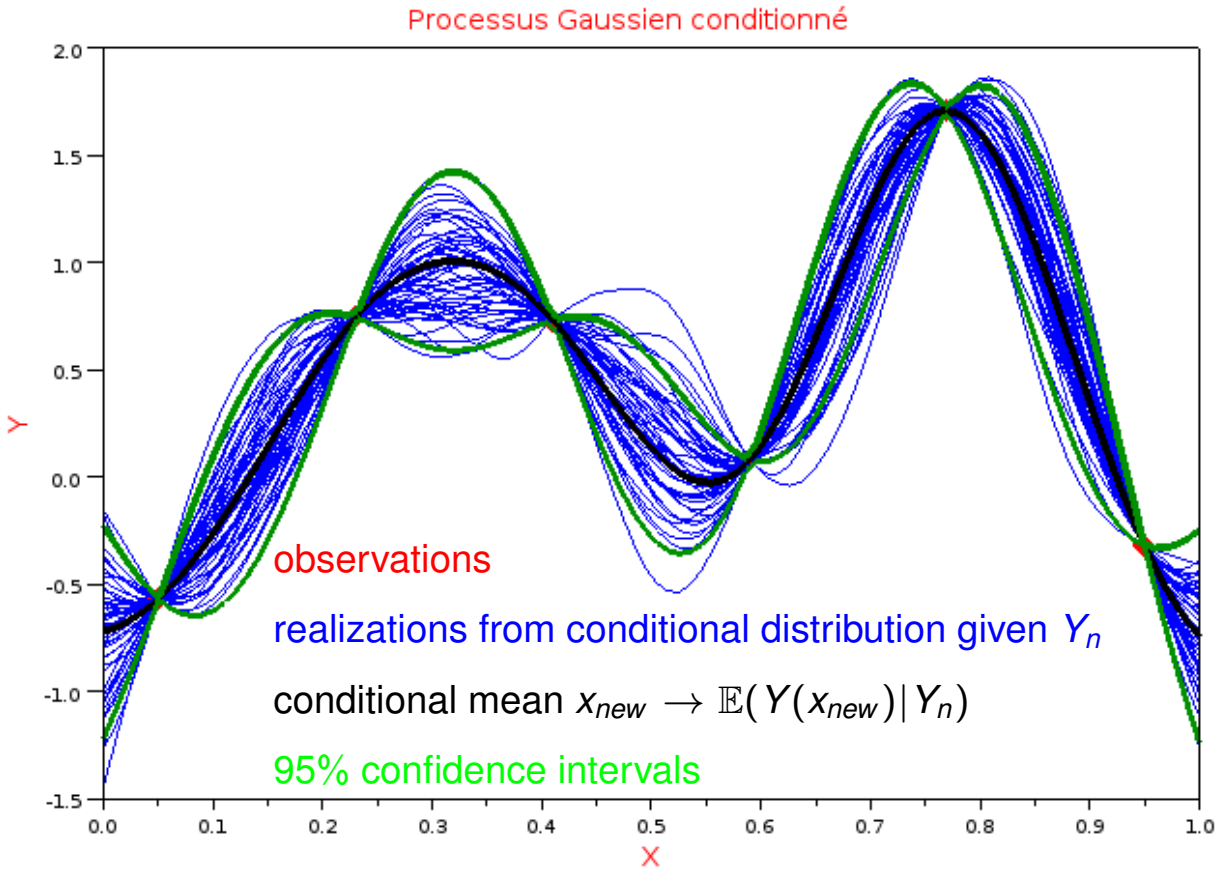


Kriging prediction with measure error

It can be desirable not to reproduce the observed value exactly :

- when the observations comes from experiments $\Rightarrow$ variability of the response for a fixed input point
- even when the response is fixed for a given input point, it can vary strongly between very close input points

Observations with measure error

We consider that at $x_1, ..., x_n$, we observe $Y(x_1) + \epsilon_1, ..., Y(x_n) + \epsilon_n$. $\epsilon_1, ..., \epsilon_n$ are independent and are Gaussian variables, with mean 0 and known variance σ^2_{mes}.

- We Let $Y_n = (Y(x_1) + \epsilon_1, ..., Y(x_n)\epsilon_n)^t$

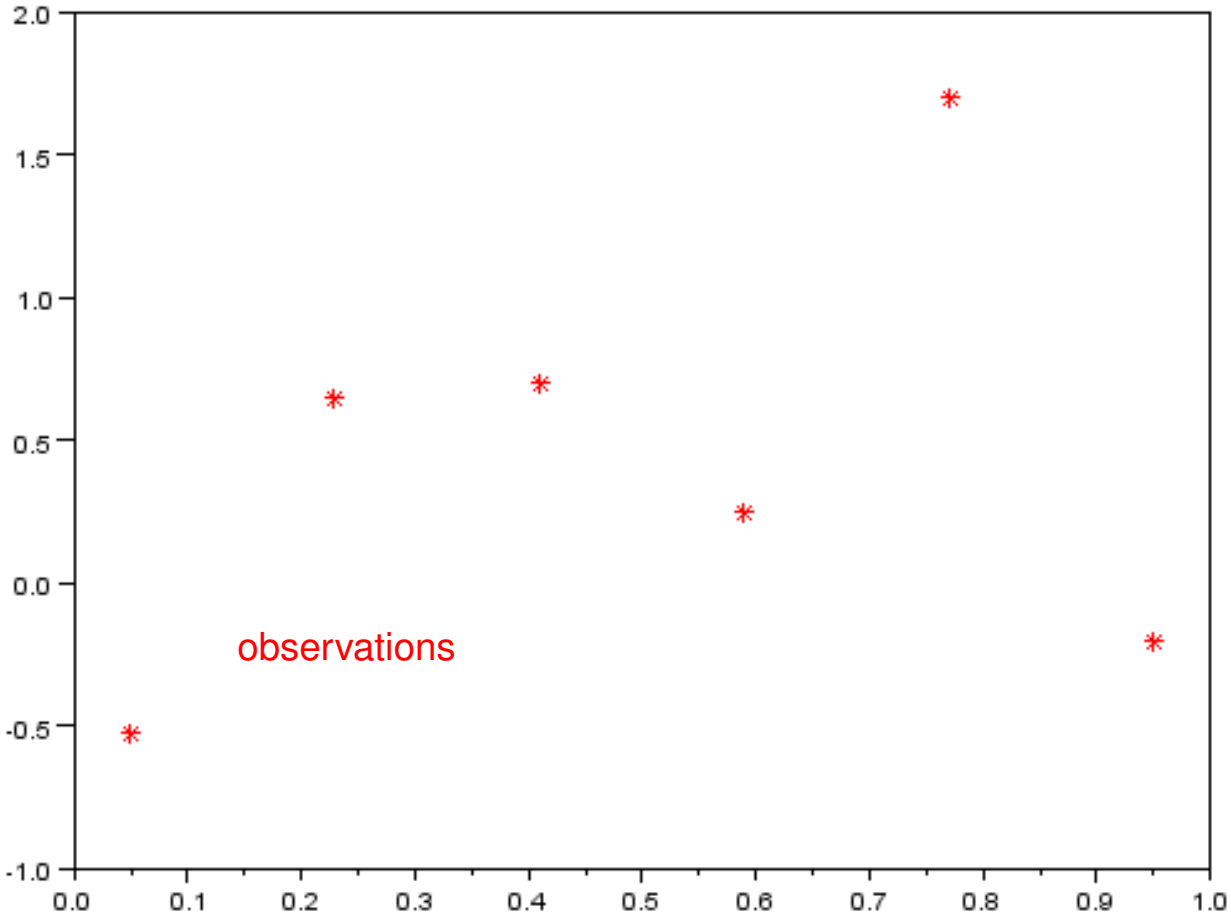
Then the Gaussian conditioning theorem still gives the conditional mean of $Y(x_{new})$ given the observed values in Y_n :

$$\hat{y}(x_{new}) := \mathbb{E}(Y(x_{new})|Y_n) = r^t(R + \sigma^2_{mes} I_n)^{-1} Y_n$$

We also have the conditional variance :

$$\hat{\sigma}^2(x_{new}) := var(Y(x_{new})|Y_n) = C(x_{new}, x_{new}) - r^t(R + \sigma^2_{mes} I_n)^{-1} r$$

Illustration of Kriging prediction with measure error



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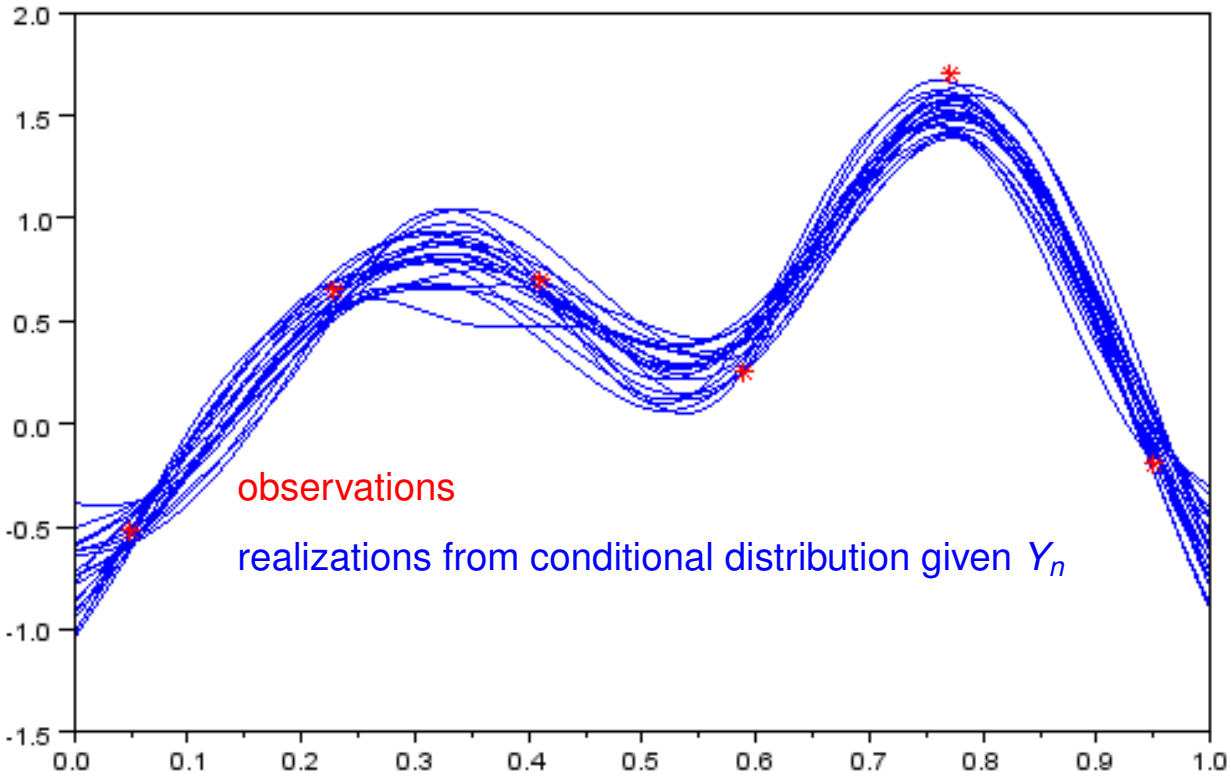

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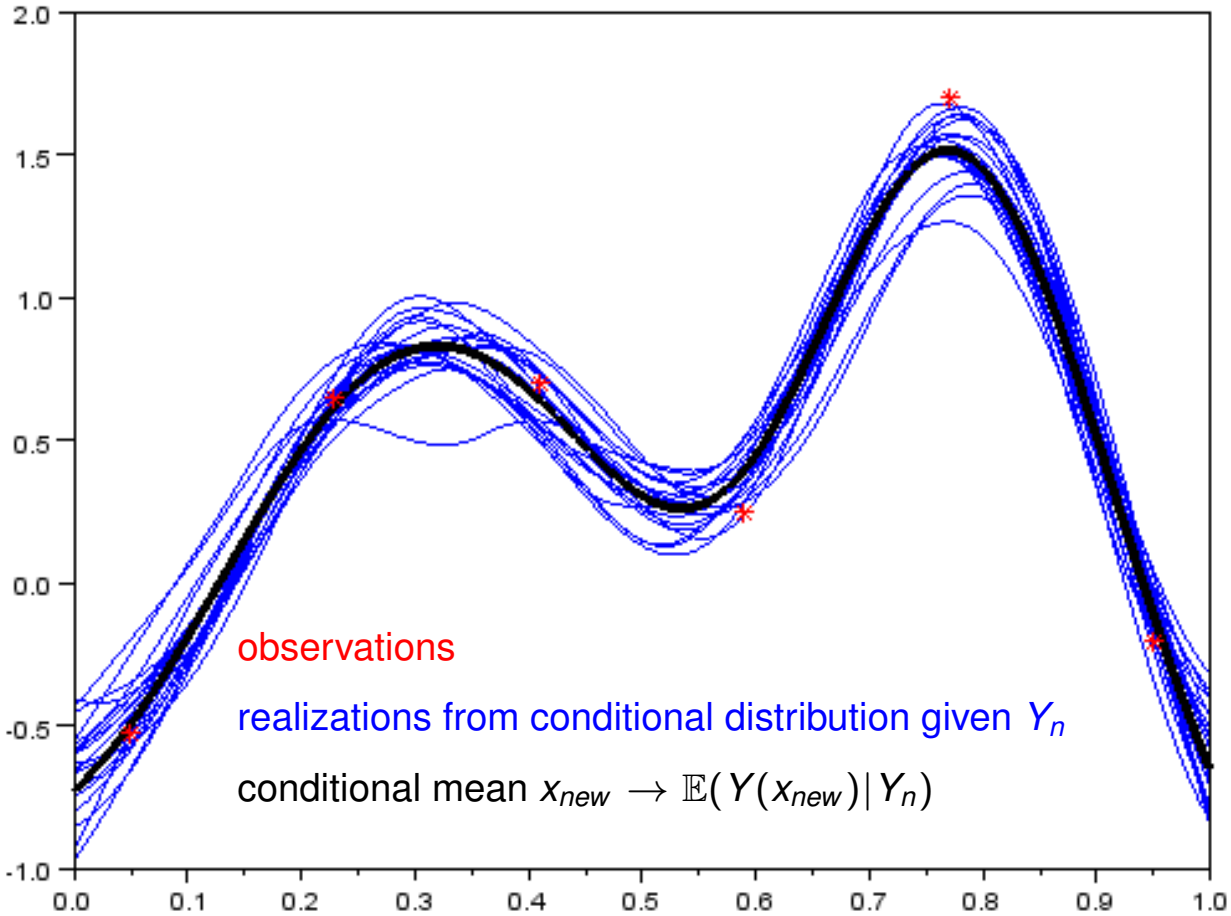

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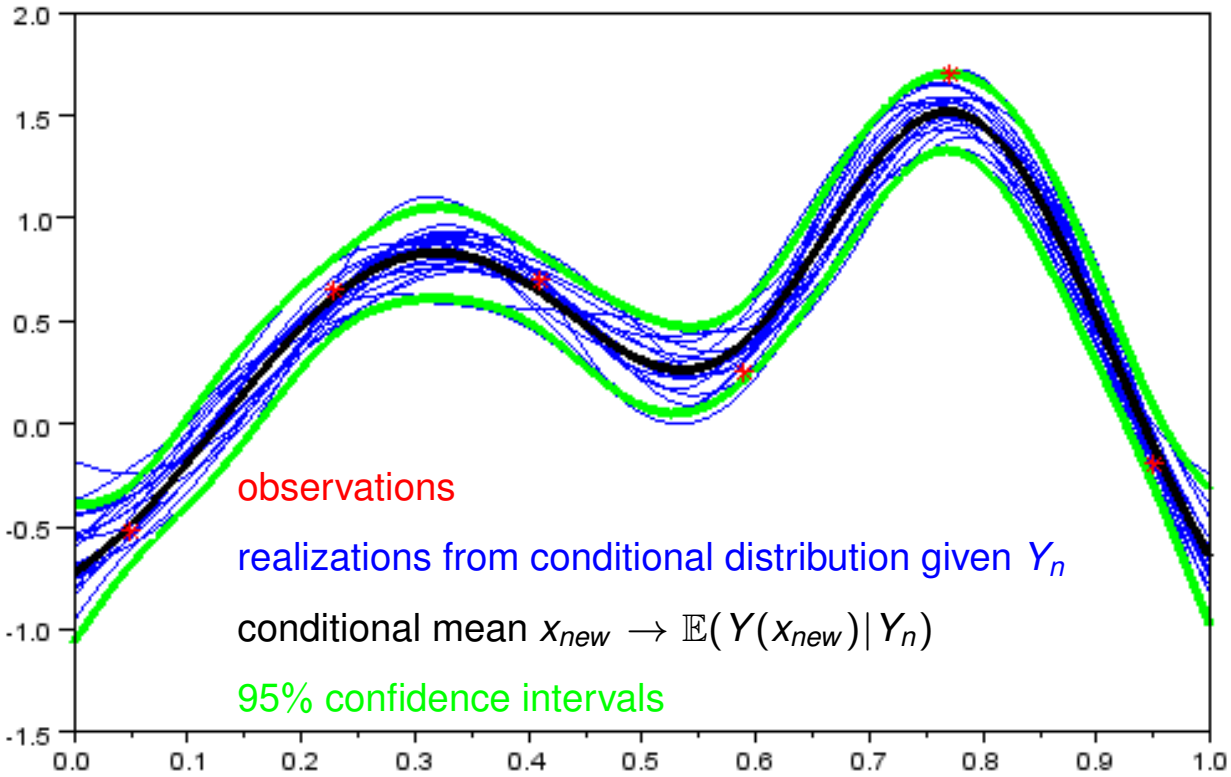


Covariance function estimation

In most practical cases, the covariance function $(x_1, x_2) \to C(x_1, x_2)$ is unknown.
It is important to choose it correctly.
In practice, it is first constrained in a parametric family of the form

$$\{C_\theta, \theta \in \Theta\}, \quad \Theta \subset \mathbb{R}^p$$

$\Rightarrow$ E.g. the multidimensional Matérn $\frac{3}{2}$ covariance function model on $\mathbb{R}^d$, with $\theta = (\sigma^2, \ell_1, ..., \ell_d)$
Then, most classically, the covariance parameter θ is automatically selected by Maximum Likelihood
In the case without measure errors :

- Let $Y_n = (Y(x_1), ..., Y(x_n))^t$ be the $n \times 1$ observation vector
- Let R_θ, be the $n \times n$ covariance matrix of Y_n, under covariance parameter θ : $(R_\theta)_{i,j} = C_\theta(x_i, x_j)$.

The Maximum Likelihood estimator $\hat{\theta}_{ML}$ of θ is then :

$$\hat{\theta}_{ML} \in \underset{\theta \in \Theta}{\operatorname{argmin}} \frac{1}{(2\pi)^{\frac{n}{2}} \sqrt{det(R_\theta)}} \exp\left(-\frac{1}{2} Y_n^t R_\theta^{-1} Y_n\right)$$

- We maximize the Gaussian probability density function of the observation vector, as a function of the covariance parameter
- Numerical optimization problem, where the cost function has a $O(n^3)$ computational cost

Summary for Kriging prediction

Most classical method :

1. From observed values gathered in the vector Y_n
2. Choose a covariance function family, parameterized by θ
   - Generally before investigating the observed values in detail and from a limited number of classical options (e.g. Matérn $\frac{3}{2}$)
3. Optimize the Maximum Likelihood criterion w.r.t $\theta \Rightarrow \hat{\theta}_{ML}$
   - Numerical optimization : gradient, quasi Newton, genetic algorithm... Potential condition-number problems
4. In the sequel, do as if the estimated covariance function $C_{\hat{\theta}_{ML}}(x_1, x_2)$ is the true covariance function (plug-in method).
5. Compute the conditional mean $x_{new} \to \mathbb{E}(Y(x_{new})|Y_n)$ and the conditional variance $x_{new} \to var(Y(x_{new})|Y_n)$ with explicit matrix vector formulas (Gaussian conditioning theorem)

1. Introduction to Gaussian processes

2. Kriging prediction
   - Conditional distribution and Gaussian conditioning theorem
   - Kriging prediction

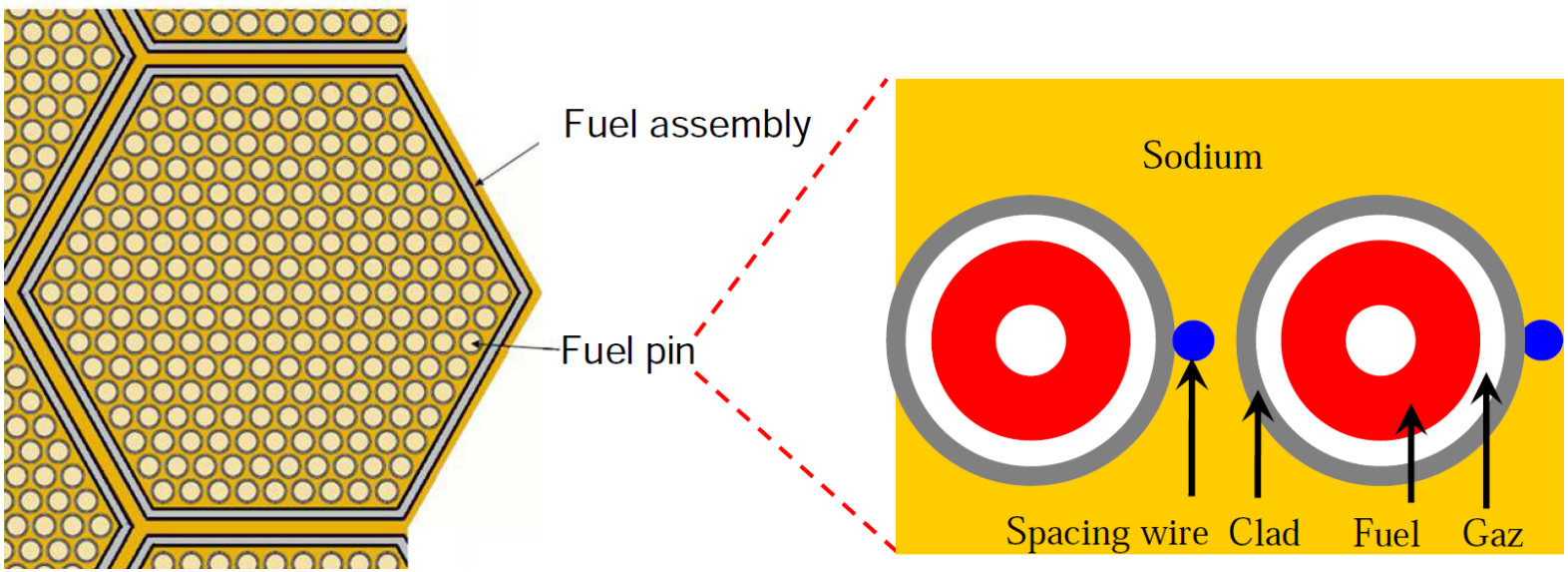
3. Application to metamodeling of the GERMINAL code

4. Application to validation of the FLICA 4 thermal-hydraulic code

GERMINAL code : presentation

Context

- GERMINAL code : simulation of the thermal-mechanical impact of the irradiation on a nuclear fuel pin
- Its utilization is part of a multi-physics and multi-objective optimization problem from reactor core design
- In collaboration with Karim Ammar (PhD student, CEA, DEN)



GERMINAL code : inputs and outputs

12 inputs $x_1, ..., x_{12} \in [0, 1]$ (normalization)

- x_1, x_2 : Schedule parameters for the exploitation of the fuel pin
- $x_3, ..., x_8$: Nature parameters of the fuel pin (geometry, plutonium concentration)
- x_9, x_{10}, x_{11} : parameters for the characterization of the power map in the fuel pin
- x_{12} : disposal volume for the fission gas produced in the fuel pin

2 scalar variable of interests

- g_1 : initial temperature. Maximum, over space, of the temperature at the initial time. Rather simple to approximate
- g_2 : fusion-margin. Minimum difference, over space and time, of the fusion temperature of the fuel and the current temperature. More difficult to approximate

general scheme

12 scalar inputs $\Rightarrow$ GERMINAL run $\Rightarrow$ spatio-temporal maps $\Rightarrow$ 2 scalar outputs

$\rightarrow$ We want to approximate 2 functions $g_1, g_2 : \mathbb{R}^{12} \rightarrow \mathbb{R}$

GERMINAL code : data bases and measure error

Data bases

For the first output g_1, we have a learning base of $n = 15722$ points (15722 couples $(x_1, g_1(x_1)), ..., (x_n, g_1(x_n))$ with $x_i \in \mathbb{R}^{12}$). We have a test base of $n_{test} = 6521$ elements.
For the second output g_2, we have $n = 3807$ and $n_{test} = 1613$

Measure errors

The GERMINAL computation scheme (GERMINAL + pre and post-treatment) had not been used for so many inputs $\rightarrow$ numerical instabilities (some very close inputs can give significantly distant outputs)
$\Rightarrow$ we incorporate the measure error parameter σ^2_{mes} to model numerical instabilities (estimated by Maximum Likelihood, together with covariance function parameters)

Metamodel

A metamodel of g is a function $\hat{g} : [0,1]^{12} \to \mathbb{R}$, that is built using the learning base only.
We consider 2 metamodels :

- The Kriging conditional mean (with Matérn $\frac{3}{2}$ covariance function and measure error variance estimated by Maximum Likelihood)
- A neural-network method, of the uncertainty platform URANIE

$\Rightarrow$ Once built, the cost of computing $\hat{g}(x_{new})$ for a new $x_{new} \in [0,1]^{12}$ is very small compared to a GERMINAL run.

Error indicator

Root Mean Square Error (RMSE) on the test base :

$$RMSE = \sqrt{\frac{1}{n_{test}} \sum_{i=1}^{n_{test}} (\hat{g}(x_{test,i}) - g(x_{test,i}))^2}$$

Results

For initial temperature g_1 (standard deviation of 344˚)

	estimated σ_{mes}	RMSE
Kriging	7.8˚	9.03˚
Neural networks		11.9˚

For Fusion Margin g_2 (standard deviation of 342˚)

	estimated σ_{mes}	RMSE
Kriging	28˚	35.9˚
Neural networks		39.7˚

- Confirmation that output g_2 is more difficult to predict than g_1
- In both cases, a significant part of the RMSE comes from the numerical instability, of order of magnitude σ_{mes}
- The metamodels have overall quite good performances (3% and 10% relative error)
- The Kriging metamodel has here comparable to slightly larger accuracy than the neural networks
- On the other hand, the neural network metamodel is significantly faster than Kriging (computational cost in $O(n)$ with n large). Nevertheless both metamodels can be considered as fast enough

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Computer code and physical system

The computer code is represented by a function f :

$$\begin{array}{rll} f & : \mathbb{R}^d \times \mathbb{R}^m & \to \mathbb{R} \\ & (x, \beta) & \to f(x, \beta) \end{array}$$

The physical system is represented by a function Y_{real}.

$$\begin{array}{rll} Y_{real} & : \mathbb{R}^d & \to \mathbb{R} \\ & x & \to Y_{real}(x) \\ Y_{obs} & : x & \to Y_{obs}(x) := Y_{real}(x) + \epsilon(x) \end{array}$$

- The inputs in x are the experimental conditions
- The inputs in β are the calibration parameters of the computer code
- The outputs $f(x, \beta)$ and $Y_{real}(x)$ are the variable of interest
- Measure error $\epsilon(x)$

Explaining discrepancies between simulation and experimental results

We have carried out experiments $Y_{obs}(x_1), ..., Y_{obs}(x_n)$. Discrepancies between simulations $f(x_i, \beta)$ and observations $Y_{obs}(x_i)$ can have 3 sources :

- misspecification of β
- measure errors on the observations $Y_{obs}(x_i)$
- Errors on the specifications of the experimental conditions x_i

$\longrightarrow$ These 3 errors can insufficient to explain the differences between simulations and experiments

Gaussian process modeling of the model error

Gaussian process model : unknown physical system $\rightarrow$ represented by a realization of a Gaussian process

$$\begin{aligned} Y_{real}(x) &= f(x,\beta) + Z(x) \\ Y_{obs}(x) &= Y_{real}(x) + \epsilon(x) \end{aligned}$$

- β : calibration parameter
  incorporation of expert knowledge with the Bayesian framework
- Z is the model error of the code. Z is modeled as the realization of a Gaussian process

Universal Kriging model

Linear approximation of the code

$$\forall x : \ f(x, \beta) = \sum_{i=1}^{m} h_i(x)\beta_i$$

$\rightarrow$ small uncertainty on β
Observations stem from a Gaussian process with linearly parameterized mean function with unknown coefficients $\Rightarrow$ universal Kriging model.

3 steps

With similar matrix vector formula and interpretation as for the 0 mean function case :

- Estimation of the covariance function of Z
- Code calibration : conditional probability density function of β
- Prediction of the physical system : conditional mean $\mathbb{E}(Y_{real}(x_{new})|Y_n)$ and conditional variance $var(Y_{real}(x_{new})|Y_n)$

Universal Kriging model : calibration and prediction formula (1/2)

Y_{real} is observed at $x_1, ..., x_n \in \mathbb{R}^d$. We consider here that we know the covariance function C of the model error Z

Notations

- Let $Y_n = (Y_{real}(x_1), ..., Y_{real}(x_n))^t$ be the observation vector. It is a Gaussian vector
- Let R be the $n \times n$ covariance matrix of $(Z(x_1), ..., Z(x_n)) : (R)_{i,j} = C(x_i, x_j)$.
- Let $x_{new} \in \mathbb{R}^d$ be a new input point for the Gaussian process Y_{real}. We want to predict $Y(x_{new})$.
- Let r be the $n \times 1$ covariance vector between $Z(x_1), ..., Z(x_n)$ and $Z(x_{new}) : r_i = C(x_i, x_{new})$
- Let H be the $n \times m$ matrix of partial derivatives of f at $x_1, ..., x_n : H_{i,j} = h_j(x_i)$
- Let h be the $m \times 1$ vector of partial derivatives of f at $X_{new} : h_i = h_i(x_{new})$
- Let σ^2_{mes} be the variance of the measure error

Then the Gaussian conditioning theorem gives the conditional mean of β given the observed values in Y_n :

$$\beta_{post} := \mathbb{E}(\beta | Y_n) = \beta_{prior} + (Q^{-1}_{prior} + H^T(R + \sigma^2_{mes} I_n)^{-1} H)^{-1} H^T (R + \sigma^2_{mes} I_n)^{-1} (Y_n - H\beta_{prior}).$$

Universal Kriging model : calibration and prediction formula (2/2)

We also have the conditional mean of $Y_{real}(x_{new})$:

$$\hat{y}_{real}(x_{new}) := \mathbb{E}(Y_{real}(x_{new})|Y_n) = h^t\beta_{post} + r^t(R + \sigma^2_{mes}I_n)^{-1}(Y_n - H\beta_{post})$$

The conditional variance of $Y_{real}(x_{new})$ is

$$\begin{aligned}\hat{\sigma}^2(x_{new}) &:= var(Y_{real}(x_{new})|Y_n) \\ &= C(x_{new}, x_{new}) - r^t(R + \sigma^2_{mes}I_n)^{-1}r \\ &\quad + (h - H^t(R + \sigma^2_{mes}I_n)^{-1}h)^t(H^t(R + \sigma^2_{mes}I_n)^{-1}H + Q^{-1}_{prior})^{-1}(h - H^t(R + \sigma^2_{mes}I_n)^{-1}r)\end{aligned}$$

Interpretation

- The prediction expression is decomposed into a calibration term and a Gaussian inference term of the model error
- When the code has a small error on the n observations, the prediction at x_{new} uses almost only the calibrated code
- The conditional variance is larger than when the mean function is known

Application to FLICA 4 thermal-hydraulic code

The experiment consists in pressurized and possibly heated water passing through a cylinder. We measure the pressure drop between the two ends of the cylinder.
Quantity of interest : The part of the pressure drop due to friction : ΔP_{fro}
Two kinds of experimental conditions :

- System parameters : Hydraulic diameter D_h, Friction height H_f, Channel width e
- Environment variables : Output pressure P_s, Flowrate G_e, Parietal heat flux Φ_p, Liquid enthalpy h_e^l, Thermodynamic title X_{th}^e, Input temperature T_e

We have 253 experimental results

Friction model of FLICA 4

Code based on the (local) analytical model

$$\Delta P_{fro} = \frac{H}{2\rho D_h} G^2 f_{iso} f_h.$$

with

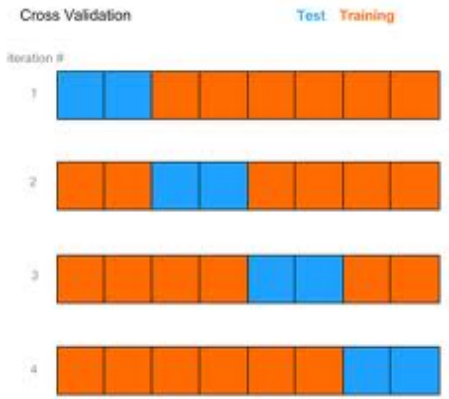
- f_{iso} : Isothermal model. Parameterized a_t and b_t.
- f_h : Monophasic model.

Prior information case with

$$\beta_{prior} = \begin{pmatrix} 0.22 \\ 0.21 \end{pmatrix}, Q_{prior} = \begin{pmatrix} 0.11^2 & 0 \\ 0 & 0.105^2 \end{pmatrix}$$

Results

We compare predictions to observations using Cross Validation



We dispose of :

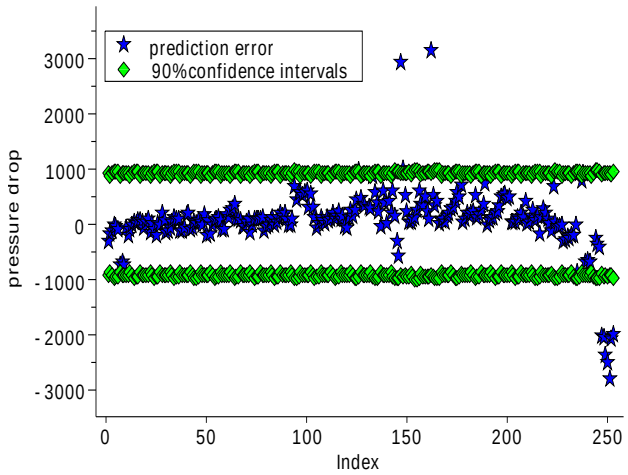
- The vector of posterior mean $\Delta\hat{P}_{fro}$ of size n.
- The vector of posterior variance σ^2_{pred} of size n.

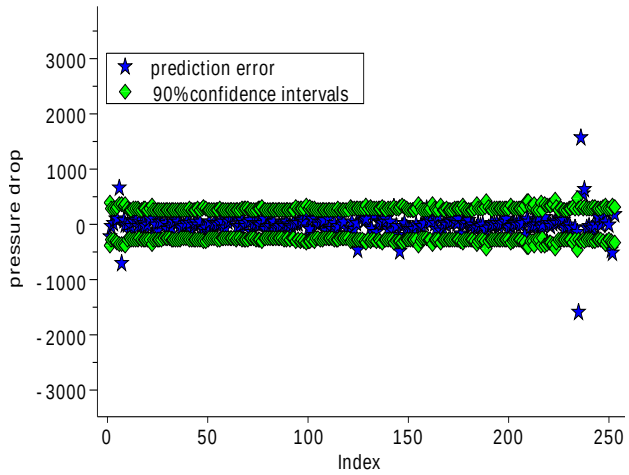
2 quantitative criteria :

- RMSE : $\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\Delta P_{fro,i} - \hat{\Delta} P_{fro}(x_i)\right)^2}$
- Confidence Interval Reliability : proportion of observations that fall in the posterior 90% confidence interval.

Results with the thermal-hydraulic code Flica IV (2/2)

	RMSE	90% Confidence Interval Reliability
Nominal code	$661Pa$	$234/253 \approx 0.925$
Gaussian Processes	$189Pa$	$235/253 \approx 0.93$





Conclusion

- We can improve the predictions of a computer code by completing it with a Kriging model built with the experimental results
- The number of experimental results needs to be sufficient. No extrapolation

For more details

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General conclusion

Standard Kriging framework

- Versatile and easy-to-use statistical model
- We can incorporate a priori knowledge in the choice of the covariance function family
- After this choice, the standard method is rather automatic
- We associate confidence intervals to the predictions
- The Gaussian framework brings numerical criteria for the quality of the obtained model

Extensions

- Kriging model can be goal-oriented : optimization, code validation, estimation of failure regions, global sensitivity analysis...
- Standard Kriging method can be computationally costly for large $n \Rightarrow$ approximate Kriging prediction and covariance function estimation is a current research domain

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Thank you for your attention !