Introduction to Gaussian process metamodel - Kriging

May 2020

Outline

Random process

Gaussian process metamodel

Conclusions

Outline

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 $\mathbb{P}\left[X = 1\right] = \frac{1}{3}$

Random vector: a vector of random variables

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

Random process

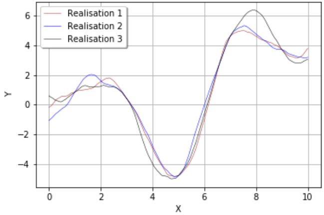
Random process Y: set of random variables indexed by x and defined in the probability space $(\Omega, \mathcal{F}, \mathcal{P})$

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

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

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

Covariance function of a stationary random process

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

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

- C_0: nugget effect
- υ: 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	$C(\tau) = \sigma^2 \exp\left(-\frac{\|\tau\|^\gamma}{\theta^\gamma}\right)$
Squared exponential	$C(\tau) = \sigma^2 \exp\left(-\frac{1}{2}\frac{\|\tau\|^2}{\theta^2}\right)$

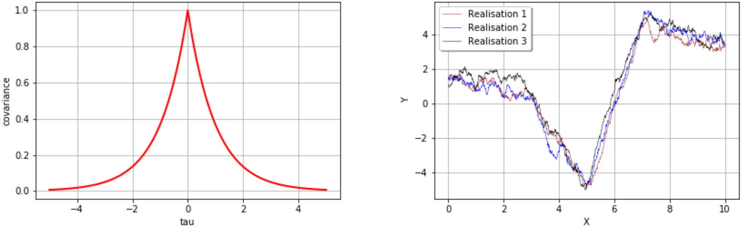
Covariance function

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

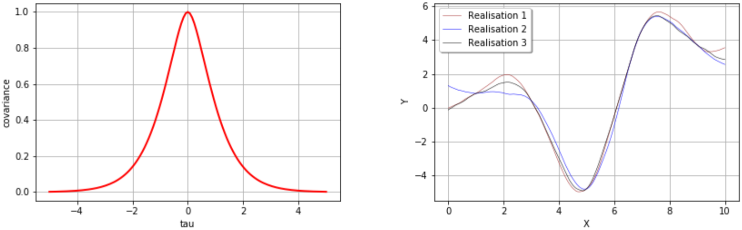
For stationary processes, the trajectories $y(x)$ are p-times differentiable if $C(\tau)$ is $2p$ times differentiable at $\tau = 0$.

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

Covariance function

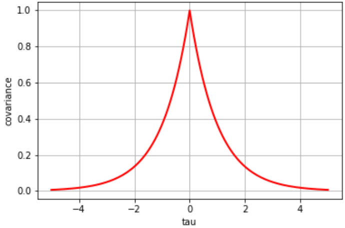


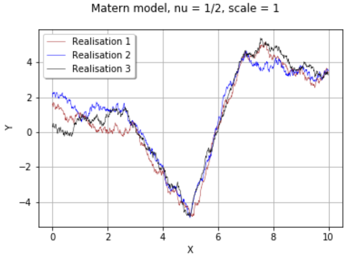
$\nu = 1/2$



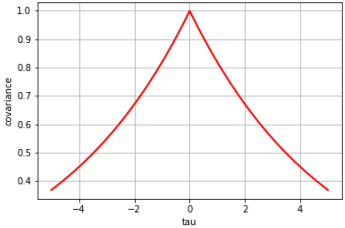
$\nu = 3/2$

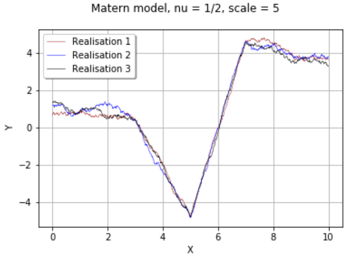
Covariance function





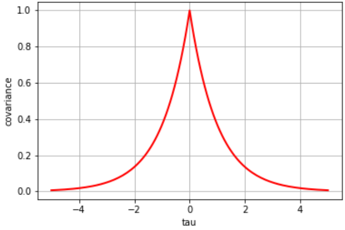
$\rho = 1$

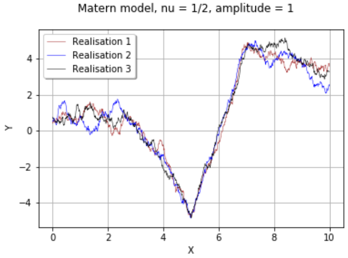




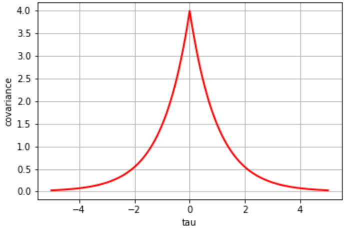
$\rho = 5$

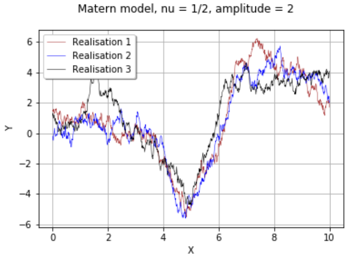
Covariance function





$\sigma = 1$





$\sigma = 2$

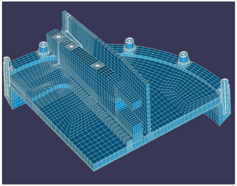
Outline

Random process

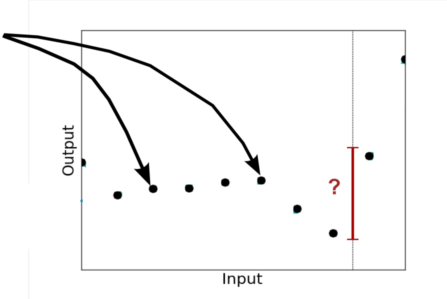
Gaussian process metamodel

Conclusions

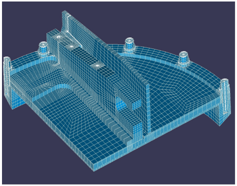
Prediction at a new point

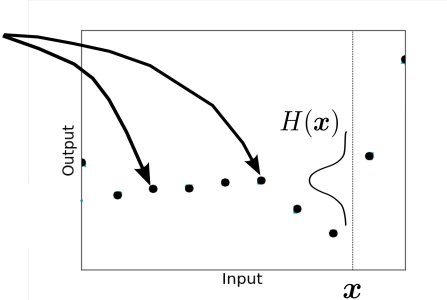


Output value at a new location?



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 :

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

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:

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

Notations:

$$\boldsymbol{k}(\boldsymbol{x}) \equiv \left\{\rho\left(\boldsymbol{x}, \boldsymbol{x}^{(1)}\right), \dots, \rho\left(\boldsymbol{x}, \boldsymbol{x}^{(N)}\right)\right\}^{\mathsf{T}}$$

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

Conditional mean:

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

Conditional variance:

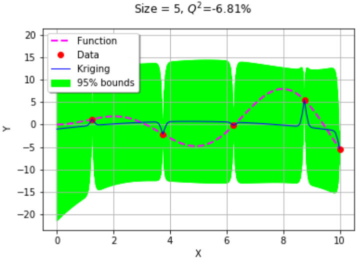
$$\boxed{\sigma^2(\boldsymbol{x}) = \sigma^2 - \boldsymbol{k}^{\mathsf{T}}(\boldsymbol{x})\, \boldsymbol{K}^{-1}\, \boldsymbol{k}^{\mathsf{T}}(\boldsymbol{x})}$$

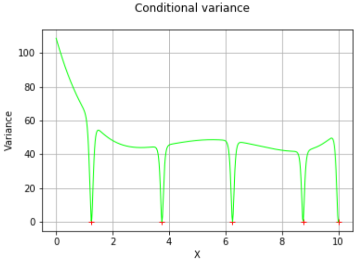
Conditional mean and variance

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

Gaussian process metamodel:

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





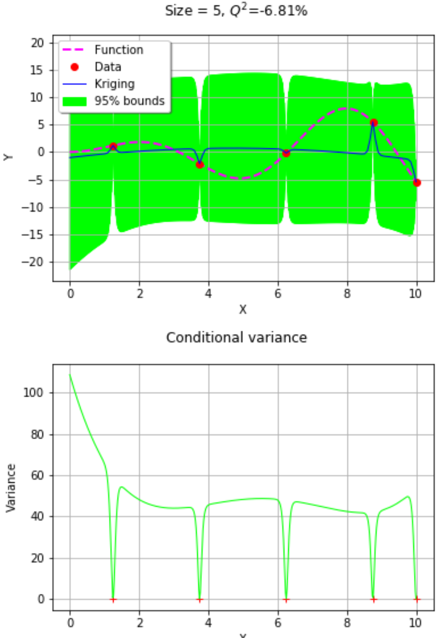
- The conditional mean is used as a metamodel (interpolator)
- The conditional variance is used as an error indicator

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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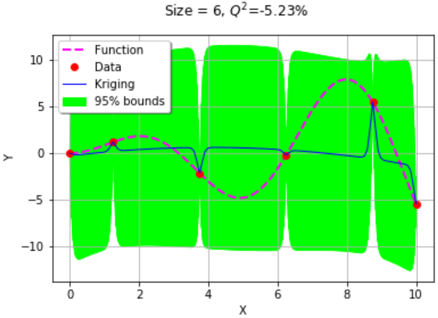

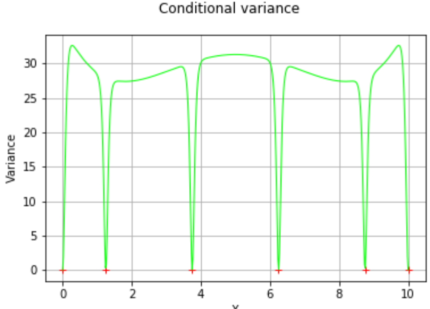

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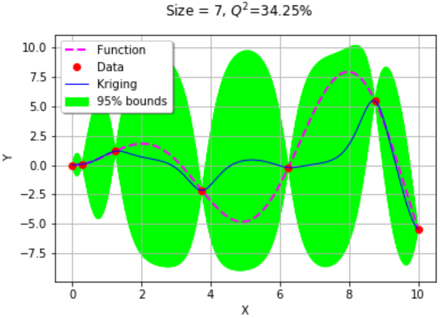

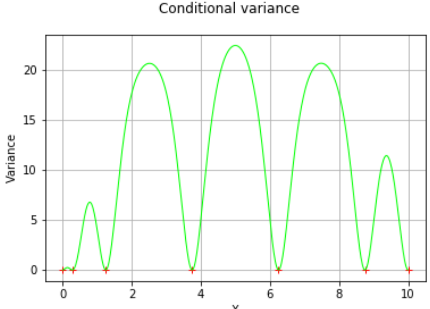

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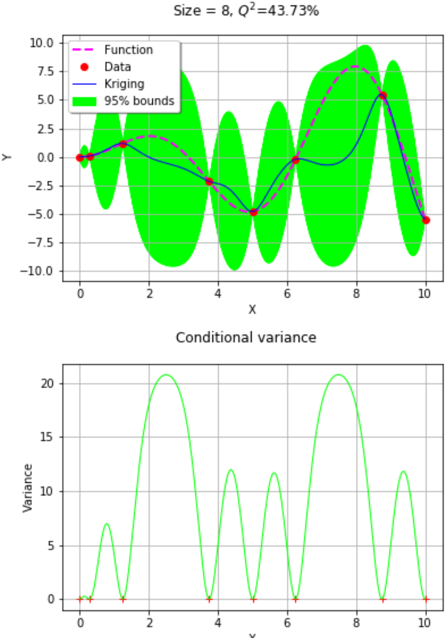

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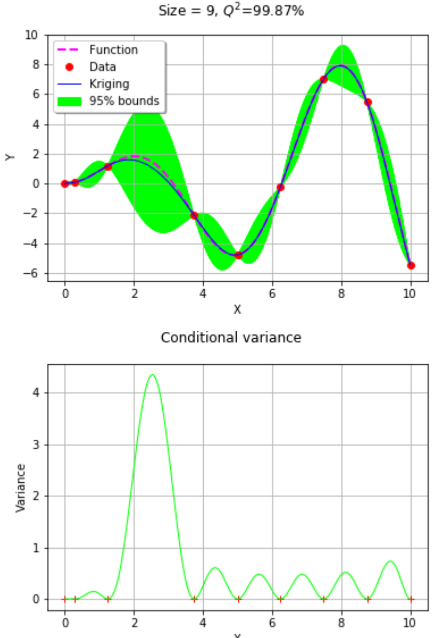

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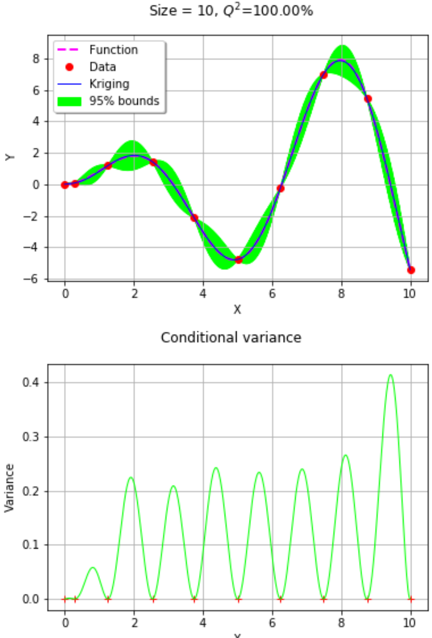

Outline

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