Introduction to Gaussian process metamodel - Kriging

May 2022

Outline

Random process

Gaussian process metamodel

Conclusions

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Conclusions

Random variable and random vector

Random variable: variable whose values depend on outcome of a random phenomenon

A random variable X is a function from a set of possible outcomes Ω to a measurable space E:

$$X : \Omega \to E$$

Ω being a sample space of the probability triple $(\Omega, \mathcal{F}, \mathcal{P})$ in which:

- $\mathcal{F}$: set of events, each event contains zero or more outcomes
- $\mathcal{P}$: probability measure, assignment of probability to events

Example: rolling a fair dice, outcome ω, set of possible outcomes: six faces $\Omega = \{1, \ldots, 6\}$. Random variable X: $X = 1$ if $\omega \in \{1, 2\}$, $X = 2$ if $\omega \in \{3, 4\}$, $X = 3$ if $\omega \in \{5, 6\}$. Probabilities assigned to its values $\mathbb{P}[X = 1] = \frac{1}{3}$

Random vector: a vector of random variables

$$\boldsymbol{X} = (X_1, \ldots, X_n)$$

Random process

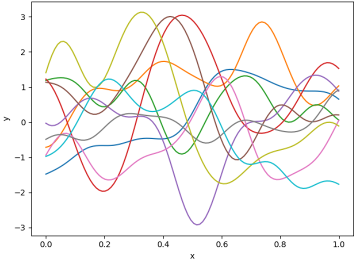
Random process Y: set of random variables indexed by x and defined in the probability space $(\Omega, \mathcal{F}, \mathcal{P})$

$$Y : \Omega \, x \, \mathcal{D} \rightarrow E$$

$\mathcal{D} \subset \mathbb{R}^d$: space of indices (e.g. spatial, temporal domains)

- At a given point $x_0 \in \mathcal{D}$, $Y(\omega, x_0)$ is a random variable.
- With a given random event $\omega_0 \in \Omega$ and index $x \in \mathcal{D}$, one obtains a function (a.k.a realization, trajectory):

$$y(\omega_0, x) : x \in \mathcal{D} \rightarrow \mathbb{R}$$



Random process

Mean:

$$\mu(x) = \mathbb{E}\left[Y(x)\right]$$

Covariance:

$$C(x, x') := C(Y(x), Y(x')) = \mathbb{E}\left[(Y(x) - m_x)(Y(x') - m_{x'})\right]$$

Stationary random process: the covariance function $C(x, x')$ depends only on $\tau = x - x'$, not on the position in the space

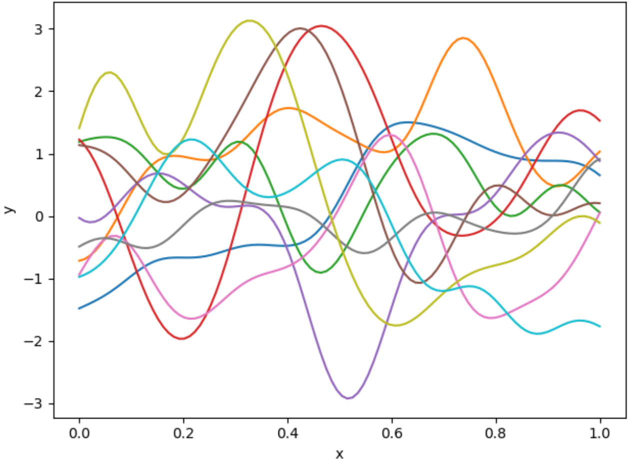
$$C(x, x') = C(x - x') = C(\tau)$$

Gaussian process: the random process $Y : \Omega \, x \, \mathcal{D} \rightarrow E$ is called a gaussian process if every finite collection of random variables is a Gaussian random vector (i.e. has a multi-variate normal distribution)

$$\forall k, \forall \{x_1, \ldots, x_k\} \in \mathcal{D}^k, \{Y(x_1), \ldots, Y(x_k)\} \sim \mathcal{N}(\mu, \boldsymbol{C}); \; \boldsymbol{C}_{ij} = C(x_i, x_j)$$

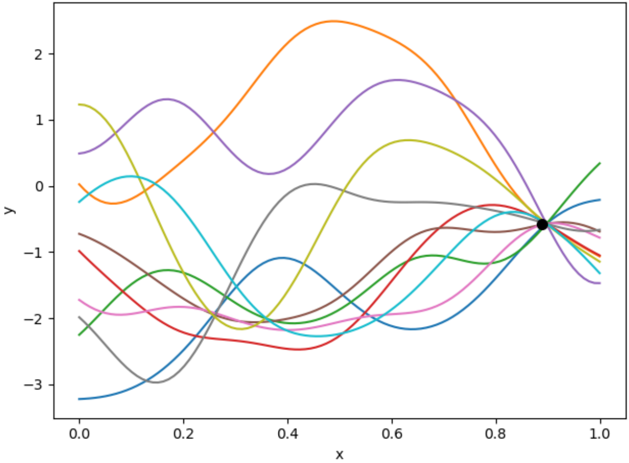
Random process

We start with a prior hypothesis on the parameterization of the mean function $\mu(x)$ and the covariance function $C(x, x')$



Random process

If we collect new data, we can update our model by forcing our process to pass through the data points



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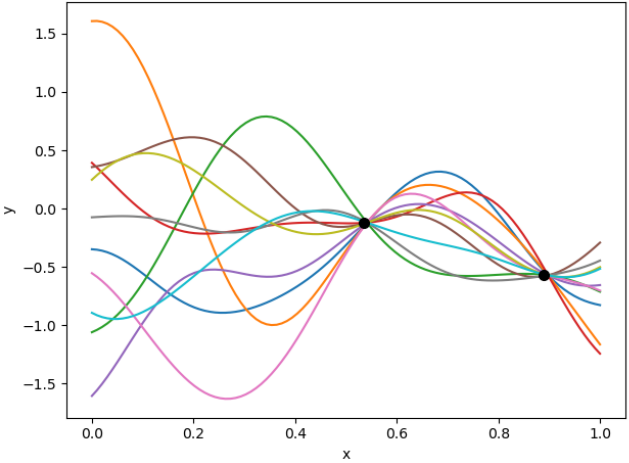

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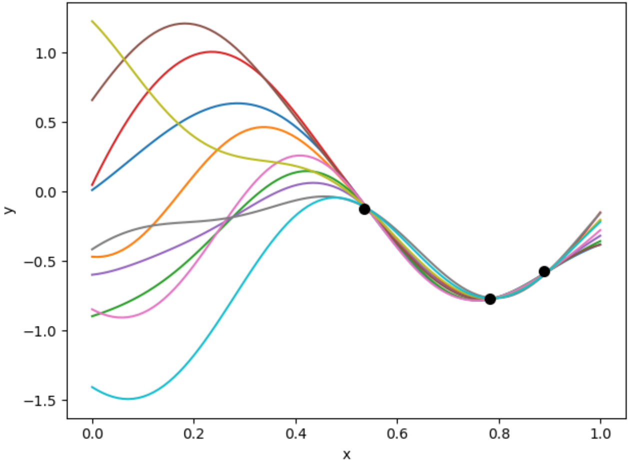

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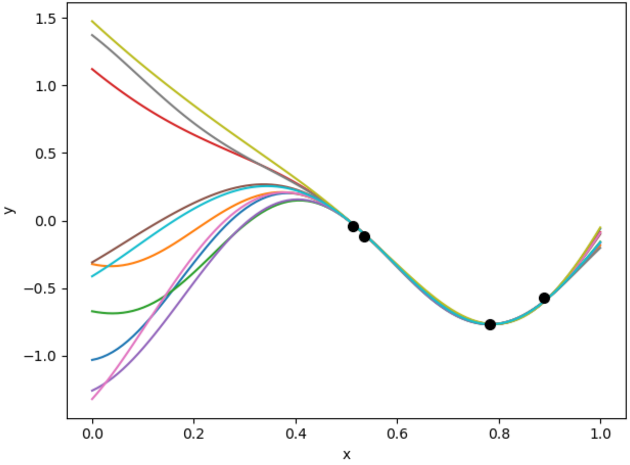

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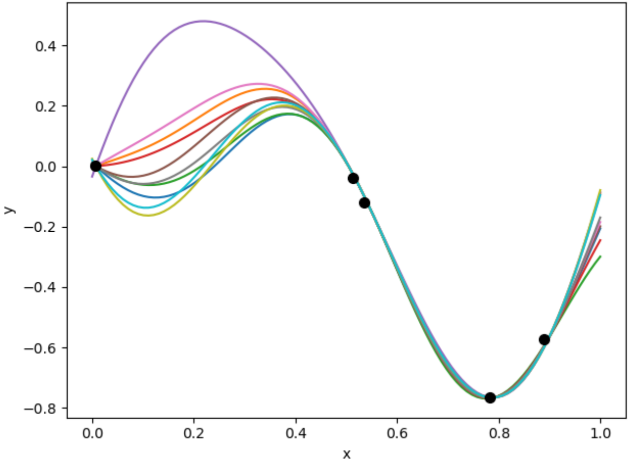


Covariance function of a stationary random process

Global form of a unidimensional covariance function (Schlather 2009):

$$C(x, x') = \delta_0 + \sigma^2 \rho\left(\frac{|x - x'|}{\theta}\right)$$

- δ_0: nugget effect
- σ^2: constant variance of the random process
- θ: correlation length

Examples of covariance functions:

Kernel	Function
Matérn	$C_\nu(\tau) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu}\lvert\tau\rvert}{\theta}\right)^\nu K_\nu\left(\frac{\sqrt{2\nu}\lvert\tau\rvert}{\theta}\right)$
Generalized exponential	$C(\tau) = \sigma^2 \exp\left(-\frac{\lvert\tau\rvert^\gamma}{\theta^\gamma}\right)$
Squared exponential	$C(\tau) = \sigma^2 \exp\left(-\frac{1}{2}\frac{\lvert\tau\rvert^2}{\theta^2}\right)$

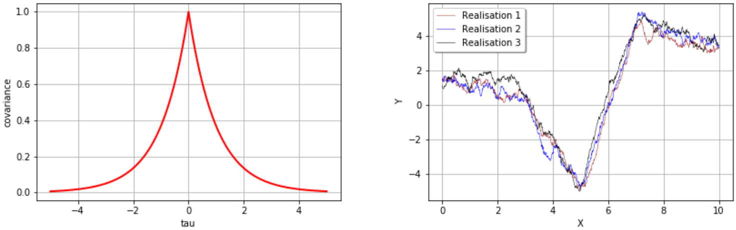
Covariance function

The regularity of the process is determined by the differentiability of $C(\tau)$ at $\tau = 0$.

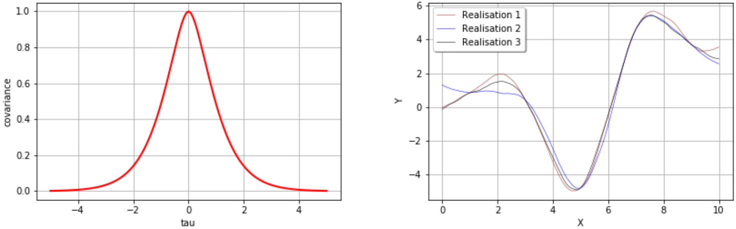
For stationary processes, the trajectories $y(x)$ are p-times differentiable if $C(\tau)$ is $2p$ times differentiable at $\tau = 0$.

ν	Matérn covariance function
$\nu = 1/2$	$C_{1/2}(\tau) = \sigma^2 exp(-\frac{\lvert\tau\rvert}{\theta})$
$\nu = 3/2$	$C_{3/2}(\tau) = \sigma^2 \left(1 + \frac{\sqrt{3}\lvert\tau\rvert}{\theta}\right) exp(-\frac{\sqrt{3}\lvert\tau\rvert}{\theta})$
$\nu = 5/2$	$C_{5/2}(\tau) = \sigma^2 \left(1 + \frac{\sqrt{5}\lvert\tau\rvert}{\theta} + \frac{5\lvert\tau\rvert^2}{3\theta^2}\right) exp(-\frac{\sqrt{5}\lvert\tau\rvert}{\theta})$

Covariance function

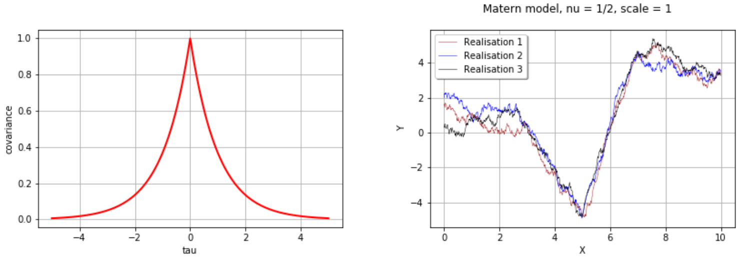


$\nu = 1/2$

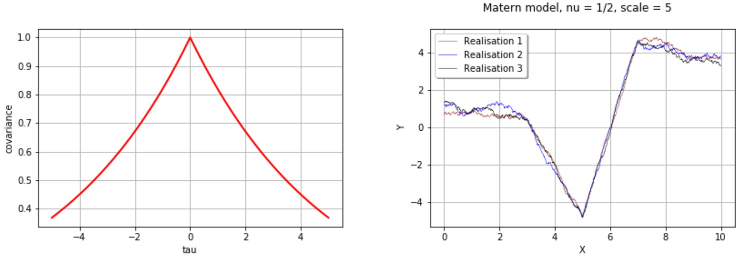


$\nu = 3/2$

Covariance function

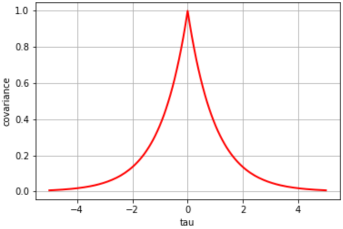


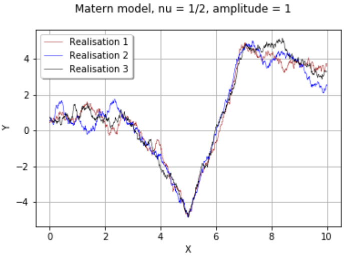
$\rho = 1$



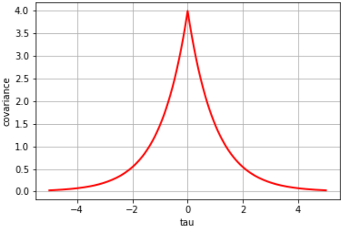
$\rho = 5$

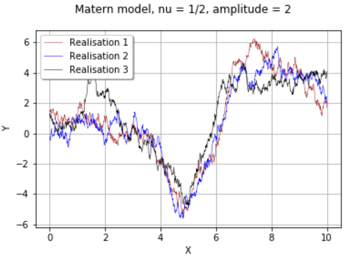
Covariance function





$\sigma = 1$

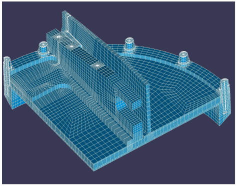


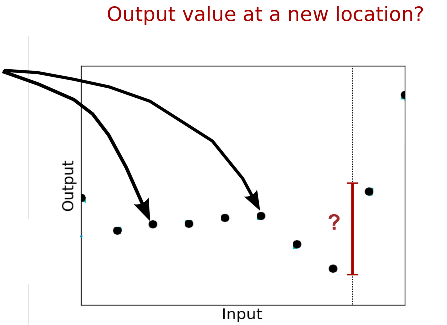


$\sigma = 2$

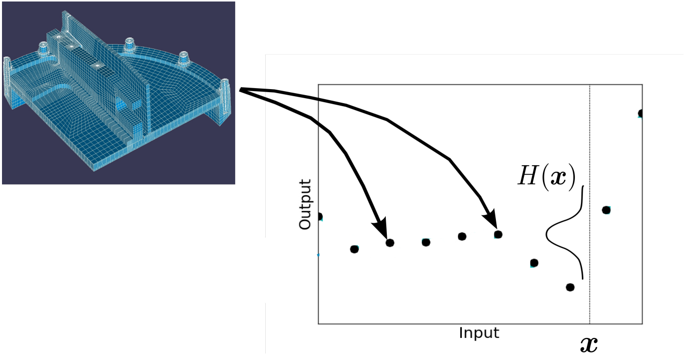
Outline

Prediction at a new point





Prediction at a new point



Assumption: The response is a realization of a Gaussian random variable whose moments depend on the design points

Gaussian process assumption

The model output is a realization of a Gaussian random process of the form :

$$Y(\boldsymbol{x}, \omega) = \boxed{\boldsymbol{r}(\boldsymbol{x}) \cdot \boldsymbol{\beta}} + \boxed{Z(\boldsymbol{x}, \omega)}$$

Trend (deterministic)

Linear regression
on a fixed basis

Random fluctuations

Gaussian process
with zero mean and
stationary

$$\mathbb{C}\mathrm{ov}_Z(\boldsymbol{x}, \boldsymbol{x}') = \sigma^2 \rho(\|\boldsymbol{x} - \boldsymbol{x}'\|)$$

Kriging

Conditional mean and variance

Experimental design: $\mathcal{X} = \left\{ \boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(N)} \right\}$

$\mathcal{Y} = \left\{ Y(\boldsymbol{x}^{(1)}), \ldots, Y(\boldsymbol{x}^{(N)} \right\}$

Notations: $\boldsymbol{k}(\boldsymbol{x}^*) \equiv \left\{ \rho\left(\boldsymbol{x}^*, \boldsymbol{x}^{(1)}\right), \ldots, \rho\left(\boldsymbol{x}^*, \boldsymbol{x}^{(N)}\right) \right\}^{\mathsf{T}}$

$$\boldsymbol{R} \equiv \left(r_j(\boldsymbol{x}^{(i)}) \right)_{1 \le i \le N, 1 \le j \le p} \quad , \quad \boldsymbol{K} \equiv \left(\rho(\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)}) \right)_{1 \le i,j \le N}$$

Conditional mean: $\boxed{\mu(\boldsymbol{x}^*) = \boldsymbol{r}^{\mathsf{T}}(\boldsymbol{x}^*)\boldsymbol{\beta} + \boldsymbol{k}^{\mathsf{T}}(\boldsymbol{x}^*)\boldsymbol{K}^{-1}\left(\mathcal{Y} - \boldsymbol{R}\boldsymbol{\beta}\right)}$

Conditional variance: $\boxed{\sigma^2(\boldsymbol{x}^*) = \sigma^2 - \boldsymbol{k}^{\mathsf{T}}(\boldsymbol{x}^*)\,\boldsymbol{K}^{-1}\,\boldsymbol{k}^{\mathsf{T}}(\boldsymbol{x}^*) - \boldsymbol{U}(x^*)^{\mathsf{T}}\,\boldsymbol{F}\,\boldsymbol{U}(x^*)}$

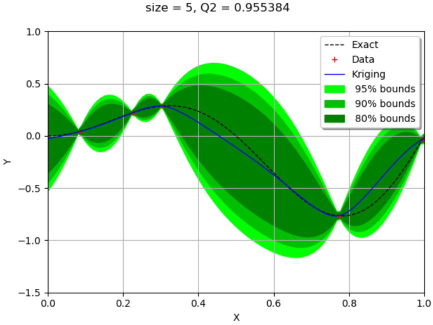
with $\boldsymbol{F} = (\boldsymbol{R}^{\mathsf{T}}\boldsymbol{K}^{-1}\boldsymbol{R})^{-1}$, $\boldsymbol{U}(x^*) = \boldsymbol{R}^t K^{-1}\boldsymbol{k}(x^*) - \boldsymbol{r}(x^*)^t$

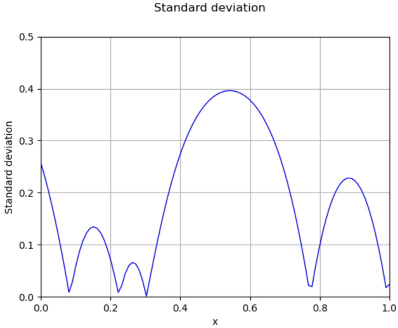
Conditional mean and variance

Consider an instructive model: $y = f(x) = x\sin(x)$

Gaussian process metamodel:

$$H(x,\omega) \;=\; \boldsymbol{r}(x)\cdot\boldsymbol{\beta} \;+\; Z(x,\omega) \qquad , \qquad \mathbb{C}\mathrm{ov}_Z(x,x') \;=\; \sigma^2 e^{-\theta(x-x')^2}$$





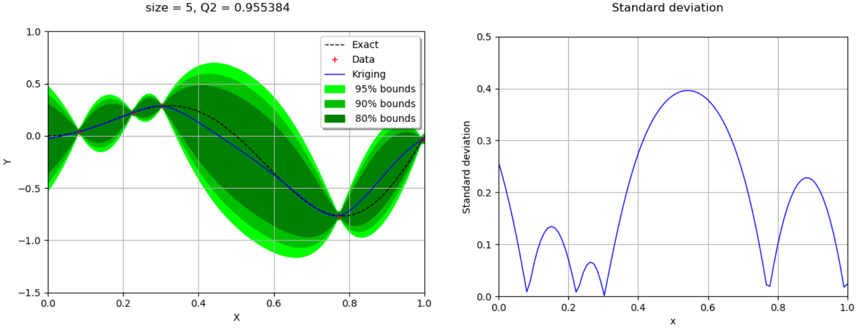
- The conditional mean is used as a metamodel (interpolator)
- The conditional variance is used as an error indicator

Parameter fitting

To apply the previous formulas, the parameters $(\boldsymbol{\beta}, \sigma, \boldsymbol{\theta})$ have to be estimated from the design points

- Optimal correlation parameter $\hat{\boldsymbol{\theta}}$ estimated by the maximum likelihood estimate (Marrel et al. 2008) or cross validation (Bachoc 2013)
- Parameters $(\hat{\boldsymbol{\beta}}, \hat{\sigma})$ estimated by empirical best linear unbiased estimator (BLUE) (Santner et al. 2003)

Sequential enrichment of the experimental design



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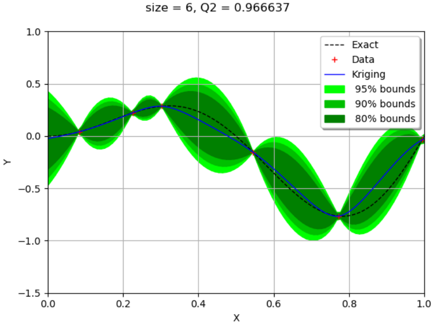

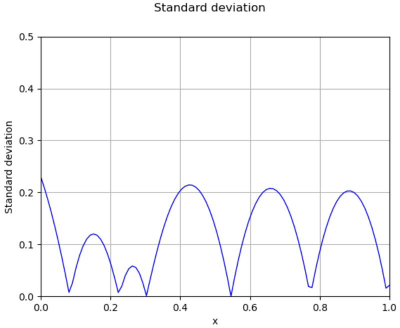

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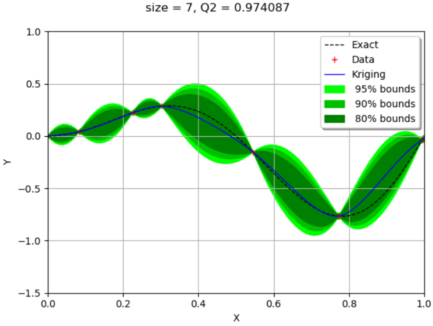

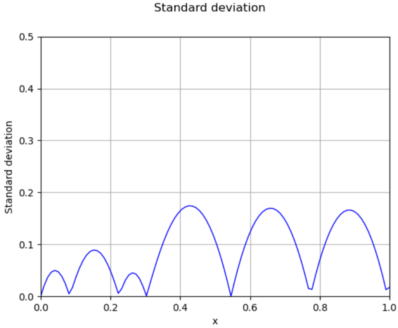

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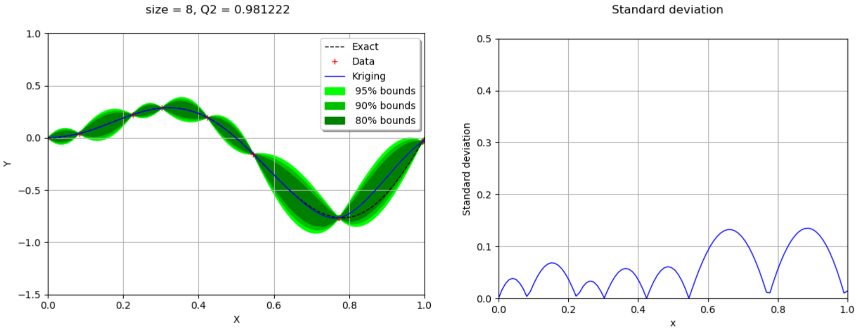

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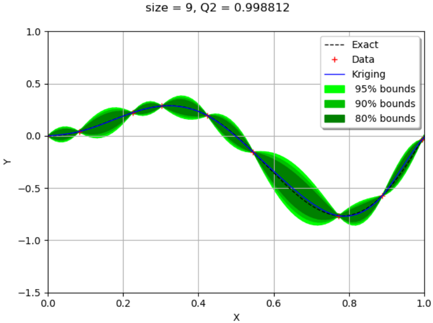

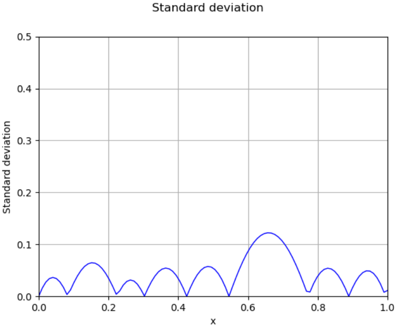

Sequential enrichment of the experimental design

Alternative and more complex enrichment strategies exist, allowing to define optimal surrogate models for different purposes:

- Optimization
- Inversion (identification of critical areas)
- Global model exploration

Additionally, when dealing with computationally intensive but parallelizable codes, some of these criteria can be extended in order to define batches of enrichment points to be evaluated

Some limitations and drawbacks

The standard GP formulation relies on several hypotheses:

- The covariance function is stationary (only depend on $\tau = |x - x'|$)
- The covariance function is continous

$\rightarrow$ Gaussian processes are not suited to model non-stationary and/or non continuous functions

- The evaluation of the likelihood requires the inversion of an $n \times n$ covariance matrix (n being the training data set size)

$\rightarrow$ The training computational cost becomes large at around $n = 1000$

Some variants of this surrogate model exist in order to partially avoid these issues

Outline

Gaussian process metamodel

- The regularity of the trajectories depends on the choice of covariance function
- Kriging allows to associate a measure of certainty to a prediction of the function
- Kriging allows the effective sequential enrichment of the experimental design

Thank you