

Introduction to Gaussian process metamodel - Kriging

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Outline

Random process

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Conclusions

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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 :

$$X : \Omega \rightarrow E$$

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 $\Omega = \{1, \dots, 6\}$. 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

$$\mathbf{X} = (X_1, \dots, X_n)$$

Random process

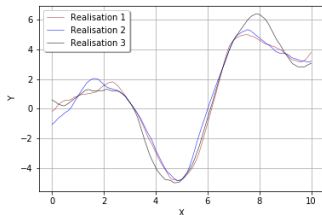
Random process Y : set of random variables indexed by x and defined in the probability space $(\Omega, \mathcal{F}, \mathcal{P})$

$$Y : \Omega \times \mathcal{D} \rightarrow E$$

$\mathcal{D} \subset \mathbb{R}^d$: 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 realisation, trajectory):

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



Random process

Mean:

$$\mu_x = \mathbb{E}[Y(x)]$$

Covariance:

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

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 $Y : \Omega \times \mathcal{D} \rightarrow E$ 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)

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

Covariance function of a stationary random process

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

$$C(x, x') = C_0 + v \rho\left(\frac{|x - x'|}{l}\right)$$

- ▶ C_0 : nugget effect
- ▶ v : constant variance of the random process
- ▶ l : correlation length

Examples of covariance functions:

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

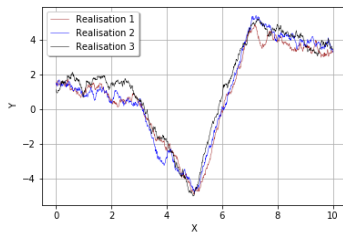
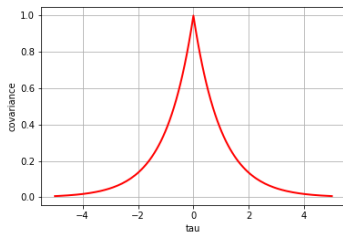
Covariance function

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

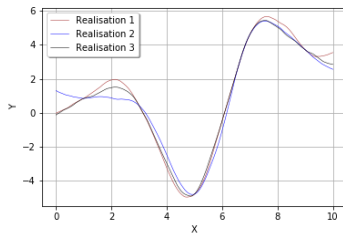
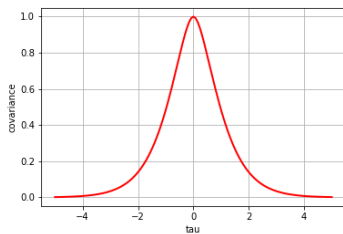
For stationary processes, the trajectories $y(x)$ are p -times differentiable if $C(\tau)$ is $2p$ times differentiable at $\tau = 0$.

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

Covariance function

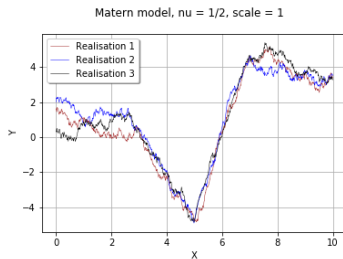
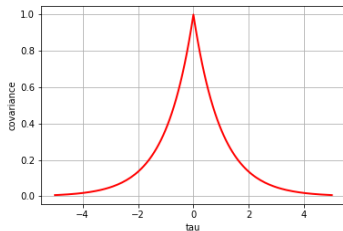


$$\nu = 1/2$$

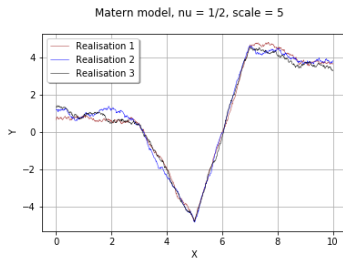
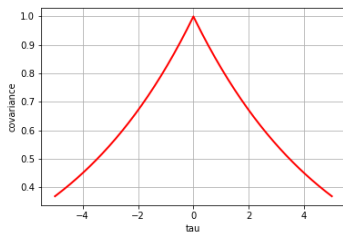


$$\nu = 3/2$$

Covariance function

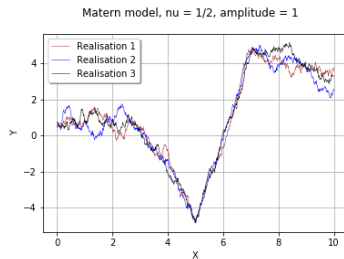
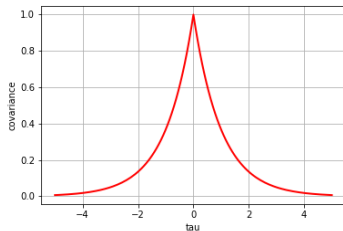


$$\rho = 1$$

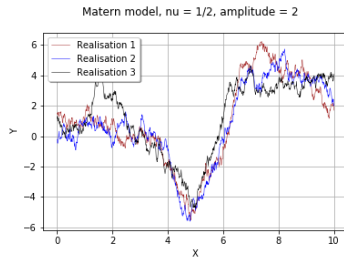
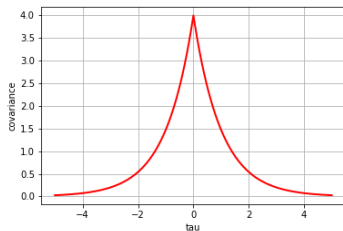


$$\rho = 5$$

Covariance function



$$\sigma = 1$$



$$\sigma = 2$$

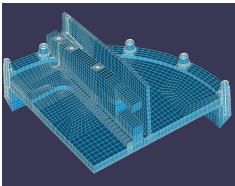
Outline

Random process

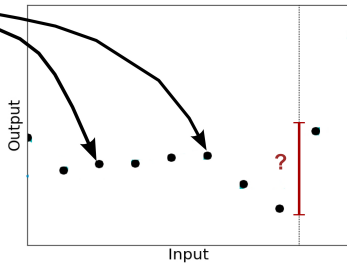
Gaussian process metamodel

Conclusions

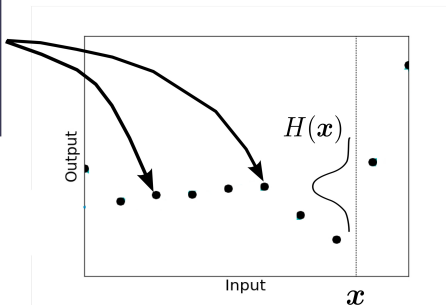
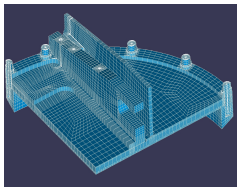
Prediction at a new point



Output value at a new location?



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 :

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

Trend (deterministic)

Linear regression
on a fixed basis

Random fluctuations

Gaussian process
with zero mean and
stationary

$$\text{Cov}_Z(\mathbf{x}, \mathbf{x}') = \sigma^2 \rho(\|\mathbf{x} - \mathbf{x}'\|)$$

Kriging

Conditional mean and variance

Experimental design:

$$\mathcal{X} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)}\}$$
$$\mathcal{Y} = \{Y(\mathbf{x}^{(1)}), \dots, Y(\mathbf{x}^{(N)})\}$$

Notations:

$$\mathbf{k}(\mathbf{x}) \equiv \{\rho(\mathbf{x}, \mathbf{x}^{(1)}), \dots, \rho(\mathbf{x}, \mathbf{x}^{(N)})\}^T$$
$$\mathbf{R} \equiv (r_j(\mathbf{x}^{(i)}))_{1 \leq i, j \leq N} \quad , \quad \mathbf{K} \equiv (\rho(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}))_{1 \leq i, j \leq N}$$

Conditional mean:

$$\mu(\mathbf{x}) = \mathbf{r}^T(\mathbf{x})\boldsymbol{\beta} + \mathbf{k}^T(\mathbf{x})\mathbf{K}^{-1}(\mathcal{Y} - \mathbf{R}\boldsymbol{\beta})$$

Conditional variance:

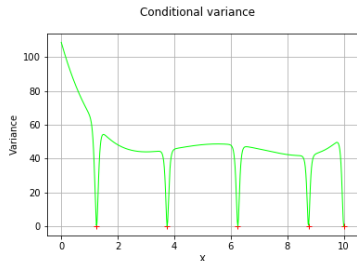
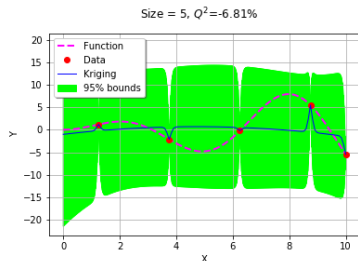
$$\sigma^2(\mathbf{x}) = \sigma^2 - \mathbf{k}^T(\mathbf{x})\mathbf{K}^{-1}\mathbf{k}(\mathbf{x})$$

Conditional mean and variance

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

Gaussian process metamodel:

$$H(x, \omega) = \mathbf{r}(x) \cdot \boldsymbol{\beta} + Z(x, \omega) \quad , \quad \text{Cov}_Z(x, x') = \sigma^2 e^{-\theta(x-x')^2}$$



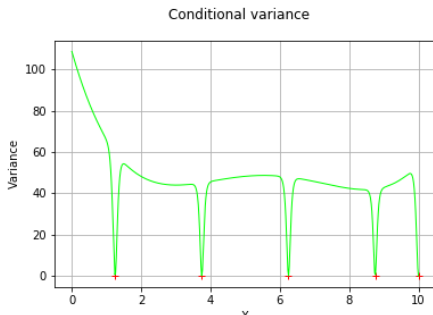
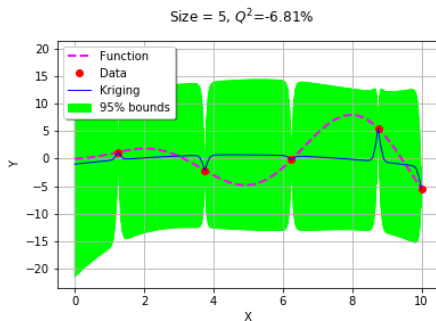
- ▶ The conditional mean is used as a metamodel (interpolator)
- ▶ The conditional variance is used as an error indicator

Parameter fitting

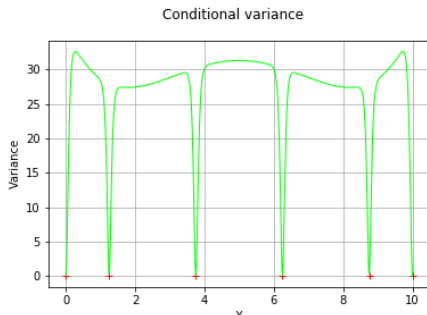
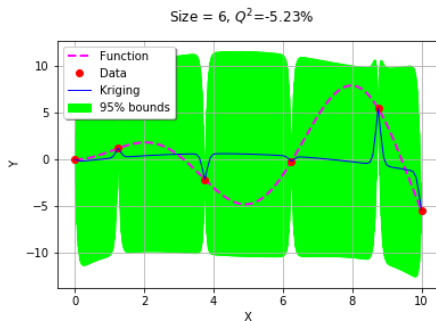
To apply the previous formulas, the parameters (β, σ, θ) have to be estimated from the design points

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

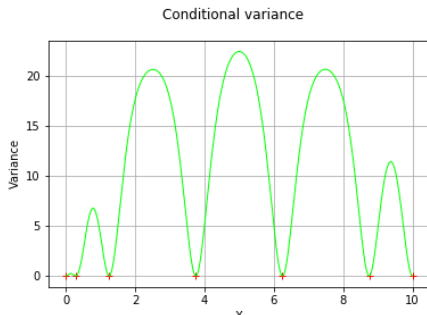
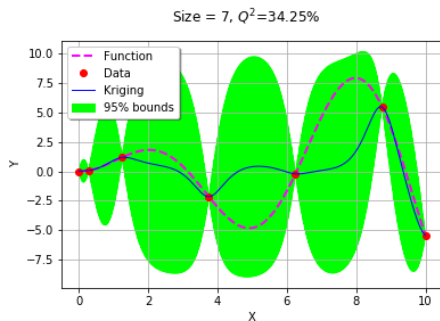
Sequential enrichment of the experimental design



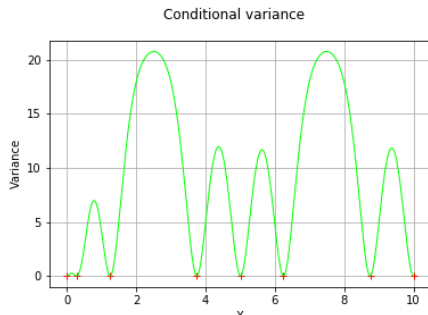
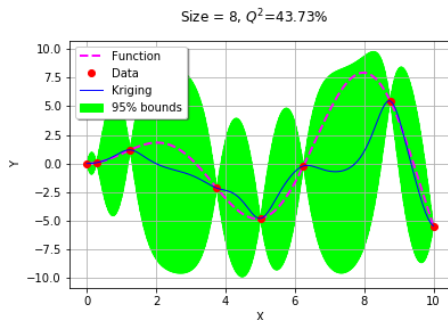
Sequential enrichment of the experimental design



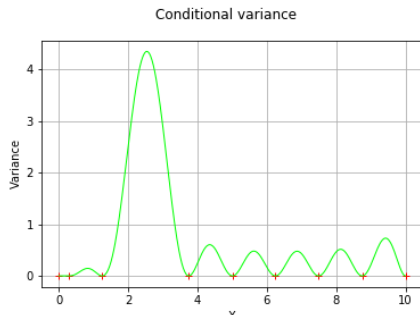
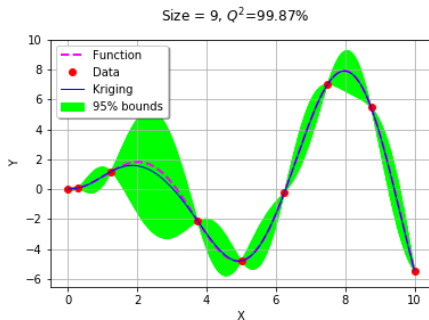
Sequential enrichment of the experimental design



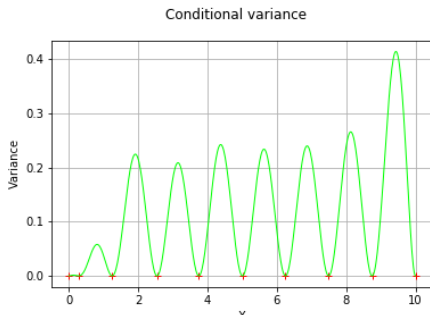
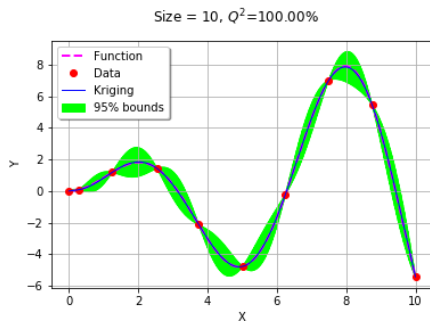
Sequential enrichment of the experimental design



Sequential enrichment of the experimental design



Sequential enrichment of the experimental design



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Random process

Gaussian process metamodel

Conclusions

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

