An introduction to Kriging metamodels

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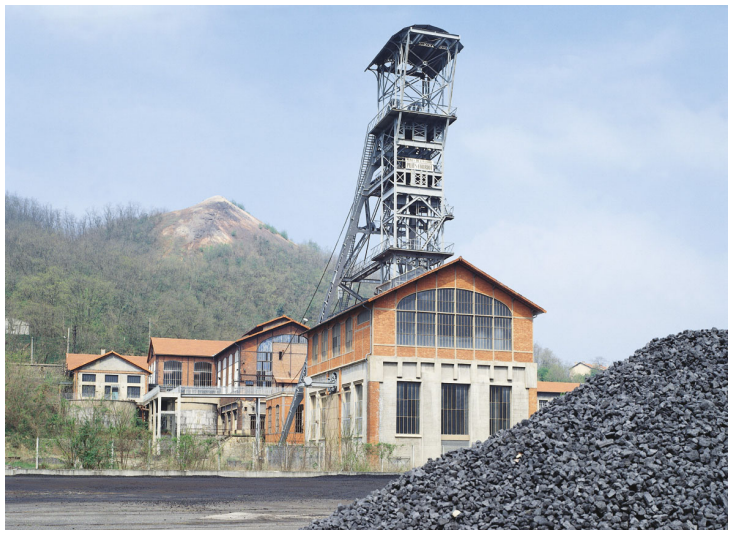


picture: mining headframe (chevalement) at Saint-Etienne

Majeure Science des données, UP4

Acknowledgements

This course is
an overview of Kriging metamodeling and Gaussian Process Regression

This material is partly recycled from previous classes by Nicolas Durrande [2], Roldolphe Le Riche [6], Xavier Bay and many others, thanks a lot !

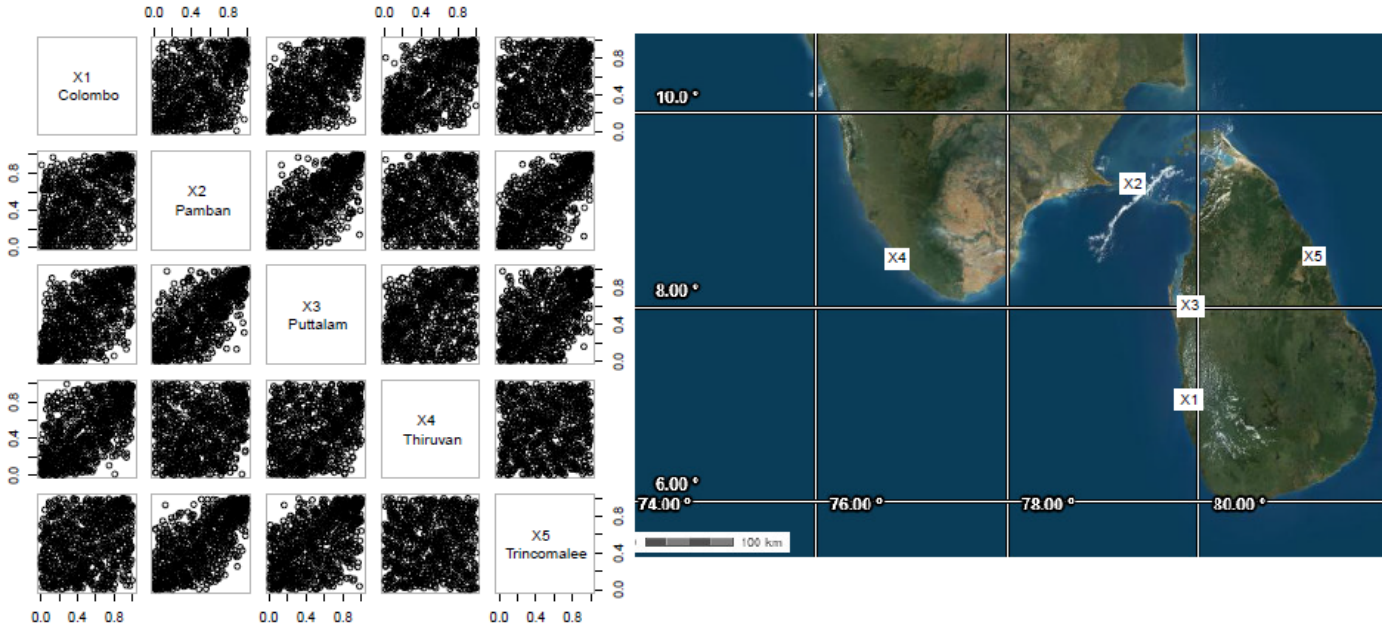
All errors are mine, do not hesitate to tell me.

Outline

Introduction

Introduction example : rainfall data

An example of rainfall data in Sri Lanka



- How to predict rainfall somewhere, if it is only measured on few specific sites ?

QUIZZ Which sites exhibits more correlation ?

QUIZZ Is this in link with spatial distance between sites ?

QUIZZ How would you do to predict between two sites ?

The Origins of Kriging

- ... ok about rain but...
- How to predict gold concentration somewhere, if it is only measured on few specific sites ?

QUIZZ

Who is this guy ?

1. Danie Spline
2. Danie Krige
3. Danie Kernel

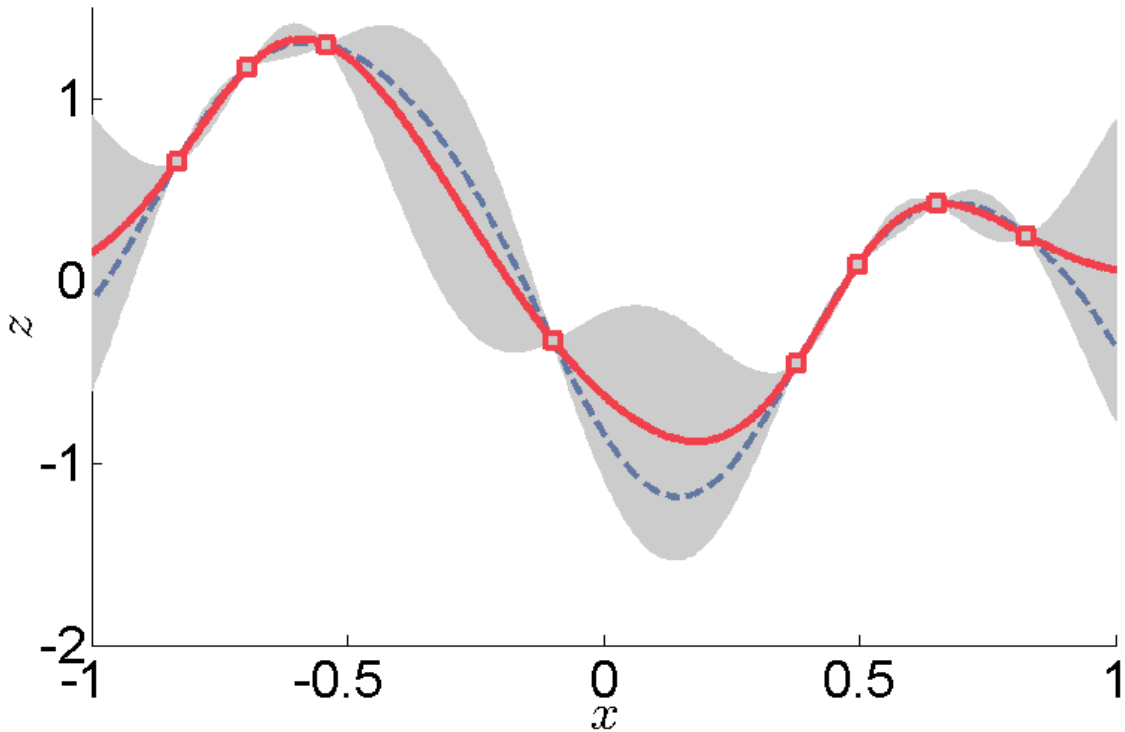
QUIZZ

Where is this mining engineer in the picture ?

A. South Africa
B. Bermuda
C. Couriot Mine in Saint-Etienne

Kriging ?

"In statistics, originally in geostatistics, kriging or Gaussian process regression is a method of interpolation for which the interpolated values are modeled by a Gaussian process governed by prior covariances (...)". Wikipedia (citation and curve)



Mathematical formalization by Georges Matheron (Ecole des Mines de Paris, student of Paul Lévy) in *Mémoires du BRGM*.

Many possible applications

Use with computer experiments

Kriging is most often used in the context of expensive experiments (simulators)

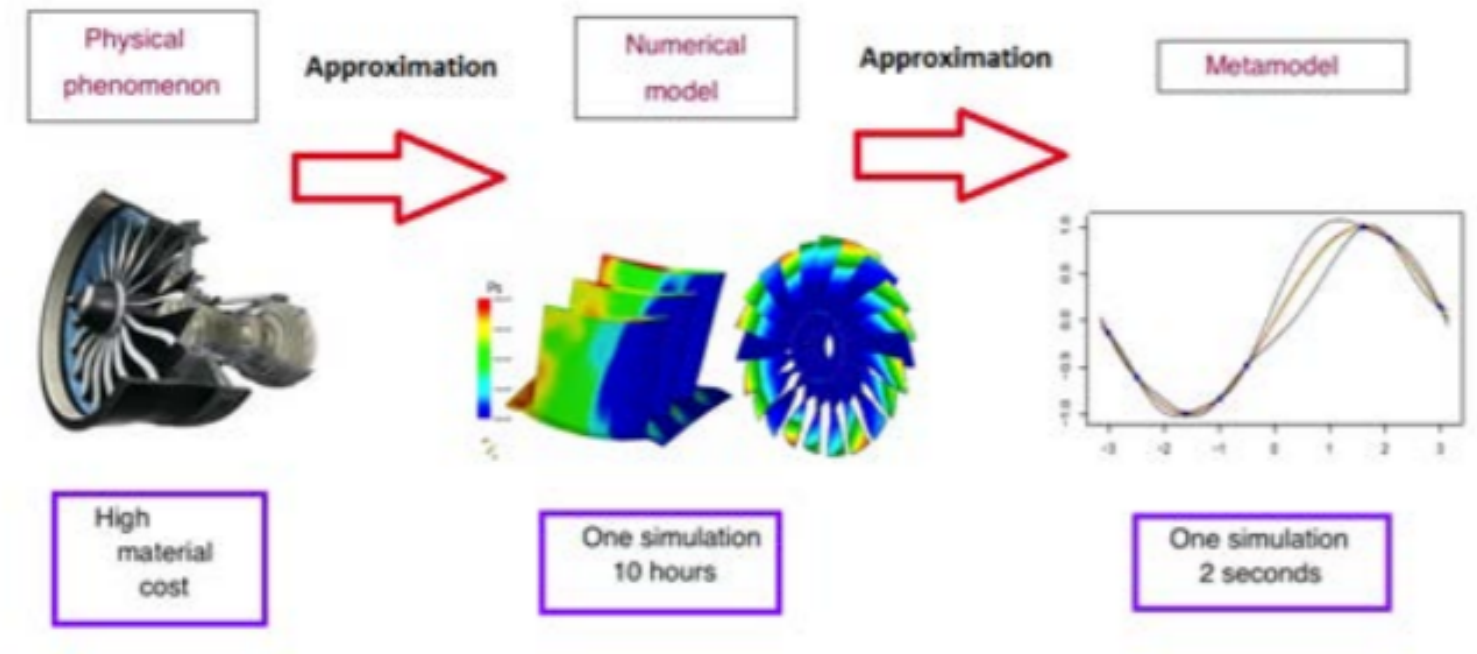


Illustration from your previous lecture Design of Experiment.

Many possible domains

Geostatistic (climate, mining)
Industry (crash tests, computer experiments)
Insurance (mortality tables, Economic Scenario Generator, nested simulations).

Context

Observations

Each experiment can be seen as a function of the input parameters.

input parameters $\in \chi \longrightarrow$ (computer/physical/...) experiment $\longrightarrow$ output $\in \mathbb{R}$

so that $y = f(x)$ where f is a **costly to evaluate function**.

In the following, we will assume that

- $x \in \chi$: There are d input variables. Usually (but not necessarily) χ is $\mathbb{R}^d$.
- $y \in \mathbb{R}$: The output is a scalar. But extensions to GP regression with multiple outputs exist.

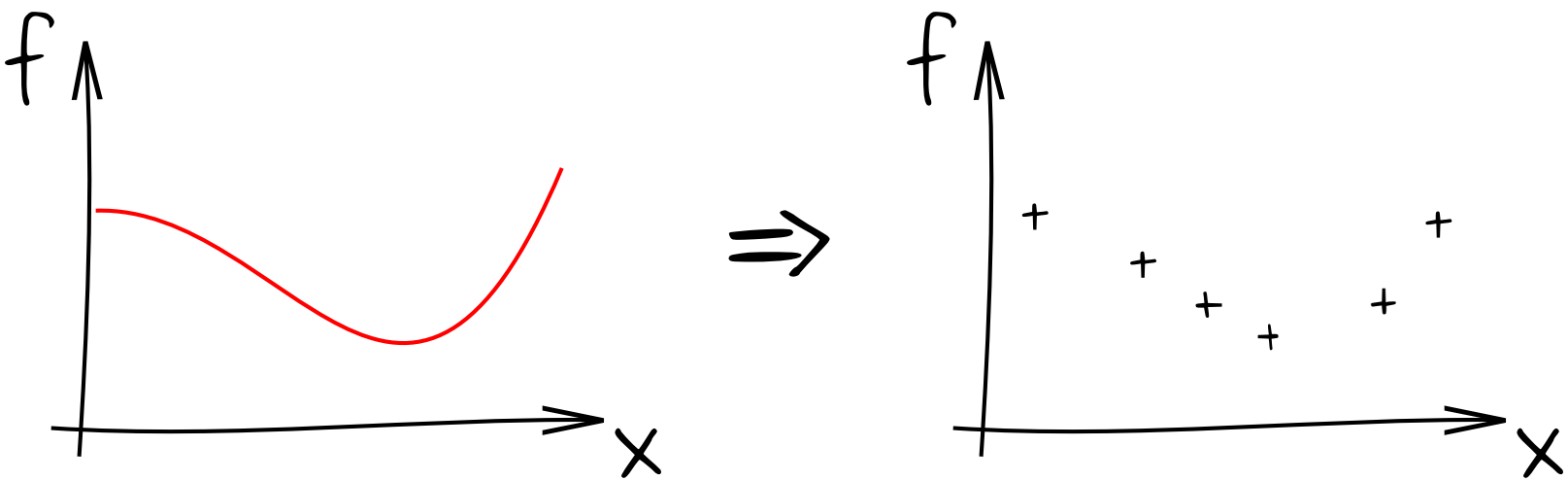
The interpolation problem

How to predict the output value for some new input parameters ?

f costly

The fact that f is **costly to evaluate** changes a lot of things...

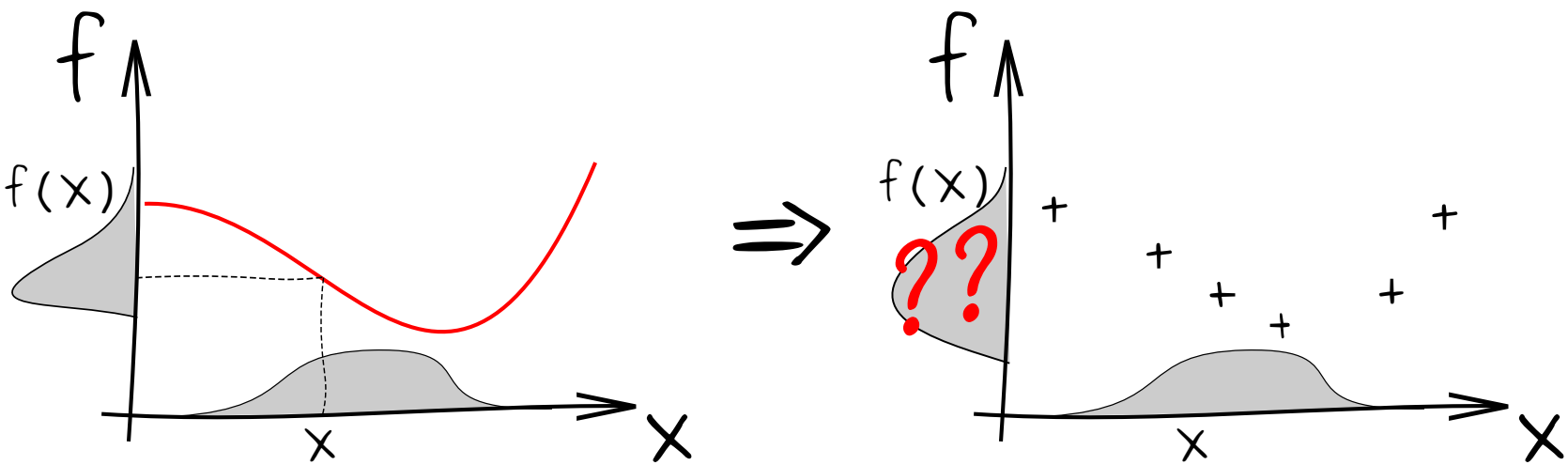
1. Representing the function is not possible...



f costly

The fact that f is **costly to evaluate** changes a lot of things...

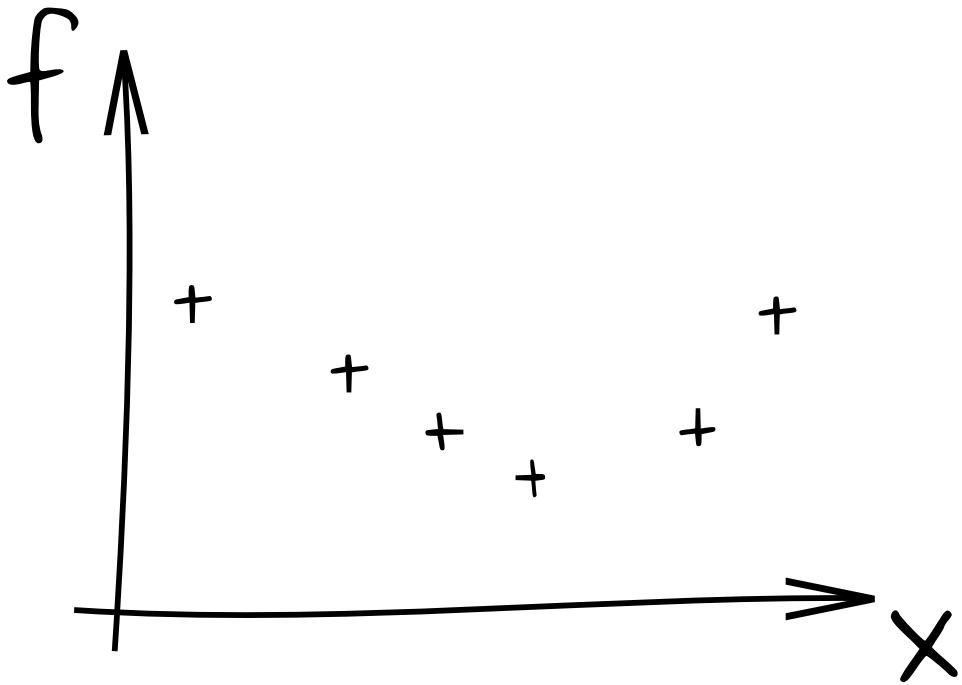
2. Uncertainty propagation is not possible...



f costly

The fact that f is **costly to evaluate** changes a lot of things...

3. Optimisation is also tricky...



4. Computing integrals is not possible...
5. Sensitivity analysis is not possible...

Need of a metamodel

Metamodel

Need to replace the costly f by a metamodel

- that can give a mean interpolation
- that can also measure the uncertainty associated with this interpolation

The presented one

Here we present Kriging metamodels, also known as Gaussian Process Regression (GPR) under some Gaussian assumptions.
Many other metamodels exist : splines, Inverse Distance Weighting, decomposition in basis functions, etc.
They are sometimes related to Kriging.

The Statistical Approach

Notations

Observations

set of possible sites :	$\chi = \mathbb{R}^d$	(e.g. rainfall $\chi = \mathbb{R}^2$)
n observations sites :	$\mathbb{X} = (x_1, \dots, x_n) \in \chi^n$	(e.g. n city locations)
n observed responses :	$\mathbf{Y}_{\mathbb{X}} = (Y_{x_1}, \dots, Y_{x_n})^\top \in \mathbb{R}^n$	(e.g. annual rainfall quantity)
indices :	$I = \{1, \dots, n\}$	

Quantity of interest

One new prediction site :	$x \in \chi$	(e.g. one new city location)
Unknown response at this site :	$Y_x \in \mathbb{R}$	(e.g. rainfall to be predicted)

Assumptions

- all Y_{x_i} are random variables with finite mean and finite variance
- Covariances matrix $\mathbf{K} = (K_{ij})_{i,j \in I}$ and vector $\mathbf{k}_x = (k_i(x))_{i \in I}$ are known.
  where $K_{ij} = \mathrm{Cov}\left[Y_{x_i}, Y_{x_j}\right]$ covariance between responses,
  and $k_i(x) = \mathrm{Cov}\left[Y_{x_i}, Y_x\right]$ covariance with target Y_x.

Simple Kriging : the model

The idea

Most natural idea : your prediction is a linear combination of observed responses.

The Simple Kriging Model

One assumes $\mathbf{Y}_{\mathbb{X}}$ and Y_x centered : $\forall x, \mathrm{E}[Y_x] = 0$. Define a predictor $M(x)$ as

$$M(x) = \sum_{i=1}^{n} \alpha_i(x) Y_{x_i} \tag{1}$$

where weights $\boldsymbol{\alpha}_x = (\alpha_i(x))_{i=1..n}$ are minimizing

$$\Delta(x) = \mathrm{E}\left[(M(x) - Y_x)^2\right] . \tag{2}$$

Check that unbiasedness holds : $\mathrm{E}[M(x)] = \mathrm{E}[Y_x]$

Simple Kriging : calculations (1)

Step 1 : Develop $\Delta(x)$, express it as a function of covariances $\mathbf{K}$ and $\mathbf{k}_x$

Recall that $\mathbf{k}_x$ is the covariance vector between Y_x and the vector $\mathbf{Y}_{\mathbb{X}}$, and $\mathbf{K}$ is the covariance matrix of $\mathbf{Y}_{\mathbb{X}}$. Using $M(x) = \boldsymbol{\alpha}_x^\top \mathbf{Y}_{\mathbb{X}}$, let us develop

$$\Delta(x) = \mathrm{E}\left[(M(x) - Y_x)^2\right] .$$

do your calculations here :

Simple Kriging : calculations (2)

Step 2 : find the weights $\boldsymbol{\alpha}_x$ that minimize $\Delta(x)$

Now let us minimize on $\boldsymbol{\alpha}_x$

$$\Delta(x) = \boldsymbol{\alpha}_x^\top \mathbf{K} \boldsymbol{\alpha}_x - 2\boldsymbol{\alpha}_x^\top \mathbf{k}_x + \text{constant}$$

do your calculations here :

Simple Kriging : Result (1)

Optimal weights

This leads to the vector of weights

$$\boldsymbol{\alpha}_x = \mathbf{K}^{-1}\mathbf{k}_x$$

where $\mathbf{k}_x$ is the covariance vector between Y_x and the vector $\mathbf{Y}_{\mathbb{X}}$, and $\mathbf{K}$ is the covariance matrix of $\mathbf{Y}_{\mathbb{X}}$.

Predictor and variance

From that follows the expression of $M(x)$ and $\Delta(x)$:

$$\begin{cases} M(x) &= \mathbf{k}_x^\top \mathbf{K}^{-1}\mathbf{Y}_{\mathbb{X}} \\ \Delta(x) &= \sigma_x^2 - \mathbf{k}_x^\top \mathbf{K}^{-1}\mathbf{k}_x \end{cases}$$

Notice that $\Delta(x)$ does not depend on observed responses $\mathbf{Y}_{\mathbb{X}}$.

Simple Kriging : Result (1)

Results remain valid for q prediction points. Given a specific instance $\mathbf{Y}_{\mathbb{X}} = \mathbf{y}$, we get :

Simple Kriging

One assumes that $\mathbf{Y}_{\mathbb{X}}$ and Y_x are centered. Kriging mean corresponds to the Best Linear Unbiased Predictor of Y_x given $\mathbf{Y}_{\mathbb{X}} = \mathbf{y}$, and Kriging variance to the mean square error $\Delta(x)$:

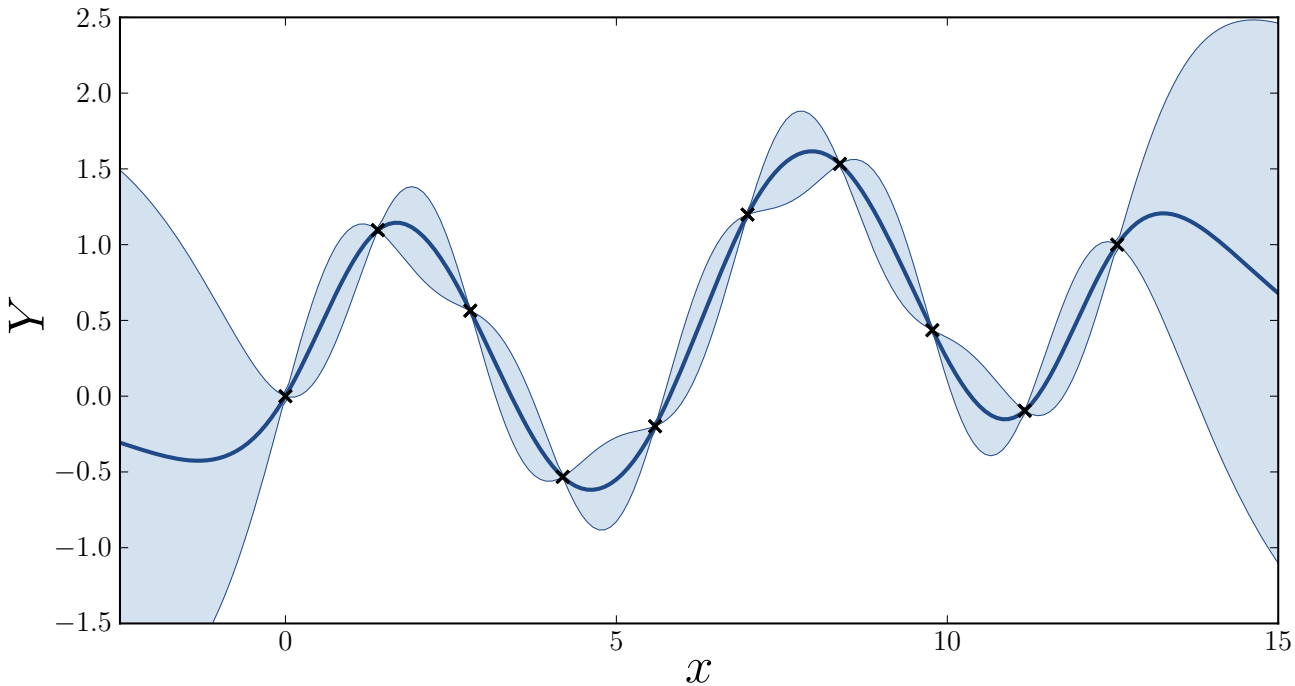
$$\left\{ \begin{array}{rcl} m(x) & = & \mathbf{k}_x^\top \mathbf{K}^{-1} \mathbf{y} \\ v(x) & = & \sigma_x^2 - \mathbf{k}_x^\top \mathbf{K}^{-1} \mathbf{k}_x \end{array} \right. \tag{3}$$

where $\mathbf{K} = \mathrm{Cov}\left[\mathbf{Y}_{\mathbb{X}}, \mathbf{Y}_{\mathbb{X}}\right]$ is $n \times n$ covariance matrix, and $\mathbf{k}_x = \mathrm{Cov}\left[\mathbf{Y}_{\mathbb{X}}, Y_{\mathbf{x}}\right]$ is a $n \times q$ covariance matrix.

At home, for $x, x' \in \chi$, determine $\Delta(x, x') = \mathrm{E}\left[(M(x) - Y_x)(M(x') - Y_{x'})\right]$, compare with $c(x, x')$ in the next section.

Simple Kriging : illustration

It can summarized by a mean function $m(x)$ and 95% confidence intervals corresponding to the variance $v(x)$ (under a distribution assumption).



The kriging predictor is interpolating $m(x_i) = Y_{x_i}$ for all i, why ?

Ordinary Kriging (1)

One assumes Y_{x_i}, $i \in I$ and Y_x have the same unknown mean μ. The predictor $M(x)$ writes as previously :

$$M(x) = \sum_{i=1}^{n} \alpha_i(x) Y_{x_i} \tag{4}$$

but unbiasedness condition $\mathrm{E}[M(x)] = \mathrm{E}[Y_{x_i}]$ implies $\sum_{i \in I} \alpha_i(x) = 1$.

QUIZZ Find the weights minimizing $\Delta(x) = \mathrm{E}\left[(Y_x - M(x))^2\right]$, subject to $\sum_{i \in I} \alpha_i(x) = 1$

Ordinary Kriging (2)

Using a Lagrange multiplier, we minimize in $\boldsymbol{\alpha}_x$

$$\Delta(x) - 2\lambda(\mathbf{1}^\top \boldsymbol{\alpha}_x - 1) = \boldsymbol{\alpha}_x^\top \mathbf{K}\boldsymbol{\alpha}_x - 2\boldsymbol{\alpha}_x^\top \mathbf{k}_x + \sigma_x^2 - 2\lambda(\mathbf{1}^\top \boldsymbol{\alpha}_x - 1) \tag{5}$$

after few calculation this gives

Ordinary Kriging

Under the assumption $\mathrm{E}[Y_{x_i}] = \mathrm{E}[Y_x] = \mu$, for all $i \in I$, Ordinary Kriging mean and variance are

$$\begin{cases} m(x) &= \boldsymbol{\alpha}_x^\top \mathbf{y} \\ v(x) &= \boldsymbol{\alpha}_x^\top \mathbf{K}\boldsymbol{\alpha}_x - 2\boldsymbol{\alpha}_x^\top \mathbf{k}_x + \sigma_x^2 \end{cases} \tag{6}$$

with $\boldsymbol{\alpha}_x = \mathbf{K}^{-1}\left(\mathbf{k}_x + \underbrace{\left(\frac{1 - \mathbf{k}_x^\top \mathbf{K}^{-1}\mathbf{1}}{\mathbf{1}^\top \mathbf{K}^{-1}\mathbf{1}}\right)}_{=\lambda} \cdot \mathbf{1}\right)$.

Ordinary Kriging can be seen as a Simple Kriging on residuals, with :

$$\begin{cases} \hat{\mu} &= \left(\mathbf{1}^\top \mathbf{K}^{-1}\mathbf{1}\right)^{-1} \mathbf{1}^\top K^{-1}\mathbf{Y}_{\mathbb{X}} \\ m(x) &= \hat{\mu} + \mathbf{k}_x^\top \mathbf{K}^{-1}(\mathbf{Y}_{\mathbb{X}} - \hat{\mu}\mathbf{1}) \end{cases} \tag{7}$$

Universal Kriging

Consider given matrices of factors, e.g. $F(\mathbb{X}) = (\mathbf{1}, \mathbb{X})$ and $F(x) = (1, x)$.
The universal Kriging predictor writes

$$M(x) = F(x)^\top \beta + \sum_{i=1}^{n} \alpha_i(x) Y_{x_i} \tag{8}$$

The vector β does not depend on x. One can show (*Sacks et al.*, 1989) :

Universal Kriging

The optimal coefficients β and $\alpha(x)$ are the same as those obtained by :

1. doing a linear regression $\mathbf{Y}_\mathbb{X} = F(\mathbb{X})^\top \beta + \epsilon$ to estimate the β_i's

$$\hat{\beta} = \left(F(\mathbb{X})^\top \mathbf{K}^{-1} F(\mathbb{X})\right)^{-1} F(\mathbb{X})^\top \mathbf{K}^{-1} \mathbf{Y}_\mathbb{X}$$

2. then doing a Simple Kriging on residuals

... so that no other results are needed ☺.

QUIZZ What happens when $F(\mathbb{X}) = \mathbf{1}$?

Advantages of the Statistical Approach

Some advantages of the "statistical approach" (compared to other approaches)

Pro

- General : only requires random variables with two moments, no Gaussian assumption, manipulate only finite vectors
- Can be extended with other regression techniques : penalizations (LASSO, ridge), cross effects, quadratic terms, link functions...

$$M(x) = \sum_i \alpha_i(x) Y_{x_i} - \lambda \left| \sum_i \alpha_i(x) \right|$$

$$M(x) = f\left(Y_{x_1}, ..., Y_{x_n}, \boldsymbol{\alpha}\right)$$

- Can be nested using other estimators

$$M(x) = \sum_i \alpha_i(x) M_i(x)$$

Cons

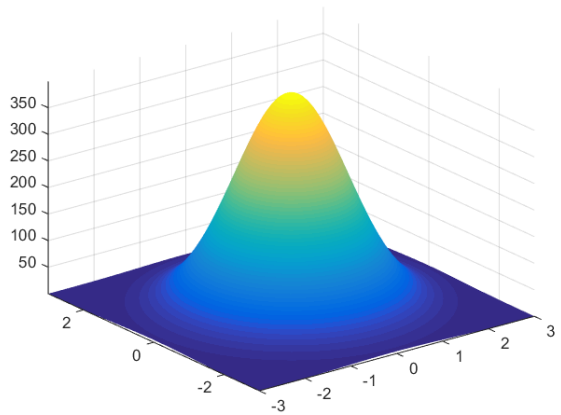
- Interpretation : No direct interpretation as a conditional process
- Theroretical : Conditional quantities sometimes hard to derive

The Gaussian Process Approach

Gaussian Vectors

A Gaussian Vector $\mathbf{Y}$ with mean $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$ is a random vector with density

$$f_{\mathbf{Y}}(y_1, \ldots, y_d) = \frac{1}{\sqrt{(2\pi)^d \det \boldsymbol{\Sigma}}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right) \tag{9}$$



- Non-degenerate if $\boldsymbol{\Sigma}$ definite positive : $\forall \mathbf{a}$ non zero, $\mathbf{a}^\top \boldsymbol{\Sigma} \mathbf{a} > 0$.
- Linear combinations of components of $\mathbf{Y}$ are Gaussian,
- thus components Y_i are Gaussian, $i = 1, \ldots, d$ (reverse not true).

Conditional Gaussian Vectors

Let $\boldsymbol{Y} = \begin{bmatrix} \boldsymbol{Y}_1 \\ \boldsymbol{Y}_2 \end{bmatrix}$ be Gaussian with mean $\boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{bmatrix}$ and covariance $\boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{bmatrix}$, then

Conditional Gaussian Vector

The conditional distribution of $\mathbf{Y}_1$ given $\mathbf{Y}_2 = \mathbf{y}_2$ is Gaussian with mean and covariance

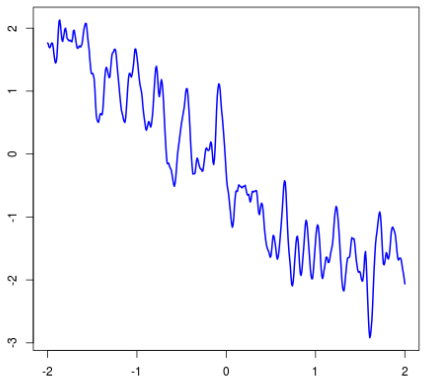
$$\begin{cases} \boldsymbol{\mu}_{2|1} &= \boldsymbol{\mu}_1 + \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{y}_2 - \boldsymbol{\mu}_2) \\ \boldsymbol{\Sigma}_{2|1} &= \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21}. \end{cases} \tag{10}$$

Random Process

A random process is a set of RV's indexed by $x \in \chi$

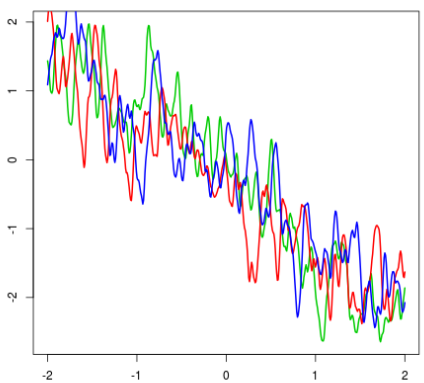
random event $\omega \in \Omega$
(e.g., weather)

$\Longrightarrow$



Repeat the random event ($3\times$)

$\Longrightarrow$



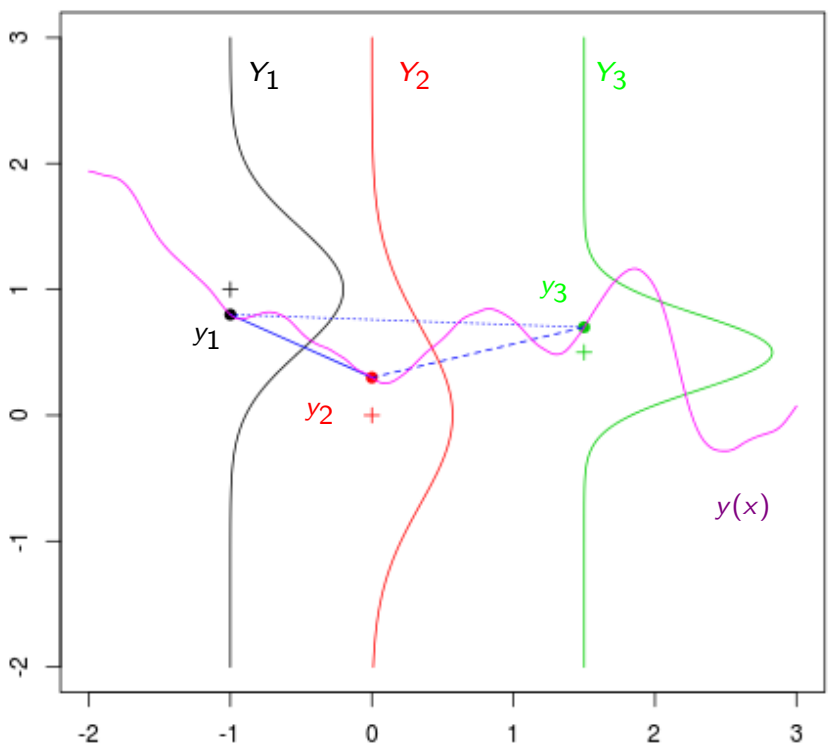
This creates 3 trajectories $y(x)$'s. They are different, yet bear strong similarities.

Gaussian Process (1) : definition

Gaussian Process : one possible definition

A stochastic process is Gaussian $\iff$ all finite subvectors are Gaussian

- implies that for any $x \in \chi$, Y_x is a Gaussian RV (reverse not true).
- implies that any finite linear combination of some Y_x's is Gaussian.



Gaussian Process (2) : characterisation

For such a Gaussian Process (GP), we denote

$$k(x, x') = \mathrm{Cov}\left[Y_x, Y_{x'}\right].$$

Gaussian Process (2) : characterisation

The distribution of a GP is fully characterised by :

- its mean function $\mu : \chi \to \mathbb{R}$:

$$\mu(x) = \mathrm{E}\left[Y_x\right]$$

- its covariance function, or *kernel*, $k : \chi \times \chi \to \mathbb{R}$:

$$k(x, x') = \mathrm{Cov}\left[Y_x, Y_{x'}\right]$$

In particular, $\forall \mathbb{X} = \begin{pmatrix} x_1 \\ \cdots \\ x_n \end{pmatrix} \in \chi^n$, $\mathbf{Y}_{\mathbb{X}} = \begin{pmatrix} Y_{x_1} \\ \cdots \\ Y_{x_n} \end{pmatrix} \sim \mathcal{N}(\mu(\mathbb{X}), \mathbf{K})$,
where $\mathbf{K} = (K_{ij})_{i,j \in I}$, $K_{ij} = \mathrm{Cov}(Y_{x_i}, Y_{x_j}) = k(x_i, x_j)$.

Gaussian Process (3) : covariance function

Conditions

... but conditions hold (detailed later) for the covariance function $k(.,.)$!

QUIZZ Should $k(x,x') = k(x',x)$? why ?

QUIZZ For any $\boldsymbol{a}$, variance of the random variable $\boldsymbol{a}^\top \mathbf{Y}_{\mathbb{X}}$? consequence on $k(.,.)$?

One example (for the moment)

The *Gaussian kernel*, or *Squared Exponential (SE) covariance function* :

$$k(x,x') = \sigma^2 \exp\left(-\frac{1}{2\theta^2}||x-x'||_2^2\right)$$

has two parameters, the variance σ^2 and the lengthscale θ.

Matrix notations for kernels

for two vectors $\mathbf{u} \in \chi^q$, $\mathbf{v} \in \chi^n$, we often use the matrix notation :

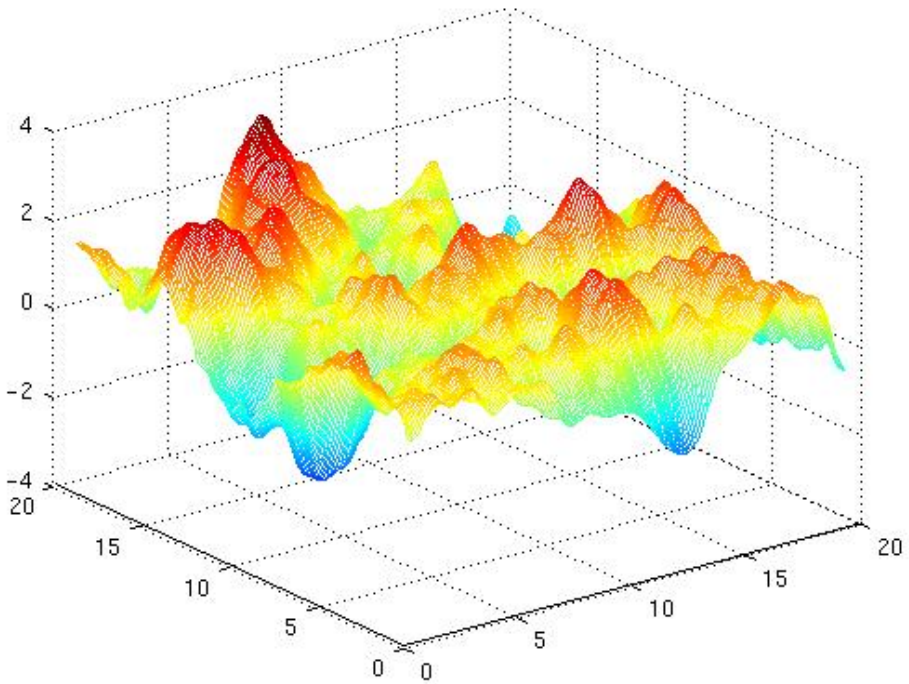
$$k(\mathbf{u},\mathbf{v}) = (k(u_i,u_j))_{i=1,\dots,q;j=1,\dots,n} \quad \in \mathbb{R}^{q\times n}$$

- $\mathbf{K} = k(\mathbb{X},\mathbb{X}) \in \mathbb{R}^{n\times n}$,
- $\mathbf{k}_x = k(\mathbb{X},x) = k(x,\mathbb{X})^\top \in \mathbb{R}^{n\times 1}$.

Gaussian Process (4) : random fields

On previous illustrations $x \in \mathbb{R}$, so that trajectories are functions $\mathbb{R} \to \mathbb{R}$.

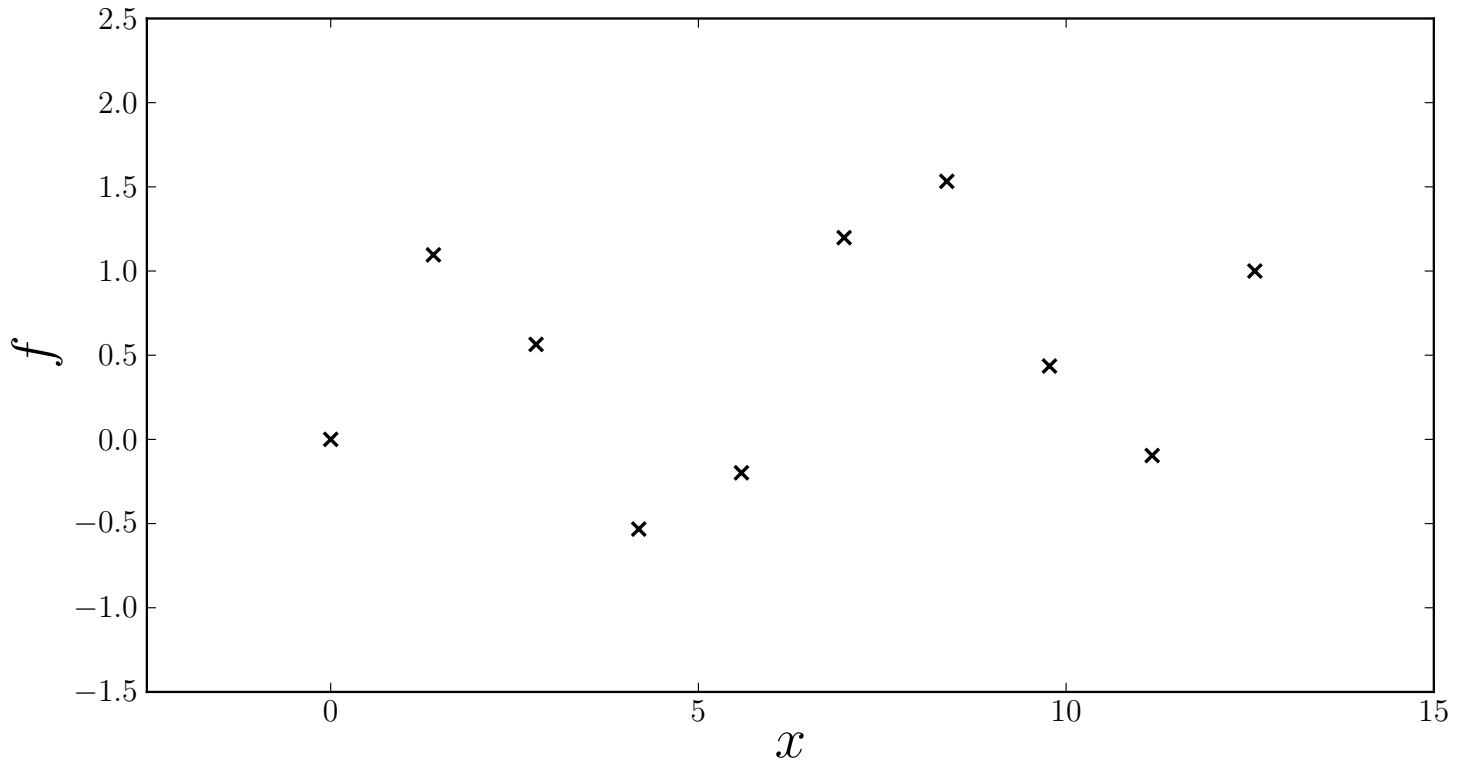
When $x \in \mathbb{R}^d$, with $d > 1$, trajectories are functions $\mathbb{R}^d \to \mathbb{R}$.



Nothing is changed, but we sometimes call the process a Gaussian Random Field.

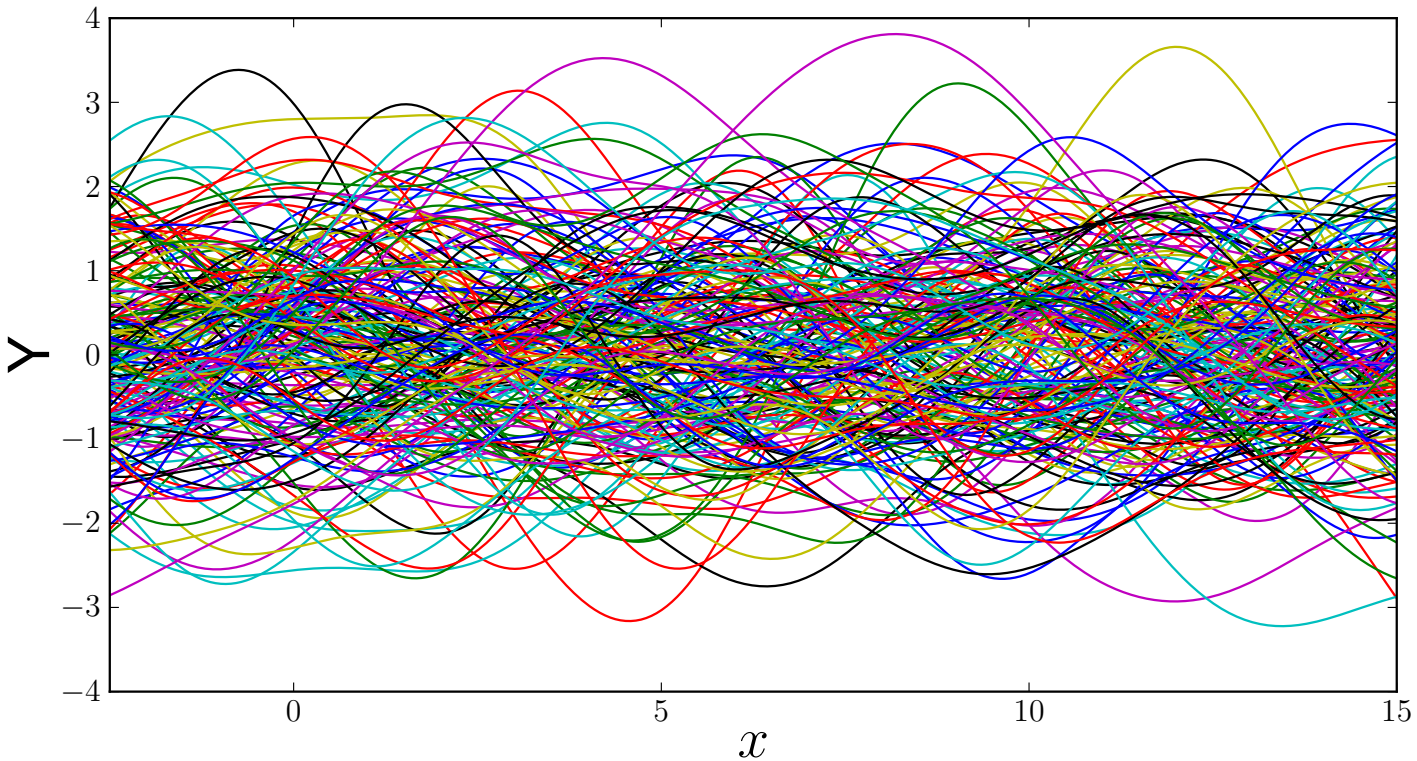
Gaussian process regression

Assume we have observed a function $f()$ over a set of points $X = (x_1, \ldots, x_n)$:



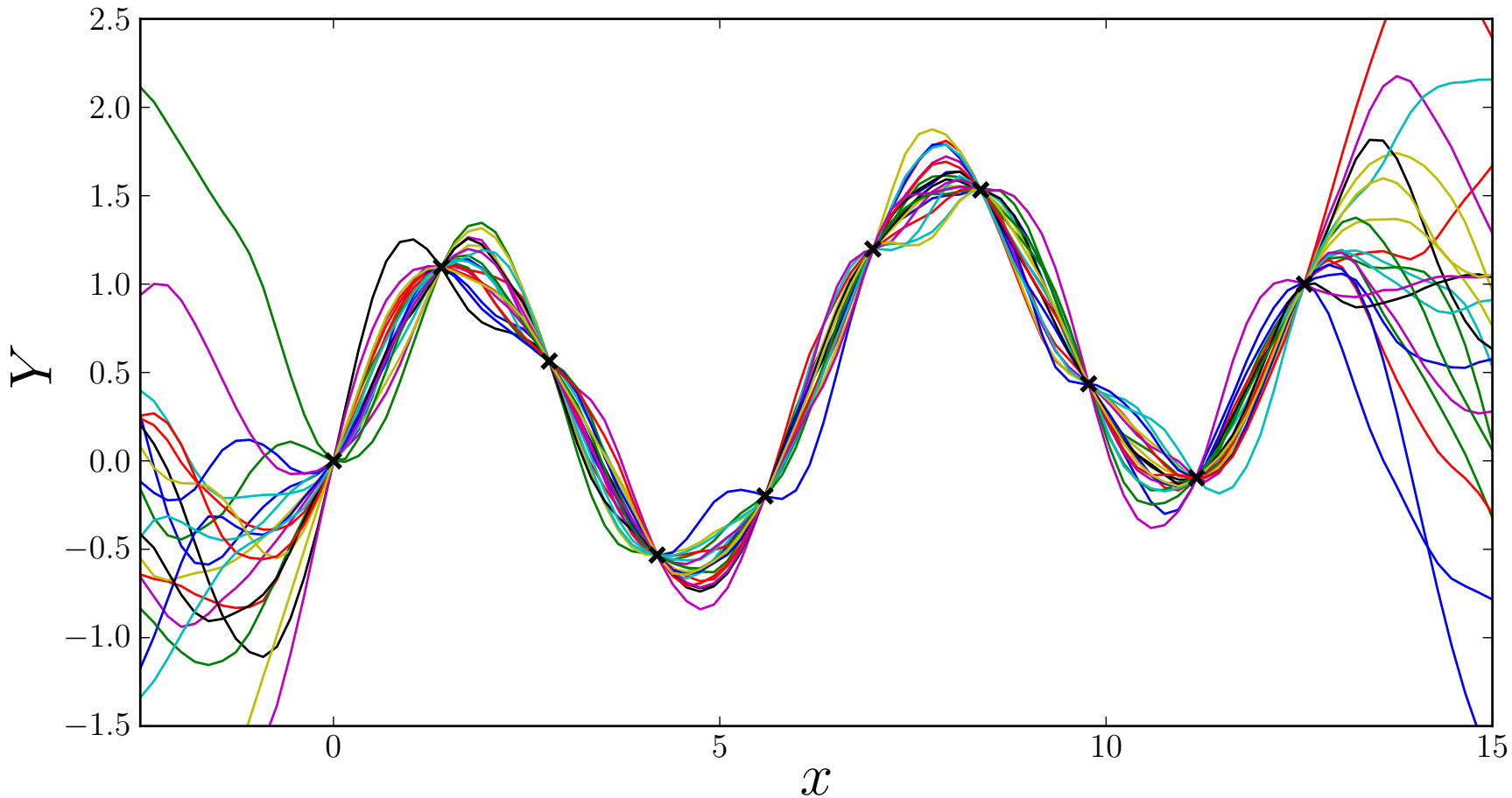
The vector of observations is $\mathbf{y} = f(\mathbb{X})$, i.e. $y_i = f(x_i)$.

Since $f()$ in unknown, we make the general assumption that it is the sample path of a Gaussian process $Y \sim \mathcal{N}(\mu(.), k(.,.))$:

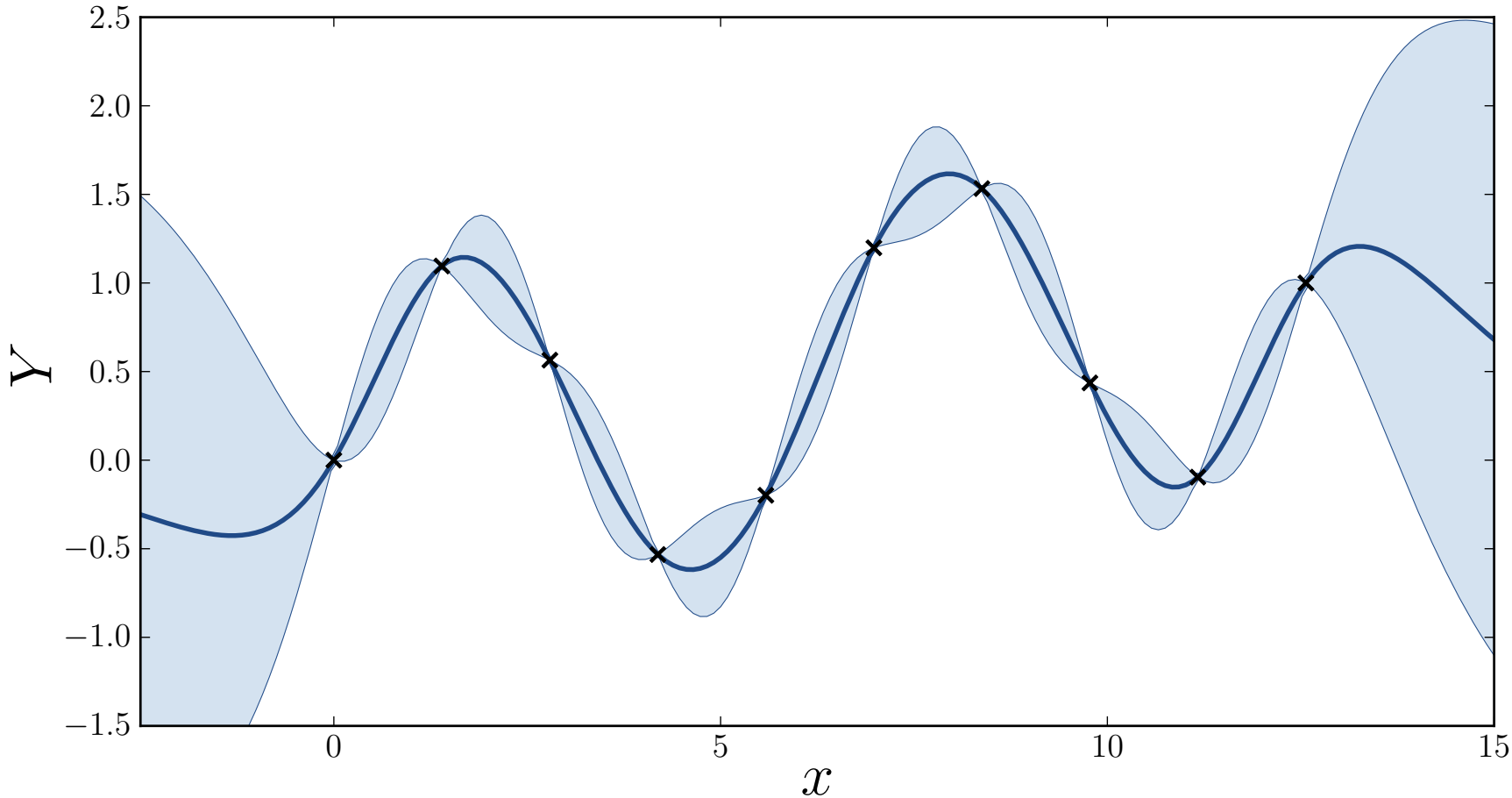


(here $\mu(x) = 0$)

If we remove all the samples that do not interpolate the observations we obtain :



It can summarized by a mean function and 95% confidence intervals.



Kriging equations (1/2)

The conditional distribution can be obtained analytically :

By definition, $(Y_x, \mathbf{Y}_{\mathbb{X}})$ is multivariate normal. Formulas on the conditioning of Gaussian vectors, in Equation (10), give the distribution of $Y_x|\mathbf{Y}_{\mathbb{X}} = \mathbf{y}$. It is $\mathcal{N}(m(.), c(.,.))$ with :

$$\begin{aligned} m(x) &= \mathrm{E}\left[Y_x|\mathbf{Y}_{\mathbb{X}}=\mathbf{y}\right] \\ &= \mu(x) + k(x,\mathbb{X})k(\mathbb{X},\mathbb{X})^{-1}(\mathbf{y} - \mu(\mathbb{X})) \\ c(x,x') &= \mathrm{Cov}\left[Y_x, Y_{x'}|\mathbf{Y}_{\mathbb{X}}=\mathbf{y}\right] \\ &= k(x,x') - k(x,\mathbb{X})k(\mathbb{X},\mathbb{X})^{-1}k(\mathbb{X},x') \end{aligned}$$

Simple Kriging, Gaussian case

For a centered process, when $\mu(x) = \mu(\mathbb{X}) = 0$, the simple Kriging predictor in Equation (3) corresponds to

$$\left\{ \begin{array}{rcl} m(x) & = & \mathrm{E}\left[Y_x|\mathbf{Y}_{\mathbb{X}}=\mathbf{y}\right] \\ v(x) & = & \mathrm{V}\left[Y_x|\mathbf{Y}_{\mathbb{X}}=\mathbf{y}\right] \end{array} \right.$$

Kriging equations (2/2)

Summary

The distribution of $Y_x|\mathbf{Y}_{\mathbb{X}} = \mathbf{y}$ is $\mathcal{N}(m(.), c(.,.))$ with mean and covariance

$$\begin{cases} m(x) & = & \mu(x) + k(x,\mathbb{X})k(\mathbb{X},\mathbb{X})^{-1}(\mathbf{y} - \mu(\mathbb{X})) \\ c(x,x') & = & k(x,x') - k(x,\mathbb{X})k(\mathbb{X},\mathbb{X})^{-1}k(\mathbb{X},x') \end{cases}$$

- $k(\mathbb{X},\mathbb{X}) = [k(x_i,x_j)]$: covariance matrix between observed outputs, sometimes named Gram matrix. It is of size $n \times n$.
- $k(x,\mathbb{X}) = [k(x,x_i),\ldots,k(x,x_n)]$: $n \times 1$ covariance vector between observed output and target Y_x.

Remarks

- It is a Gaussian distribution : gives confidence intervals, can be sampled, this is actually how the previous slides were generated.
- It is Bayesian : $Y_x|\mathbf{Y}_{\mathbb{X}} = \mathbf{y}$ is the posterior distribution of Y_x once $\mathbf{Y}_{\mathbb{X}} = \mathbf{y}$ is observed.
- It is named *Gaussian Process Regression*, often identified with the term *Kriging*.

Properties

A few remarkable properties of Gaussian Process Regression (GPR) models

- They (can) interpolate the data-points
- The prediction variance does not depend on the observations **y**
- The mean predictor does not depend on the scale of variances parameters
- They (usually) come back to the a priori trend $\mu(x)$ when we are far away from the observations.

proofs left as exercise

Kriging of noisy data

An important special case, noisy data $\mathbf{Z}_{\mathbb{X}} = \mathbf{Y}_{\mathbb{X}} + \epsilon_{\mathbb{X}}$.
where $\varepsilon(.) \sim \mathcal{N}(0, n(.,.))$ independent of $Y(.)$. Then,

$$\begin{cases} \mathrm{Cov}(Y_{x_i} + \epsilon_{x_i}, Y_{x_j} + \epsilon_{x_j}) &= k(x_i, x_j) + n(x_i, x_j) \\ \mathrm{Cov}(Y_x, Y_{x_i} + \epsilon_{x_i}) &= k(x, x_i) \end{cases}$$

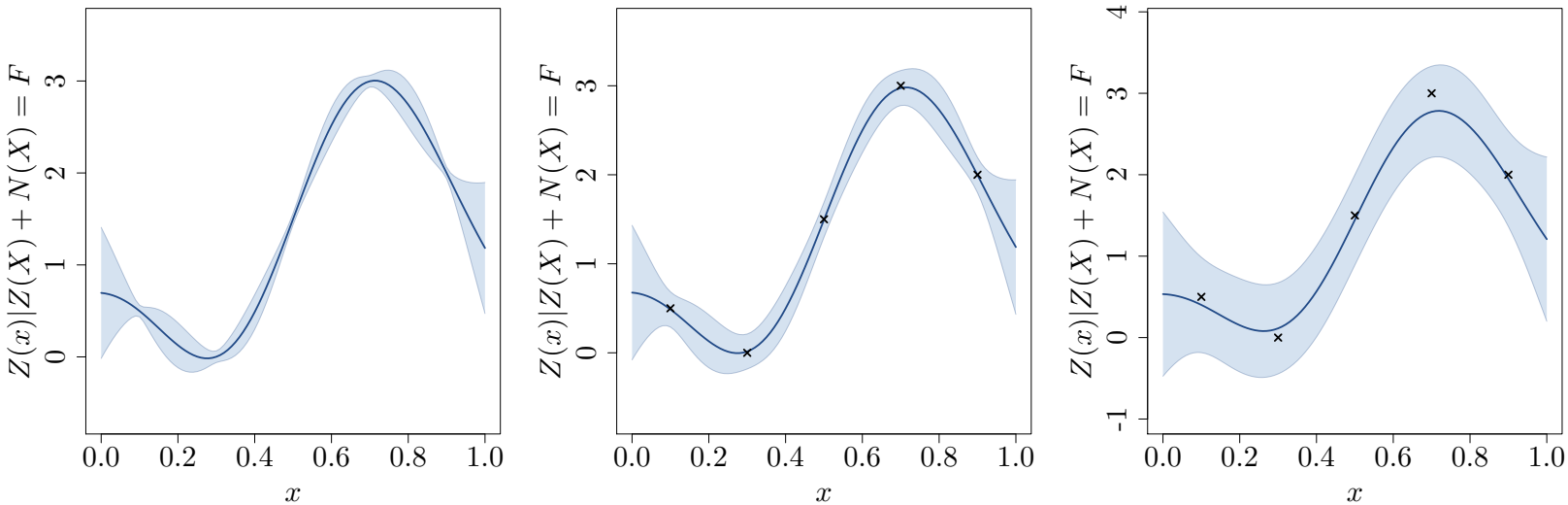
The expressions of GPR with noise become (just apply Gaussian vector conditioning with the above), when $x \notin \mathbb{X}$ and ϵ_x, $\epsilon_{x'}$, $\epsilon_{\mathbb{X}}$ mutually independent.

$$\begin{aligned} m(x) &= \mathrm{E}\left[Z_x | \mathbf{Z}_{\mathbb{X}} = \mathbf{z}\right] \\ &= \mu(x) + k(x, \mathbb{X}) \left(k(\mathbb{X}, \mathbb{X}) + n(\mathbb{X}, \mathbb{X})\right)^{-1} (\mathbf{z} - \mu(\mathbb{X})) \\ c(x, x') &= \mathrm{Cov}\left[Z(x), Z(x') | Z(\mathbb{X}) = \mathbf{z}\right] \\ &= k(x, x') - k(x, \mathbb{X}) \left(k(\mathbb{X}, \mathbb{X}) + n(\mathbb{X}, \mathbb{X})\right)^{-1} k(\mathbb{X}, x') \end{aligned}$$

Remarks

- this is the same distribution as the one of $Y_x | \mathbf{Z}_{\mathbb{X}} = \mathbf{z}$, $x \notin \mathbb{X}$.
- usually $n(\mathbb{X}, \mathbb{X})$ diagonal, called nugget effect.
- can be used to help the inversion of $k(\mathbb{X}, \mathbb{X})$

Examples of models with observation noise for $n(x, x') = \tau^2 \delta_{x,x'}$:



The values of τ^2 are respectively 0.001, 0.01 and 0.1.

Kriging with noise kernel (nugget) does not interpolate the data.

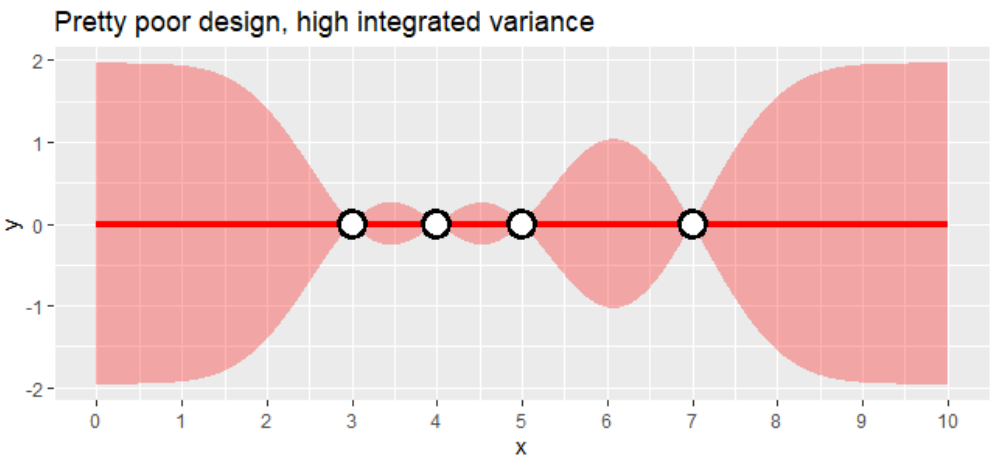
A small τ^2 (e.g., 10^{-10}) often used to make the covariance matrix invertible (more on regularization of GPs in [7]).

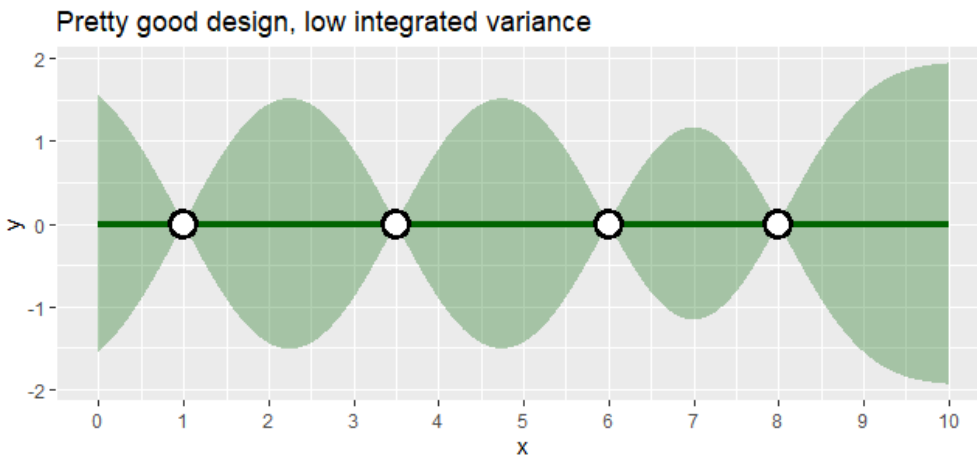
Kriging based Design

Write here $k(\mathbb{X},\mathbb{X}) = \mathrm{Cov}\left[\mathbf{Y}_{\mathbb{X}}, \mathbf{Y}_{\mathbb{X}}\right] = \mathbf{K}$ and $k(\mathbb{X},x) = \mathrm{Cov}\left[\mathbf{Y}_{\mathbb{X}}, Y_x\right] = k(x,\mathbb{X})^\top = \mathbf{k}_x$.

Lower prediction variance is better : optimize $\mathbb{X}$ in order to minimize the sum of prediction variances over χ for a given measure μ.

$$IMSE(\mathbb{X}) = \int_\chi v(x)d\mu(x) = \int_\chi \left(\sigma_x^2 - k(x,\mathbb{X})k(\mathbb{X},\mathbb{X})^{-1}k(x,\mathbb{X})\right) d\mu(x)$$





Other criterions : maximizing entropy or Mutual Information *Krause et al.*, 2008.

to be continued...

in the rest of the lecture, we will detail more results on

- Kernels, covariance functions.
- (Hyper)-parameters estimation.

Kernels

What is a kernel ?

Small recap

In former slides we assumed that some matrices where given :

- covariances matrices $k(\mathbb{X}, \mathbb{X})$ between observed outputs $\mathbf{Y}_{\mathbb{X}}$
- covariances $k(\mathbb{X}, x)$ between observed outputs and target Y_x

We have seen that there was a function $k : \chi \times \chi \to \mathbb{R}$ that was able to create valid covariance matrices : this function is named the kernel.

Kernel types

- Stationary kernels : such that $k(x, x') = k(x - x')$ for any x, x'.
  Correlation only depends on the distance and the direction between two points : insensitive to translations, sensitive to rotations.
- Isotropic kernels : such that $k(x, x') = k(||x - x||_2)$ for any x, x'.
  Correlation only depends on the euclidean distance between two points :. insensitive to translations, insensitive to rotations.

We will define Kernel properties in this section.

Motivation

We have seen two approach of the same Kriging model, using either

- Statistical approach (BLUP)
- Conditional Gaussian Process Approach

Both were assuming the knowledge of covariances $k(\mathbb{X}, \mathbb{X})$ between observed outputs $\mathbf{Y}_{\mathbb{X}}$, and covariances $k(\mathbb{X}, x)$ between observed outputs and target Y_x.

We now investigate the impact of the covariance function $k(.,.)$.
For this, we first need to sample trajectories of $Y(.)$...

Sampling trajectories from a Kernel

How to sample

sample a Gaussian Vector $\mathcal{N}(\mu, \mathbf{\Sigma})$ at specific locations (on a fine grid).

- method 0 : use direct simulator of multivariate normal. e.g. in R : MASS : :mvrnorm(n=..., mu=..., Sigma=...) to sample n paths. ☺
  See the document `GaussianSampleSimulation.Rmd`
- method 1 : sample $\mu + \boldsymbol{A}\boldsymbol{Z}$ where $\mathbf{\Sigma} = \boldsymbol{A}\boldsymbol{A}^\top$ (Cholesky decomposition) and $\boldsymbol{Z}$ standard normal
- method 2 : same with $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Lambda}^{1/2}$ obtained from a spectral decomposition $\mathbf{\Sigma} = \boldsymbol{U}\mathbf{\Sigma}\boldsymbol{U}^{-1}$.

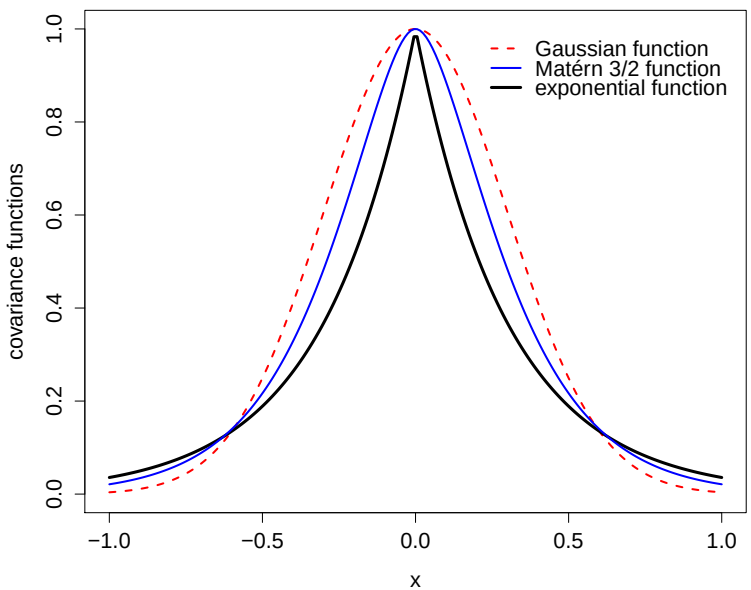
An example

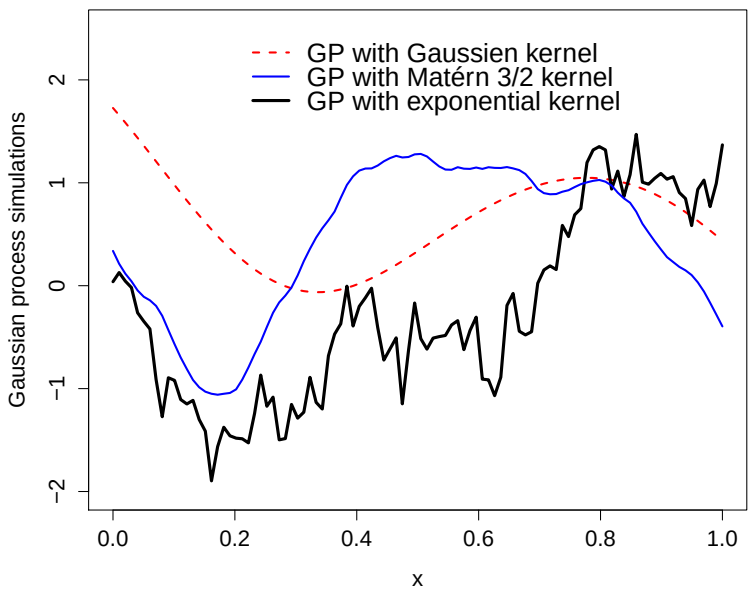
Say $k(x, x') = \sigma^2 \exp\left(-(x - x')^2/\theta^2\right)$ and in pseudo-R : build a fine grid `X`, choose mean function `mu()`, build the covariance matrix, `K[i,j]=k(X[i],X[j])`, eigenanalysis, `Keig = eigen(K)`, and sample the path $y =$ `mu[X] + Keig$vectors %*% diag(sqrt(Keig$values)) %*% matrix(rnorm(n))`

⇒ See also Shiny App : `https://github.com/NicolasDurrande/shinyApps`

Kernel impact

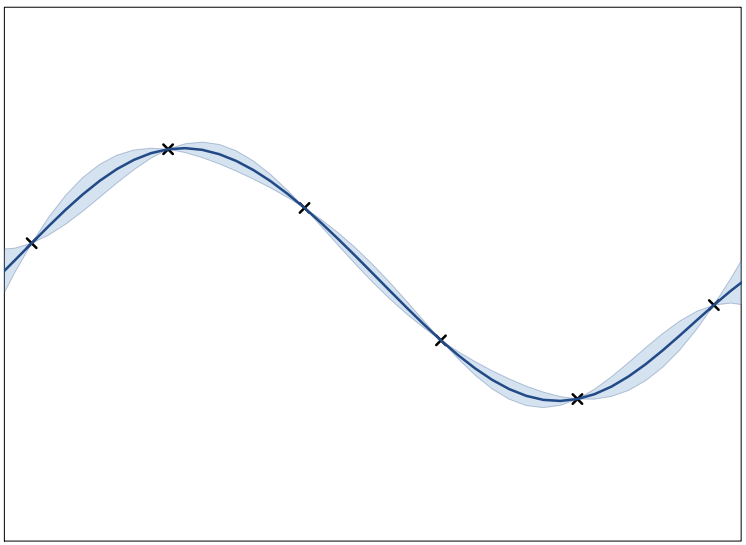
A summary illustration of Kernel impact on trajectories



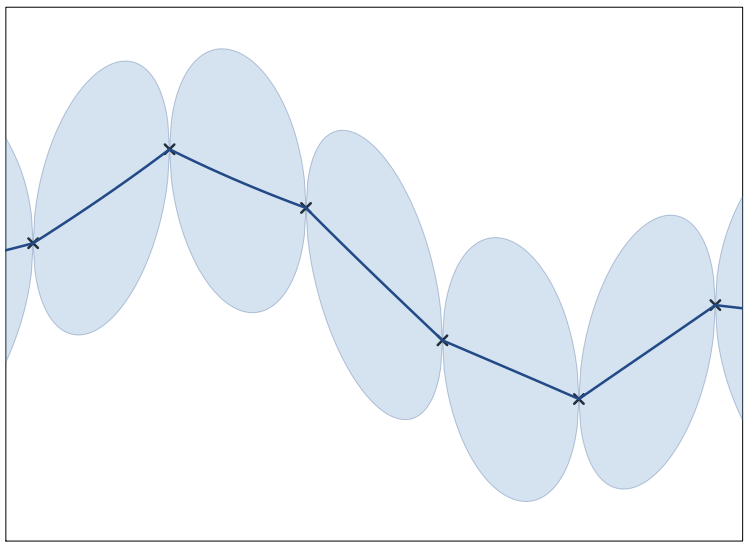


Changing the kernel has a huge impact on the model :

Gaussian kernel:

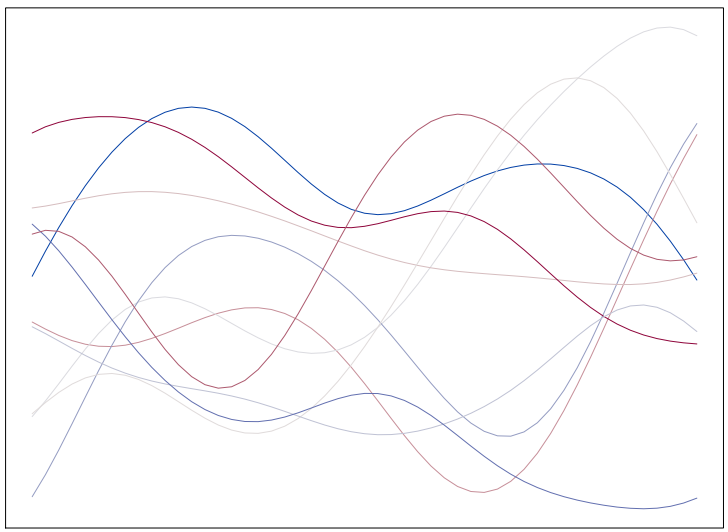


Exponential kernel:

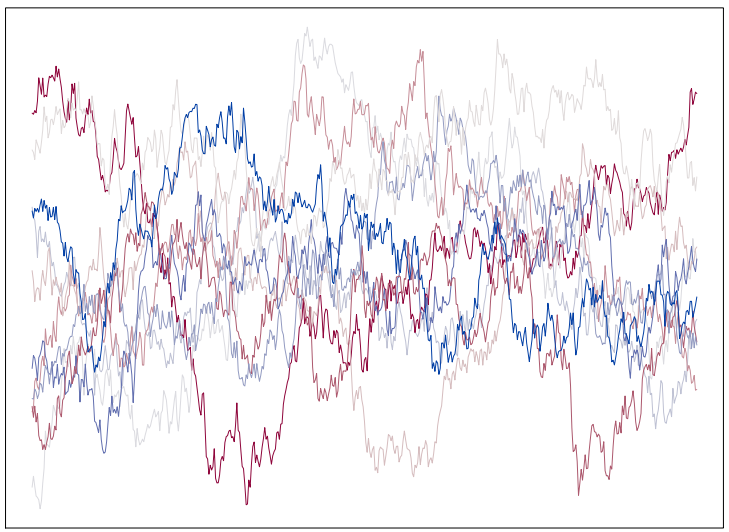


This is because changing the kernel means changing the prior on f

Gaussian kernel:

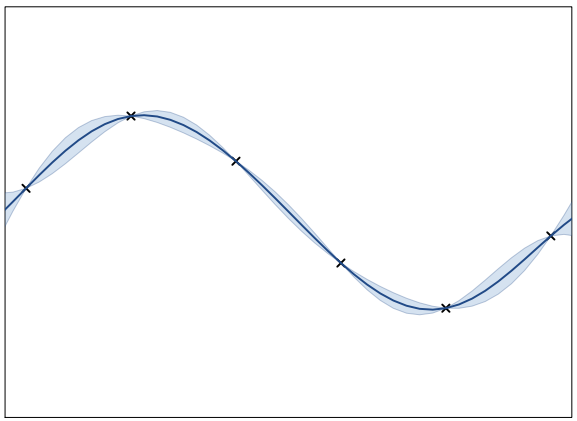


Exponential kernel:

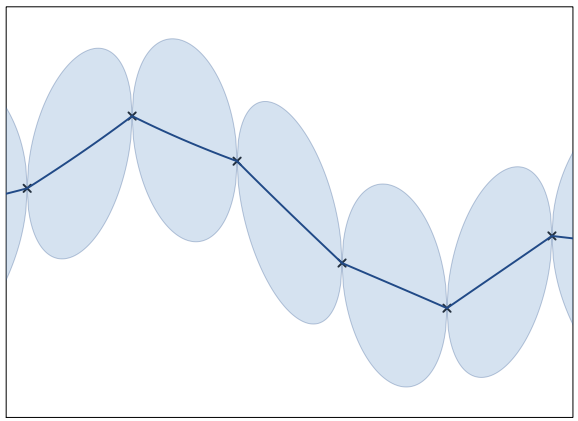


There is no kernel that is intrinsically better... it depends !

Gaussian kernel:



Exponential kernel:



The kernel has to be chosen according to the prior belief on the behaviour of the function to study :

- is it continuous, differentiable, how many times ?
- is it stationary ?
- is it monotonous, bounded ? Cf. [8]
- ...
- Default : constant trend μ (empirical mean or $\widehat{\mu}$ from max likelihood [10]) and Matérn 5/2 kernel.

Valid kernels

A kernel satisfies the following properties

Kernel requirement

- It is symmetric : $k(x, x') = k(x', x)$
- It is positive semi-definite (psd) :

$$\forall n \in \mathbb{N}, \forall x_i \in \chi, \forall \boldsymbol{a} \in \mathbb{R}^n, \sum_{i=1}^{n}\sum_{j=1}^{n} a_i a_j k(x_i, x_j) \geq 0$$

Furthermore any symmetric psd function can be seen as the covariance of a Gaussian process. This equivalence is known as the Loeve theorem.

What would happen if a kernel was not positive semi-definite ?

Many other results, such as integral representations, can be found in the literature (see *Abrahamsen*, 1997, *Rasmussen*, 2003...). e.g : $k(\tau) = \mathbb{E}\left[\exp(-\tau V)\right]$, where V is a non-negative RV, is a valid isotropic kernel in any dimension.

Popular kernels in 1D

There are a lot of functions that have already been proven psd :

constant	$k(x,x') = \sigma^2$
white noise	$k(x,x') = \sigma^2 \mathbf{1}_{\{x=x'\}}$
Brownian	$k(x,x') = \sigma^2 \min(x,x')$
power-exponential	$k(x,x') = \sigma^2 \exp\left(-\lvert x-x'\rvert^p/\theta\right)$, $0 < p \leq 2$
Matérn 3/2	$k(x,x') = \sigma^2 \left(1+\lvert x-x'\rvert\right) \exp\left(-\lvert x-x'\rvert/\theta\right)$
Matérn 5/2	$k(x,x') = \sigma^2 \left(1+\lvert x-x'\rvert/\theta + 1/3\lvert x-x'\rvert^2/\theta^2\right) \exp\left(-\lvert x-x'\rvert/\theta\right)$
squared exponential	$k(x,x') = \sigma^2 \exp\left(-(x-x')^2/\theta^2\right)$
linear	$k(x,x') = \sigma^2 x x'$
$\vdots$	

- The parameter σ^2 is called the **variance** and θ the **length-scale**.
- General factorized form : $k(x,x') = \sigma^2 r(x,x')$, $r(,)$ the correlation function. In this case, $k(x,\mathbb{X})k(\mathbb{X},\mathbb{X})^{-1} = r(x,\mathbb{X})r(\mathbb{X},\mathbb{X})^{-1}$.

here `https://bit.ly/2K7hnzx` : are there oscillating correlation functions ?

Kernel design : making new from old

Many operations can be applied to psd functions while retaining this property

Kernels can be :

- Summed
  - On the same space $k(x, x') = k_1(x, x') + k_2(x, x')$
  - On the tensor space $k(x, x') = k_1(x_1, x_1') + k_2(x_2, x_2')$
- Multiplied
  - On the same space $k(x, x') = k_1(x, x') \times k_2(x, x')$
  - On the tensor space $k(x, x') = k_1(x_1, x_1') \times k_2(x_2, x_2')$
- Composed with a function
  - $k(x, x') = k_1(h(x), h(x'))$

- to create new (non stationary) kernels, increase their dimension.
- All these transformations can be combined.

isotropy

Lengthscales parameters per dimension

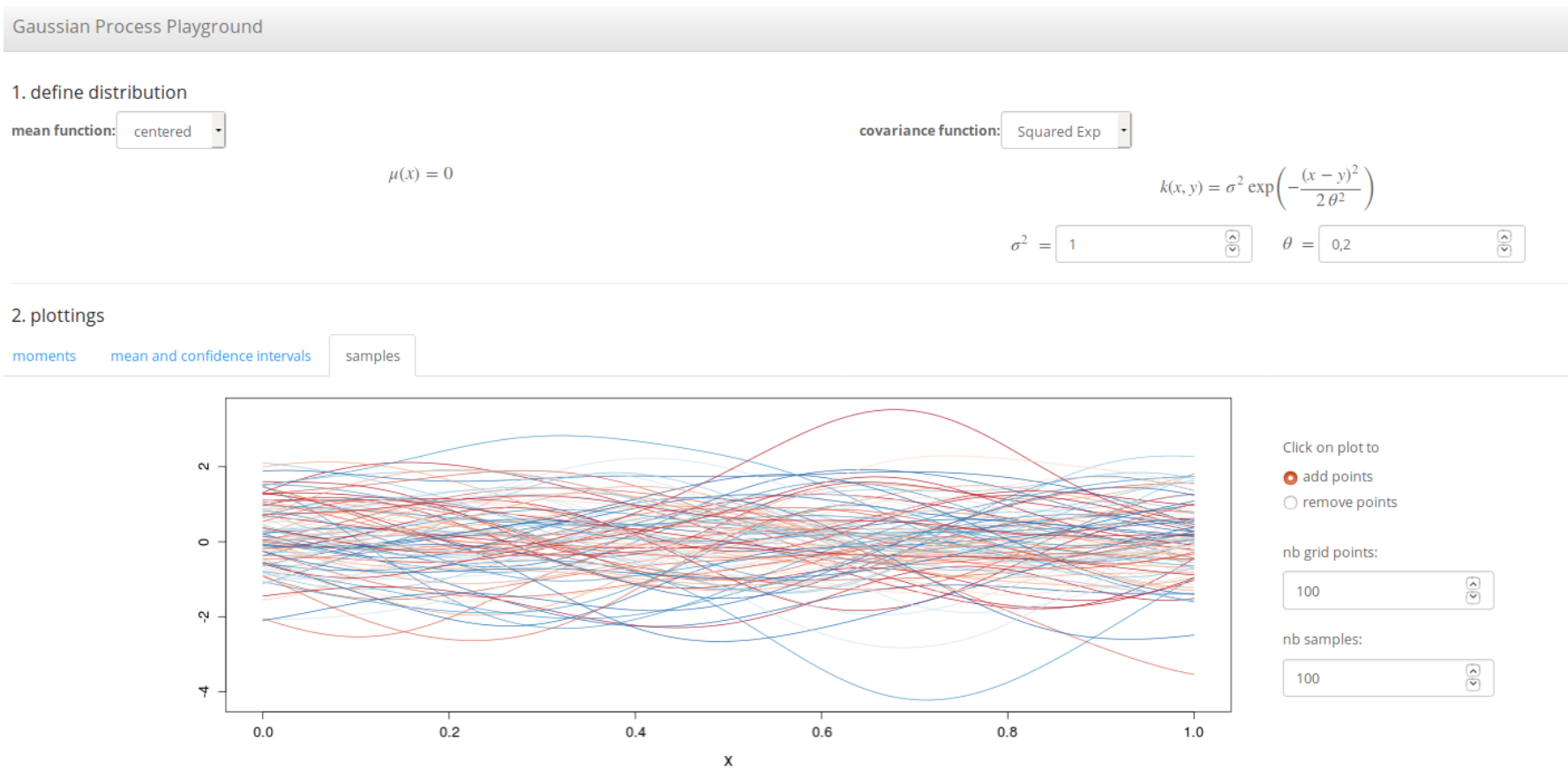
In higher dimension one can introduce one length-scale parameter per dimension. The usual Euclidean distance between two points $||x - y|| = (\sum (x_i - y_i)^2)^{1/2}$ is thus replaced by

$$||x - y||_\theta = \left(\sum_{i=1}^{d} \frac{(x_i - y_i)^2}{\theta_i^2} \right)^{1/2}.$$

If the parameters θ_i are equal for all the dimensions, the covariance (or the process) is called **isotropic**.

Trajectories with squared exponential kernel

and the Shiny App @ `https://github.com/NicolasDurrande/shinyApps`



Trajectories with the Brownian kernel

Gaussian Process Playground

1. define distribution

mean function: centered

$$\mu(x) = 0$$

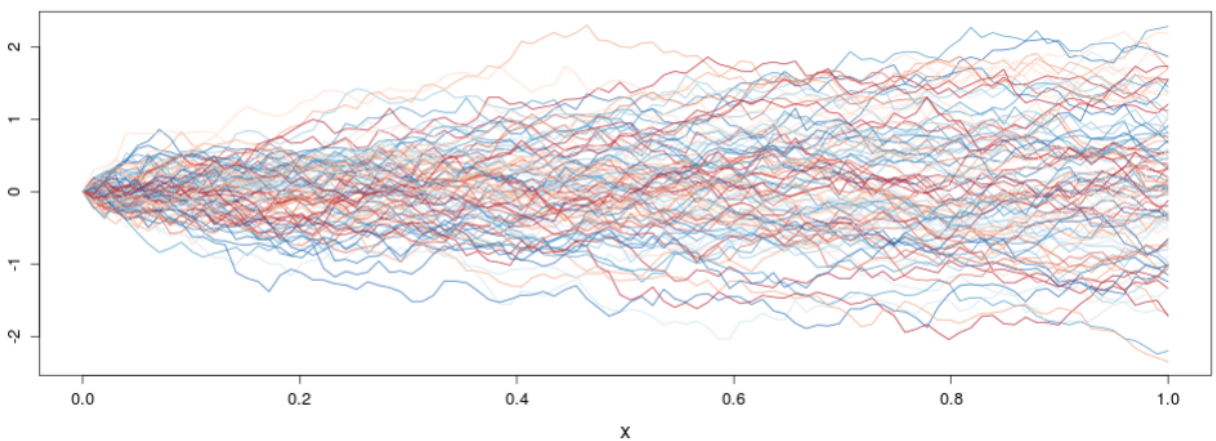
covariance function: Brownian

$$k(x, y) = \sigma^2 \min(x, y)$$

$\sigma^2 =$ 1

2. plottings

moments | mean and confidence intervals | samples



Click on plot to
- add points
- remove points

nb grid points: 100

nb samples: 100

Trajectories with the Matérn 3/2 kernel

Gaussian Process Playground

1. define distribution

mean function: centered

$$\mu(x) = 0$$

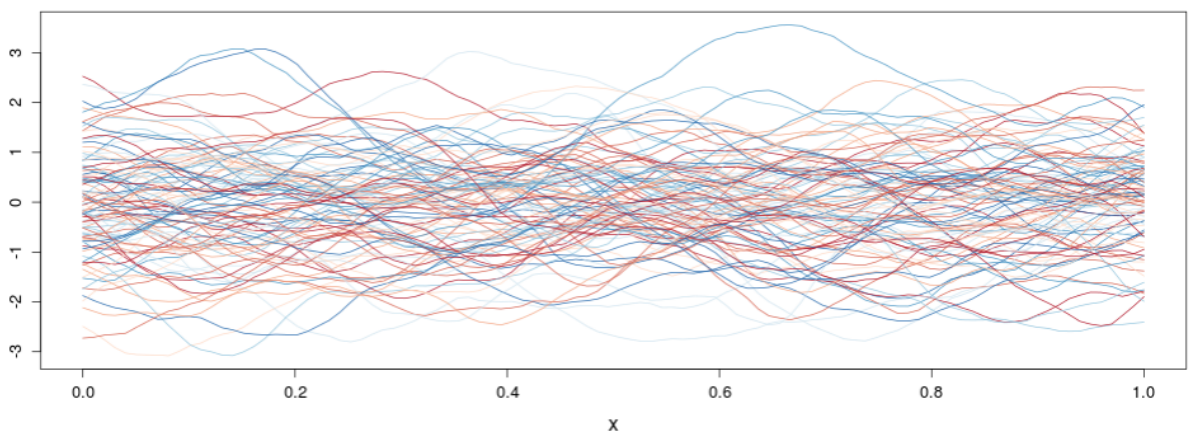
covariance function: Matern 3/2

$$k(x,y) = \sigma^2 \left(1 + \sqrt{3}\frac{|x-y|}{\theta}\right) \exp\left(-\frac{|x-y|}{\theta}\right)$$

σ^2 = 1 θ = 0,2

2. plottings

moments | mean and confidence intervals | samples



Click on plot to
- add points
- remove points

nb grid points: 100

nb samples: 100

Trajectories with the exponential kernel

Gaussian Process Playground

1. define distribution

mean function: centered

$$\mu(x) = 0$$

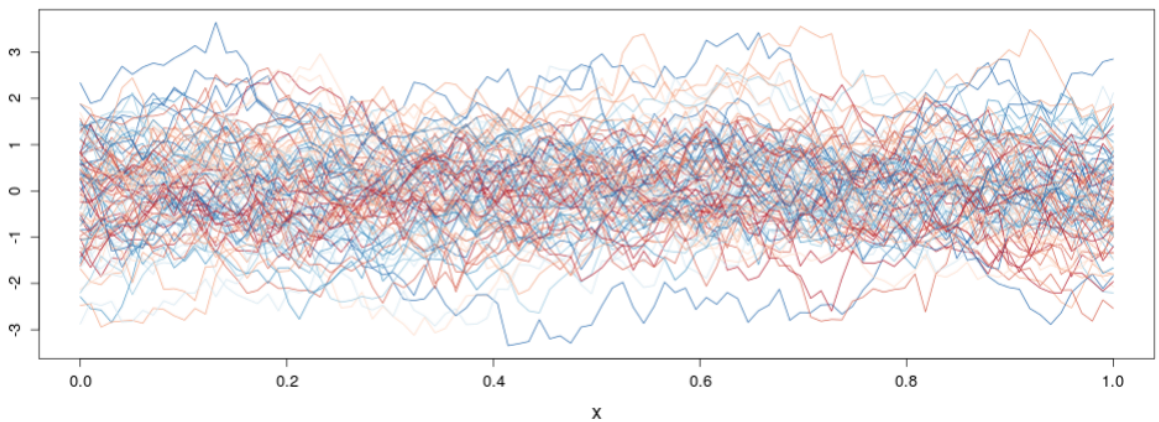
covariance function: Exponential

$$k(x, y) = \sigma^2 \exp\left(-\frac{|x - y|}{\theta}\right)$$

σ^2 = 1 θ = 0,2

2. plottings

moments | mean and confidence intervals | samples



Click on plot to
- add points
- remove points

nb grid points: 100

nb samples: 100

Regularity and covariance function

Regularity of sample path

The regularity and frequency content of the $y(x)$ are controlled by the kernel (and its length-scale), cf. *Abrahamsen*, 1997, Corollary 2.4.2.

The behavior of $k(\tau)$ at $\tau = 0$ define the regularity of the process.

Regularity of sample path

For stationary processes (depend on $\tau = x - x'$ only), the trajectories are p times differentiable (in the mean square sense) if $k(\tau)$ is $2p$ times differentiable at $\tau = 0$

Examples

- trajectories with squared exponential kernels are infinitely differentiable = very (unrealistically ?) smooth.
- trajectories with Matérn 5/2 and 3/2 kernels are twice and once differentiable.
- trajectories with power-exponential are not differentiable excepted when $p = 2$.
- e.g. in dim 1, trajectories with exponential kernel, $k(x, x') = \exp(-|x - x'|)$ are not differentiable (due to $|.|$)

Popular multi-dimensional kernels (1/2)

radial kernels

constant	$k(x,x') = \sigma^2$
white noise	$k(x,x') = \sigma^2 \delta_{x,x'}$
exponential	$k(x,x') = \sigma^2 \exp\left(-\|\|x-x'\|\|_\theta\right)$
Matérn 3/2	$k(x,x') = \sigma^2 \left(1+\sqrt{3}\|\|x-x'\|\|_\theta\right) \exp\left(-\sqrt{3}\|\|x-x'\|\|_\theta\right)$
Matérn 5/2	$k(x,x') = \sigma^2 \left(1+\sqrt{5}\|\|x-x'\|\|_\theta + \frac{5}{3}\|\|x-x'\|\|_\theta^2\right) \exp\left(-\sqrt{5}\|\|x-x'\|\|_\theta\right)$
squared expo.	$k(x,x') = \sigma^2 \exp\left(-\frac{1}{2}\|\|x-x'\|\|_\theta^2\right)$

where $||x-x'||_\theta = \left(\sum_{i=1}^d \frac{(x_i - x_i')^2}{\theta_i^2}\right)^{1/2}$.

Popular multi-dimensional kernels (2/2)

Tensor-product kernel

A common general recipee : a product of univariate kernels,

$$k(x, x') = \sigma^2 \prod_{i=1}^{d} r_i(x_i, x_i')$$

which has $d + 1$ parameters.

Parameter estimation

Estimating of lengthscales

We have seen

- Some properties of covariance kernel
- Some families of valid kernels
- The impact of the family on the sample paths and the model

Now, we mainly aim, for a given family, at :

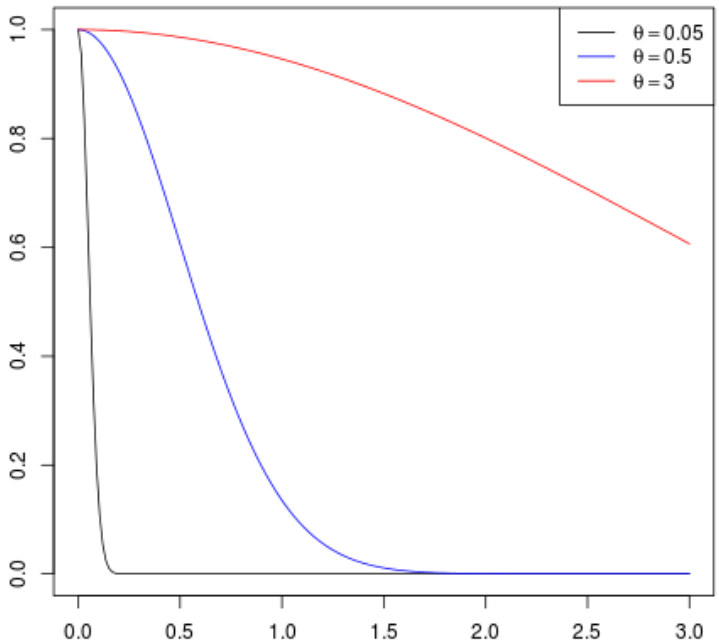
estimating lengthscales and variance parameter.

and eventually choosing the right family.

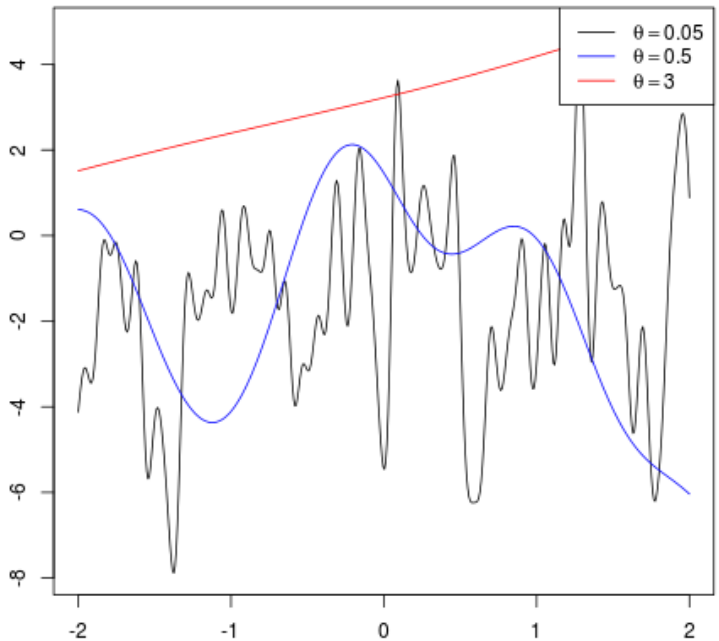
Effect of θ, squared exponential kernel

Let us first look at the impact of the lengthscale :

$k(|x - x'|)$



trajectories $y(x)$



Parameter estimation

We have seen previously that the choice of the kernel and its parameters (σ^2, the θ's, the trend and other parameters) have a great influence on the model.

In order to choose a prior that is suited to the data at hand, we can :

1. infer from variation of the response at given distance
2. maximize the model likelihood
3. minimise the model prediction error
4. use correlations (if multiple observations of the field)
5. etc.

We will detail the three first approaches, the fourth one in TP2.

Variogram

Process variations

Assume the covariance kernel is isotropic, so that it only depends on distances between points.

$$k(x, x') = k(||x - x'||_2) \tag{11}$$

Assume $\tau = ||x - x'||_2$ the euclidean distance between points. Define

$$\gamma(\tau) = \frac{1}{2}\mathrm{V}\left[Y_x - Y_{x'}\right] = \frac{1}{2}\mathrm{E}\left[(Y_x - Y_{x'})^2\right] \tag{12}$$

One can easily see that $\gamma(h) = \frac{1}{2}\mathrm{V}\left[Y_x\right] + \mathrm{V}\left[Y_{x'}\right] - 2\mathrm{Cov}\left[Y_x, Y_{x'}\right]$, and

Variogram function

Let $\tau = ||x - x'||_2$ the function γ is called the variogram function :

$$\gamma(\tau) = k(0) - k(\tau) = \frac{1}{2}\mathrm{E}\left[(Y_x - Y_{x'})^2\right] \tag{13}$$

Estimating $\gamma(.)$ or $k(.)$ is equivalent.

Estimation of $\gamma(.)$

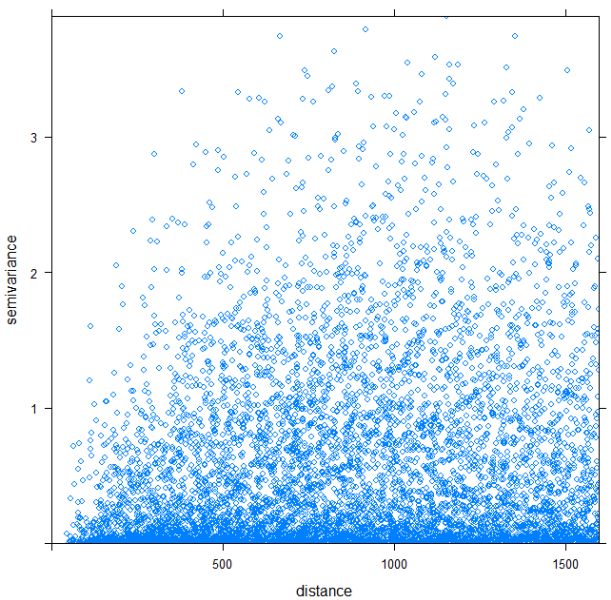
Observations of the responses are $Y_{x_i} = y_i$, $i \in \{1, \ldots, n\}$.

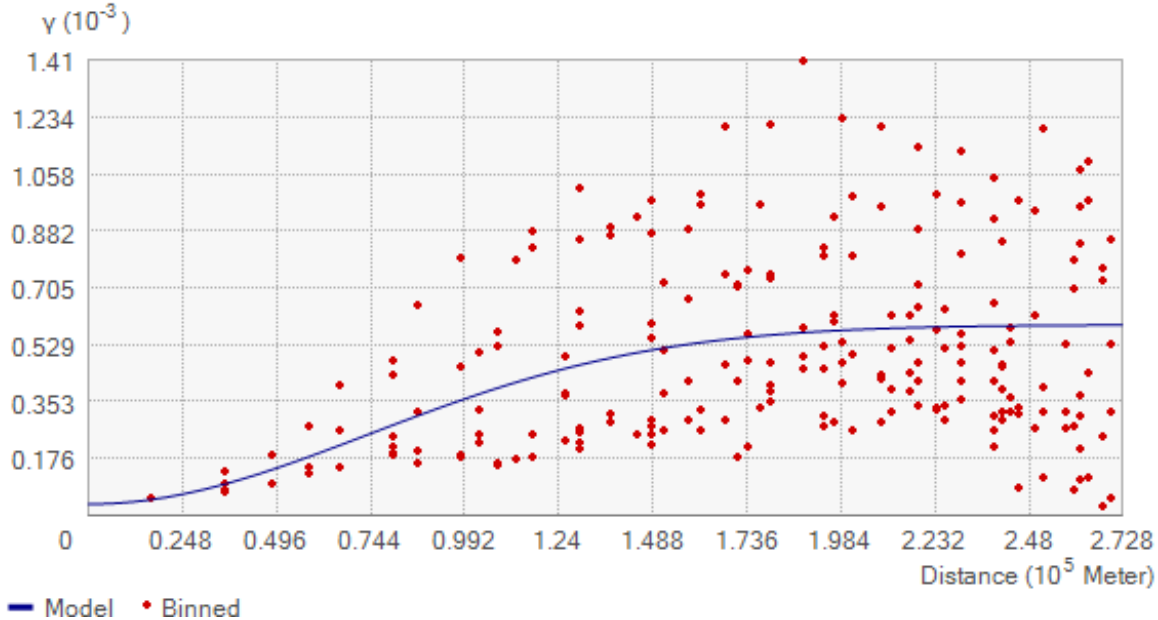
$$\text{Let } \begin{cases} \tau_{ij} &= ||x_i - x_j||_2 & \text{be the euclidean distance between } x_i \text{ and } x_j, \\ \gamma_{ij} &= \frac{1}{2}(y_i - y_j)^2 & \text{be the observed variation of } Y \text{ between } x_i \text{ and } x_j \end{cases} \tag{14}$$

The observed Scatterplot is called the Variogram cloud (*nuée variographique*)

$$\{(\tau_{ij}, \gamma_{ij})\}_{i \in I, j \in I}. \tag{15}$$

Many techniques to infer the shape of the function $\gamma(\tau)$ from this set of points.





Likelihood (1)

Likelihood

Recall the definition :
The **likelihood** of a distribution with a density f_U given observations $u^1, \ldots, u^p$ is :

$$L = \prod_{i=1}^{p} f_U(u^i)$$

- The likelihood measures the adequacy between observations and a distribution.
- One aim at maximizing the likelihood L or $\log(L)$
- Parameters obtained in this way are Maximum Likelihood Estimators (MLE)

Likelihood (2)

In the GPR context, it is possible to maximise the likelihood L or $\log(L)$ with respect to the kernel and model parameters in order to find a well suited prior.

A statistic with one observation !

We often have only **one observation** of the vector $\mathbf{y}$. The likelihood is $L = f_{\mathbf{Y}_{\mathbb{X}}}(\mathbf{y})$:

Log-Likelihood for one GP observation

$$\log L = -\frac{n}{2}\log(2\pi) - \frac{1}{2}\log\det(k(\mathbb{X},\mathbb{X})) - \frac{1}{2}(\mathbf{y}-\mu(\mathbb{X}))^\top k(\mathbb{X},\mathbb{X})^{-1}(\mathbf{y}-\mu(\mathbb{X})).$$

The likelihood is usually a multi-modal function in θ's and must be optimized with global optimization algorithms.

Likelihood (3)

In the stationary case, using $k(\mathbb{X},\mathbb{X}) = \sigma^2 r(\mathbb{X},\mathbb{X})$, MLE estimation leads to estimators of μ and σ^2 as a function of $r(\mathbb{X},\mathbb{X})$.

$$\left\{ \begin{array}{lcl} \hat{\mu} & = & (\mathbf{1}^\top r(\mathbb{X},\mathbb{X})^{-1}\mathbf{1})^{-1}\mathbf{1}^\top r(\mathbb{X},\mathbb{X})^{-1}\mathbf{y} \\ \hat{\sigma}^2 & = & \frac{1}{n}(\mathbf{y}-\hat{\mu}\mathbf{1})^\top r(\mathbb{X},\mathbb{X})^{-1}(\mathbf{y}-\hat{\mu}\mathbf{1}) \end{array} \right. \tag{16}$$

Replacing μ and σ^2 by their estimators in $\log L$, we end up in maximizing the so-called Concentrated log-Likelihood *Jones*, 2001

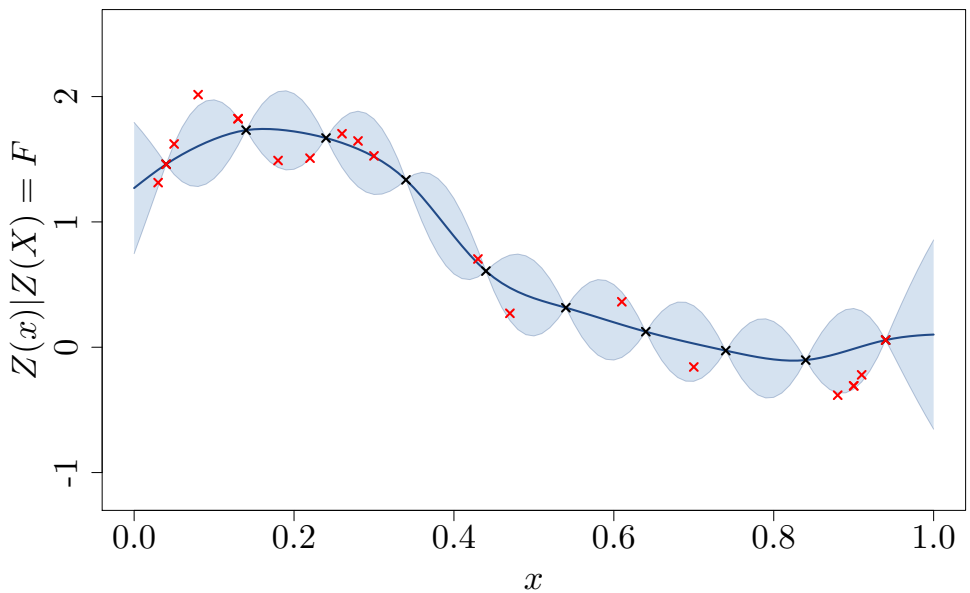
Concentrated log-Likelihood

$$\log L^{(C)} = -\frac{n}{2}\log\hat{\sigma}^2 - \frac{1}{2}\log\det r(\mathbb{X},\mathbb{X}) \tag{17}$$

Model quality (1)

We have seen that given some observations $\mathbf{y} = f(\mathbb{X})$, it is very easy to build lots of models, either by changing the kernel parameters or the kernel itself.

The question is now how to measure the quality of a model, to build the best one.
Principle : introduce new data and to compare them to the model prediction.



Since GPR models provide a mean and a covariance structure for the error they both have to be assessed.

Model quality (2)

Let $\mathbb{X}_t$ be the test set and $\mathbf{y}_t = f(\mathbb{X}_t)$ be the associated observations.

The accuracy of the mean can be measured by computing :

$$\text{Mean Square Error} \qquad MSE = \text{mean}((\mathbf{y}_t - m(\mathbb{X}_t))^2)$$

$$\text{A "normalized" criterion} \qquad Q_2 = 1 - \frac{\sum(\mathbf{y}_t - m(\mathbb{X}_t))^2}{\sum(\mathbf{y}_t - \text{mean}(\mathbf{y}_t))^2}$$

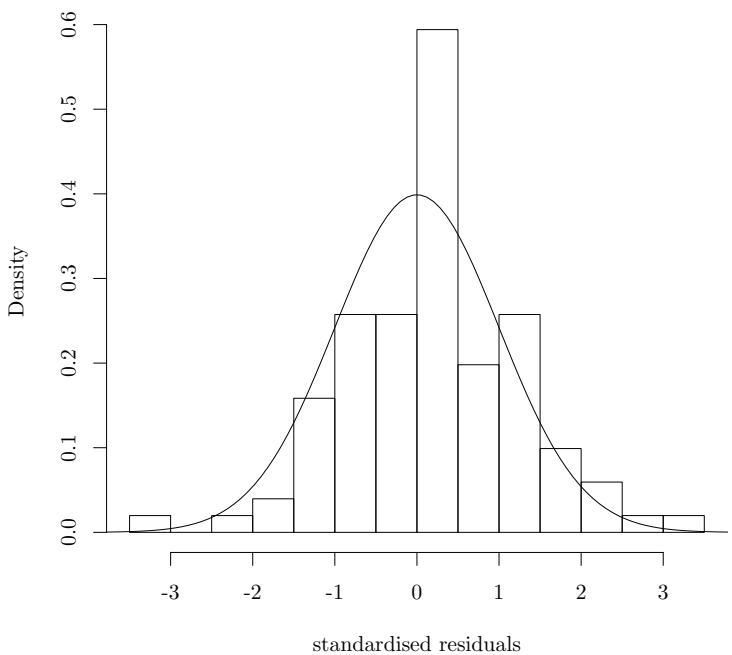
On the above example we get $MSE = 0.038$ and $Q_2 = 0.95$.

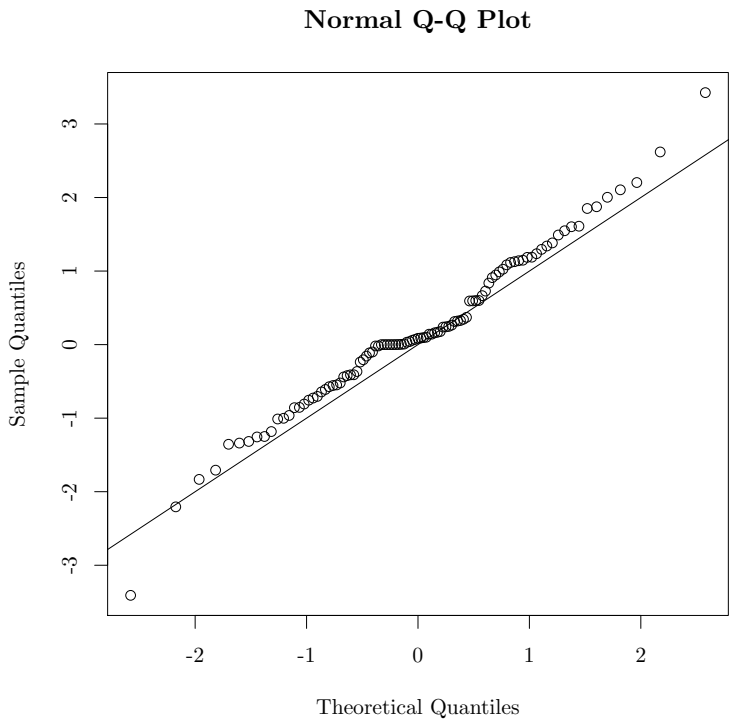
Model quality (3)

The predicted distribution can be tested by normalizing the residuals.

According to the model, $\mathbf{y}_t \sim \mathcal{N}(m(\mathbb{X}_t), c(\mathbb{X}_t, \mathbb{X}_t))$.

$c(\mathbb{X}_t, \mathbb{X}_t)^{-1/2}(\mathbf{y}_t - m(\mathbb{X}_t))$ should thus be independents $\mathcal{N}(0, 1)$:





Leave-One-Out (1)

When no test set is available, another option is to consider cross validation methods such as leave-one-out.

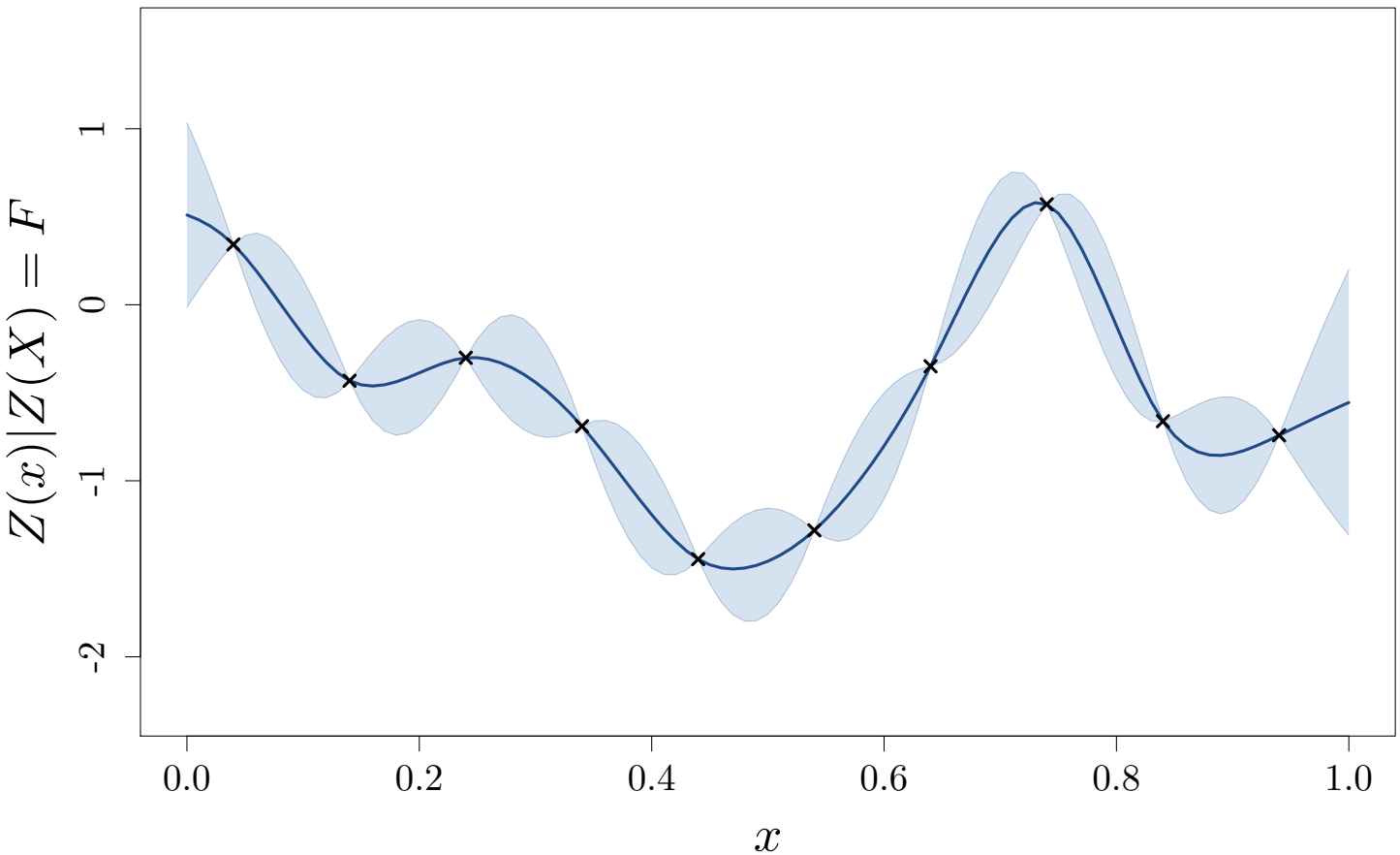
The steps are :

1. build a model based on all observations except one
2. compute the model error at this point

This procedure can be repeated for all the design points in order to get a vector of error.

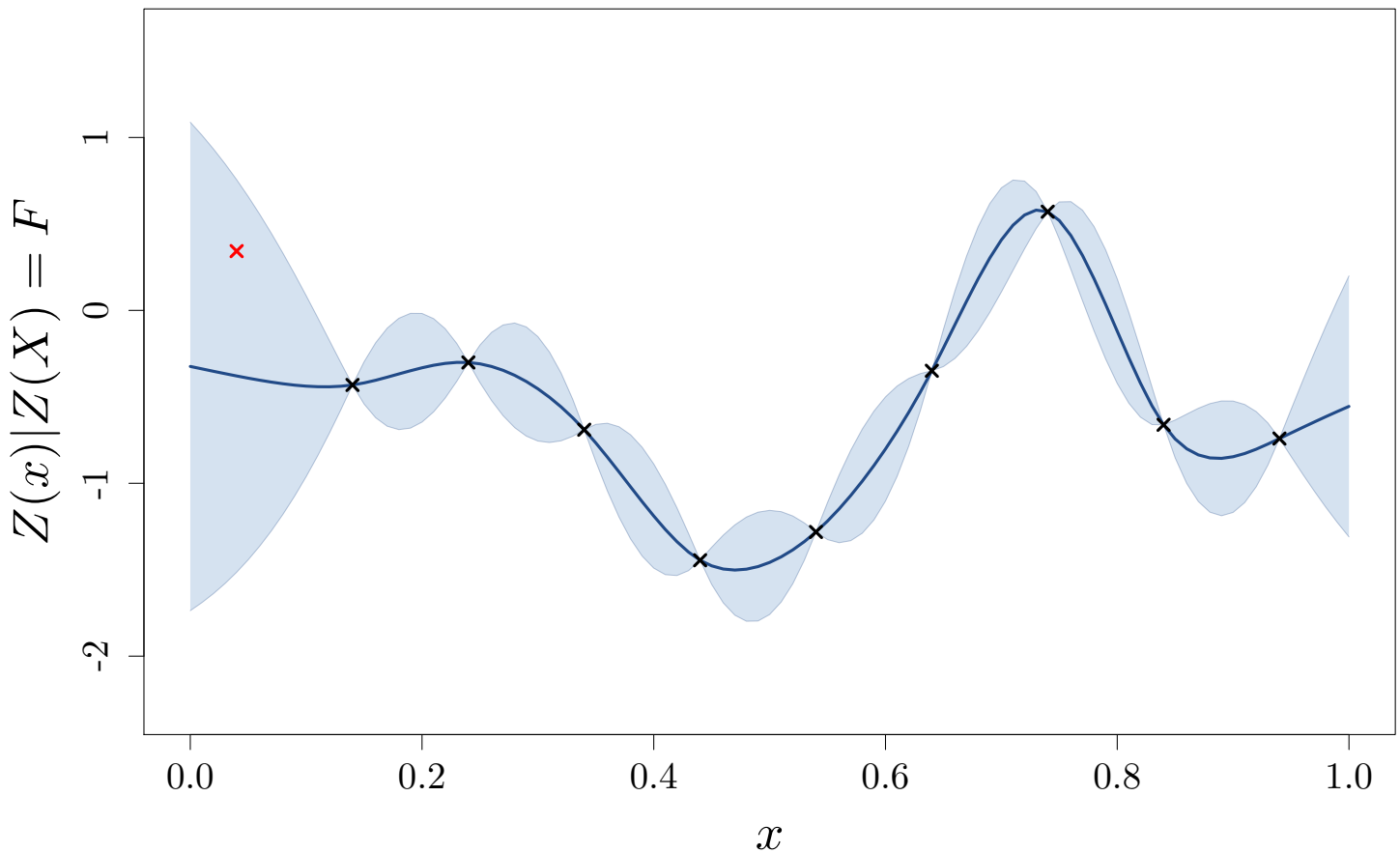
Leave-One-Out (2)

Model to be tested :



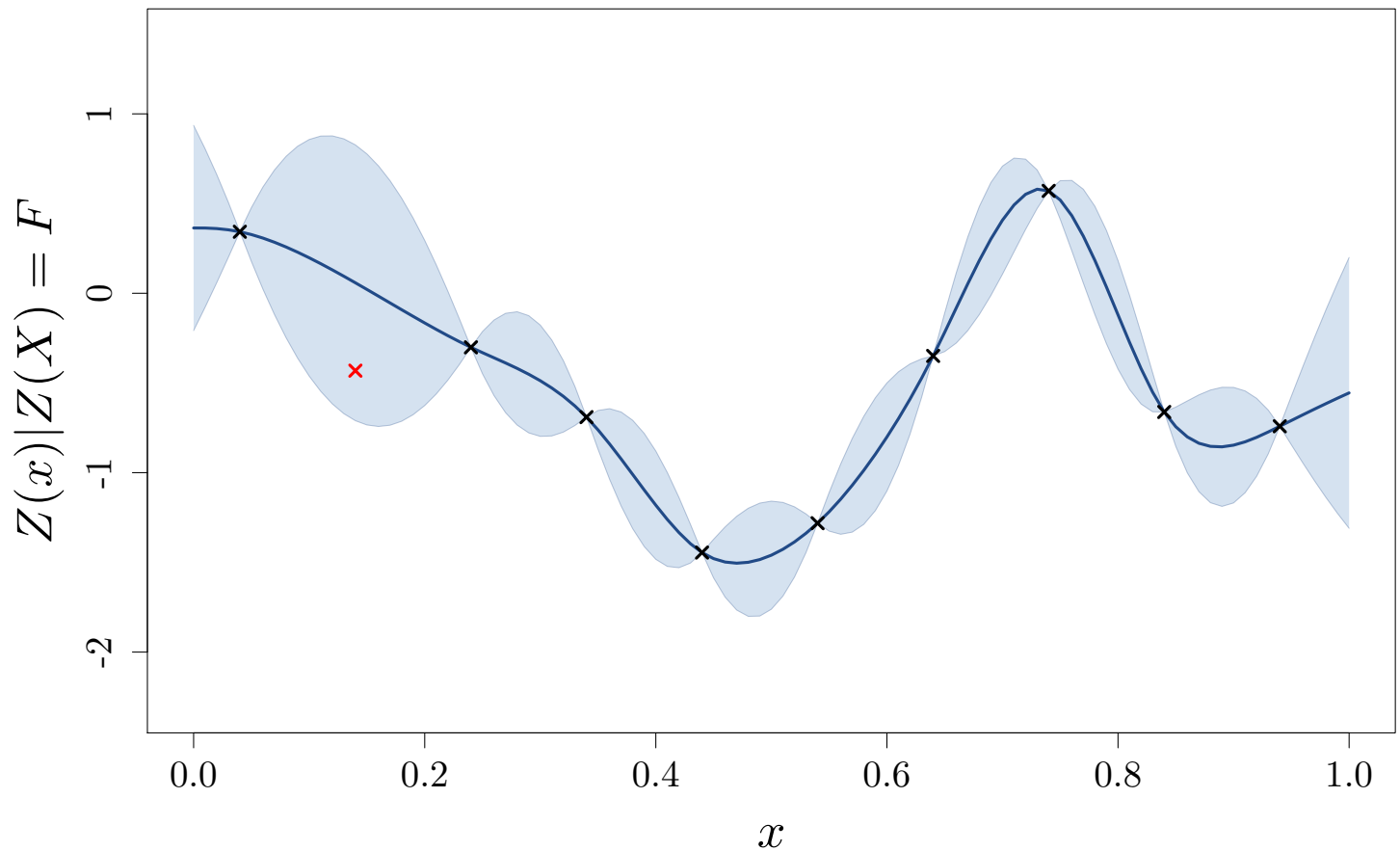
Leave-One-Out (3)

Step 1 :



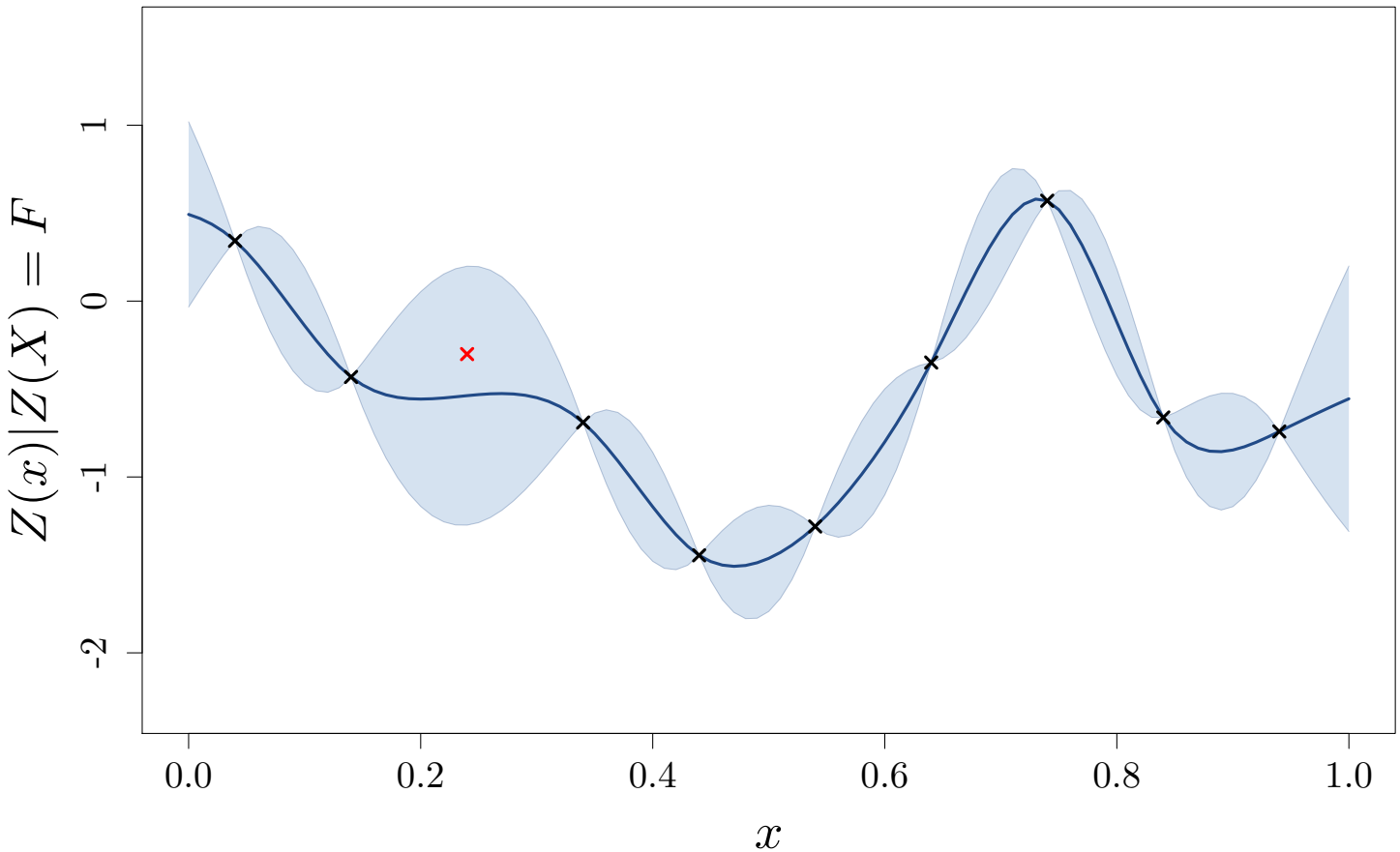
Leave-One-Out (4)

Step 2 :



Leave-One-Out (5)

Step 3 :

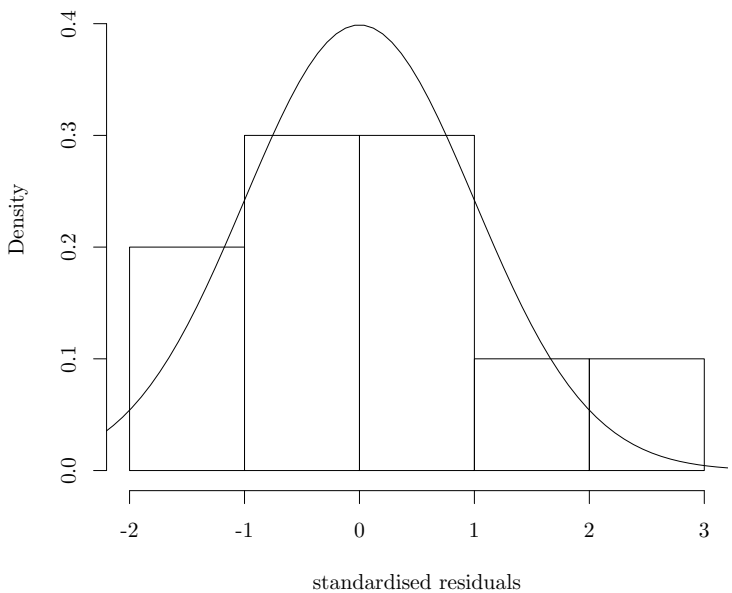


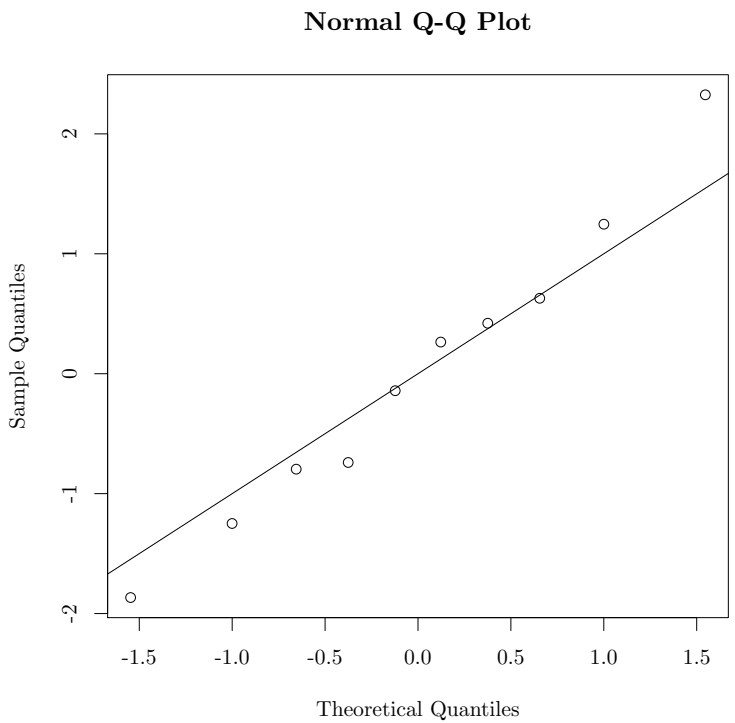
Leave-One-Out (6)

We finally obtain :

$$MSE = 0.24 \text{ and } Q_2 = 0.34.$$

We can also look at the residual distribution. For leave-one-out, there is no joint distribution for the residuals so they have to be standardized independently.

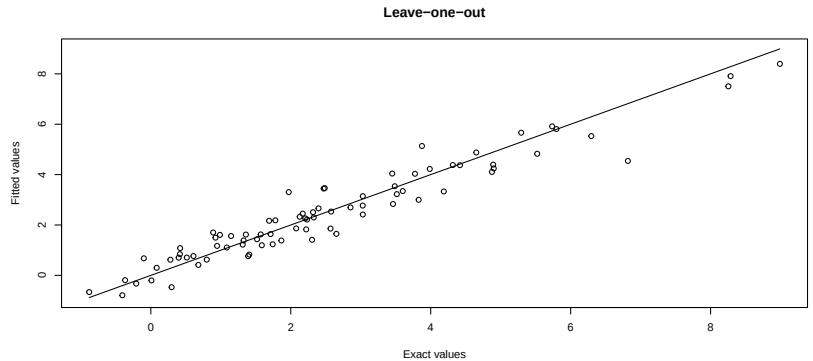


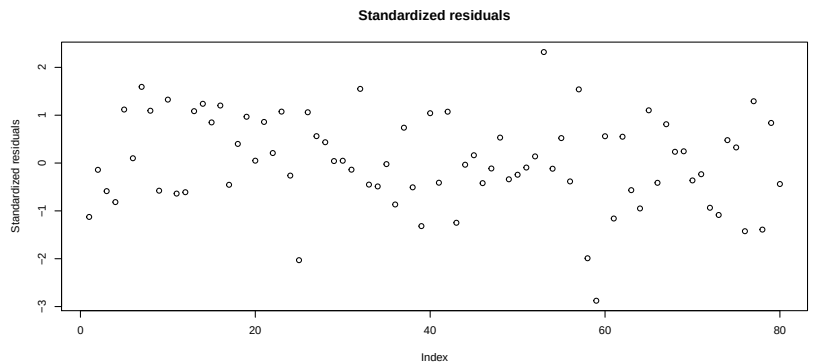


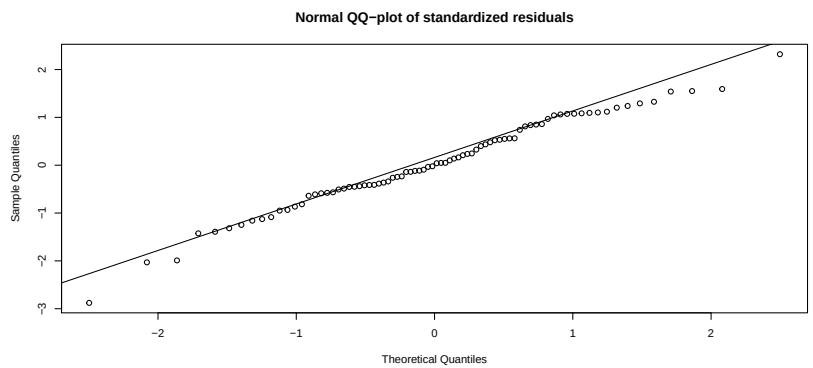
Sample code in R

(with 6D Hartman function)

```
library(DiceKriging)
library(DiceDesign)
X <- lhsDesign(n=80,...
    dimension=6)$design
X <- data.frame(X)
y <- apply(X, 1, hartman6)
mlog <- km(design = X,
response = -log(-y))
plot(mlog)
```







Conclusion

Kriging issues

Some Kriging Issues

- Too large n : $k(\mathbb{X}, \mathbb{X})$ is $n \times n$ and takes $\mathcal{O}(n^3)$ operations for its inversion $\Rightarrow$ not directly applicable beyond $n = 1000$. Solutions : inducing points [3], nested kriging [11].
- $k(X, X)$ is ill-conditioned : regularize it, 3 variants in [7] (nugget, pseudo-inverse and distribution-wise GP).
- Maximizing the likelihood (for infering the GP parameters) or minimizing the cross-validation error are multi-modal problems in $\mathcal{O}(d)$ dimensions : use global optimization algorithms.

Advantages of the Statistical Approach

Some advantages of the "statistical approach" (compared to other approaches)

Pro

- General : only requires random variables with two moments, no Gaussian assumption, manipulate only finite vectors
- Can be extended with other regression techniques : penalizations (LASSO, ridge), cross effects, quadratic terms, link functions...

$$M(x) = \sum_i \alpha_i(x) Y_{x_i} - \lambda \left| \sum_i \alpha_i(x) \right|$$

$$M(x) = f\left(Y_{x_1}, ..., Y_{x_n}, \boldsymbol{\alpha}\right)$$

- Can be nested using other estimators

$$M(x) = \sum_i \alpha_i(x) M_i(x)$$

Cons

- Interpretation : No direct interpretation as a conditional process
- Theroretical : Conditional quantities sometimes hard to derive

Advantages of the Conditional Process Approach

Some advantages of the "Conditional Process" approach

Pro

- Beautiful : clearly defined conditional distribution, clear quantities of interest, e.g. $\mathrm{Cov}\left[Y_x, Y_{x'} | \mathbf{Y}_{\mathbb{X}}\right]$
- Conditional trajectories can be obtained.
- Natural expression for covariances, nice modeling of the underlying prior process.
- Natural Bayesian interpretation : prior/posterior process.
- Can be extended to other processes (max-stable, elliptical,..).

Cons

- Hard : extensions can be hard to calculate (conditional law when no stability...)
- Formal : requires defining a whole process, understanding the conditional law.

A tiny summary

What we have seen

- Kriging as a Best Linear Unbiased Predictor.
  Take home message : weights on the form $k(\mathbb{X}, \mathbb{X})^{-1} k(\mathbb{X}, x)$.
- Kriging as a Conditional Gaussian Process.
  Take home message : Kriging mean and varaiance are mean and variance of Y_x given observations $\mathbf{Y}_{\mathbb{X}} = \mathbf{y}$.
- Some results on Kernels.
  Take home message : kernel families are related to the regularity of the process. Parameters can be estimated by cross-validation (LOO) or by MLE.

Perspectives

- There is a huge literature and remaining problems... An excellent reference book : *Rasmussen*, 2003, (cited 20 000 times !) available online
  `http://www.gaussianprocess.org/gpml/`
  Take home message : keep an eye on this book. see also
  `https://bit.ly/2K7hnzx`.

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