



Computer experiments Overview of GP-based approaches

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with acknowledgments to M. Binois, Y. Deville, N. Durrande for nice illustrations!

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Outline

- 1 Analyzing a time-consuming black box : Metamodeling and applications
- 2 Functions approximation : Three complementary point of views (geostatistics, Gaussian process, reproducing kernel Hilbert space)
- 3 Gaussian process engineering : Playing with kernels
- 4 Gaussian process in practice : Inference, validation

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Metamodeling – Computer experiments

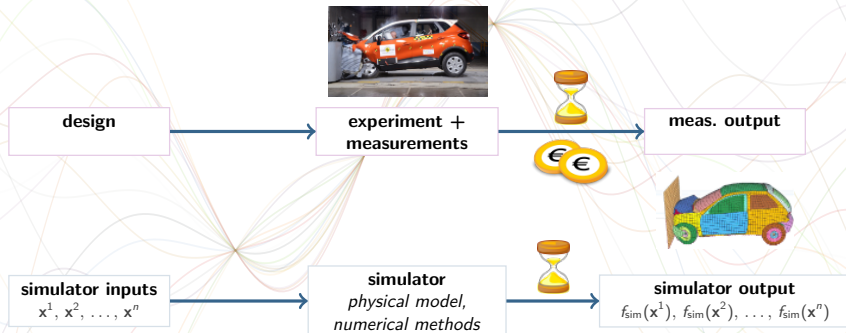


design

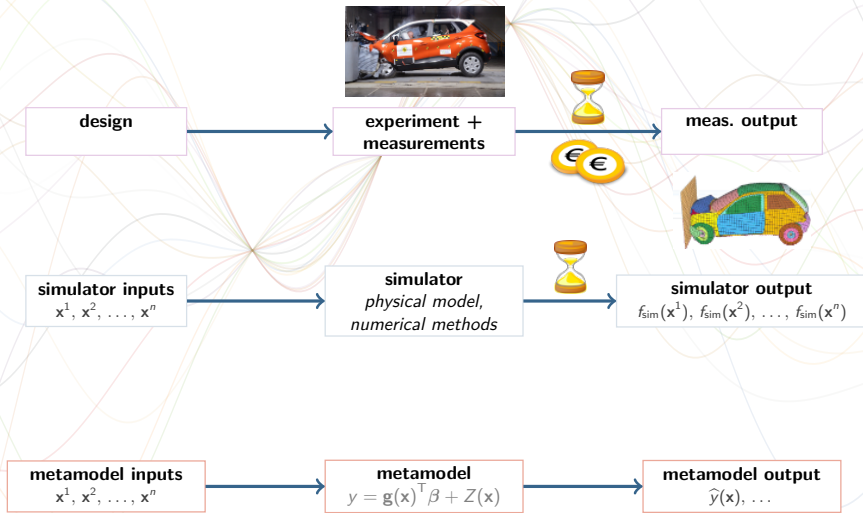
Metamodeling – Computer experiments



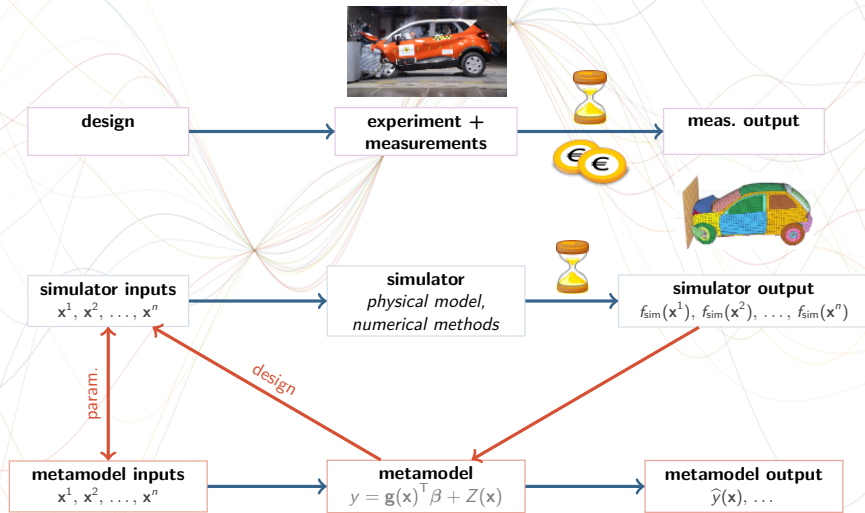
Metamodeling – Computer experiments



Metamodeling – Computer experiments



Metamodeling – Computer experiments



Metamodels : Why Gaussian processes are famous ?

- A **metamodel** is a **fast** model which approximates a time-consuming model. It can be **any regression model**, probabilistic or deterministic
 - ▶ Linear model, random forest, neural network, spline, polynomial chaos, ...

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- **Requirement : an uncertainty measure assessing ignorance at unknown area**
 - ▶ This claims in favor of probabilistic models
- **Gaussian processes (GP)** have nice features :
 - ▶ Their uncertainty measure have a closed-form
 - ▶ They are **flexible** (parameterized by two functions) and can handle prior information on data
 - ▶ They generalize splines

→ In this course, we focus on GP (regression) models

Gaussian processes

Gaussian processes are stochastic processes (or random fields) s.t. every finite dimensional distribution is Gaussian \rightarrow **Parameterized by two functions**

$$Y = (Y(x))_{x \in T} \sim GP(\underbrace{m(\mathbf{x})}_{\text{trend}}, \underbrace{k(\mathbf{x}, \mathbf{x}')}_{\text{kernel}})$$

- The trend can be any function.
- The kernel is **positive semidefinite** :

$$\forall n, \alpha_1, \dots, \alpha_n, \mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}, \quad \sum_{i=1}^n \alpha_i \alpha_j k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) \geq 0.$$

It contains the **spatial dependence**.

Gaussian processes and approximation / interpolation

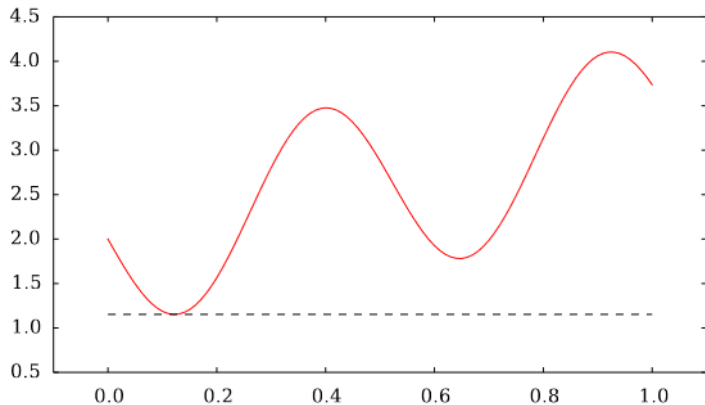
GPs conditional distributions are Gaussian, and the conditional expectation coincides with the orthogonal projection onto a linear space :

- Closed-form expressions are available
 - The conditional mean is linear in the conditioner
 - The conditional variance does not depend on it!
- very useful for adding new points in sequential strategies

In the background, Y is conditioned on $Y(x^{(1)}) = y_1, \dots, Y(x^{(n)}) = y_n$.

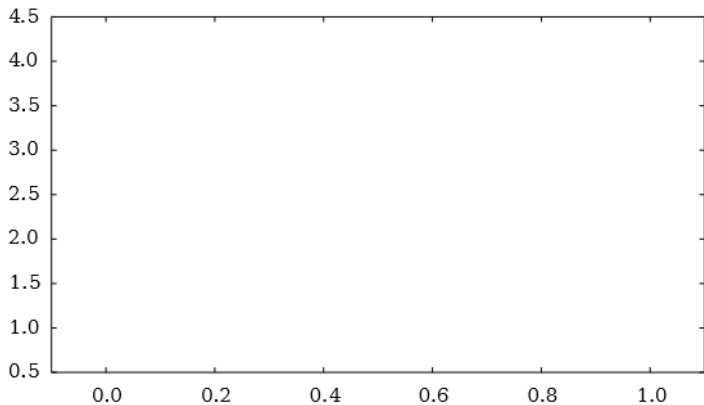
Bayesian optimization

How to find the global minimum of a function... when each evaluation is costly ?



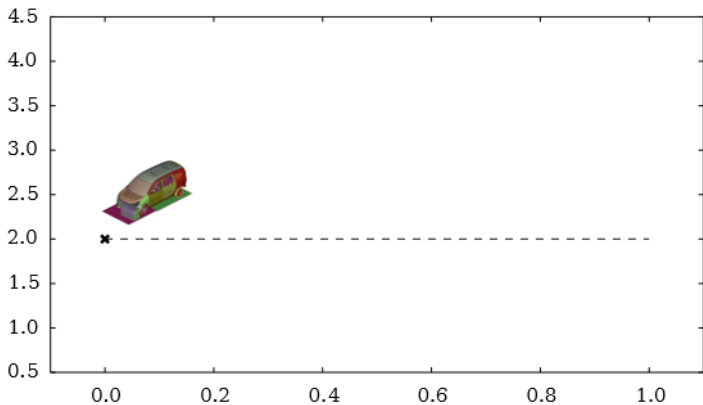
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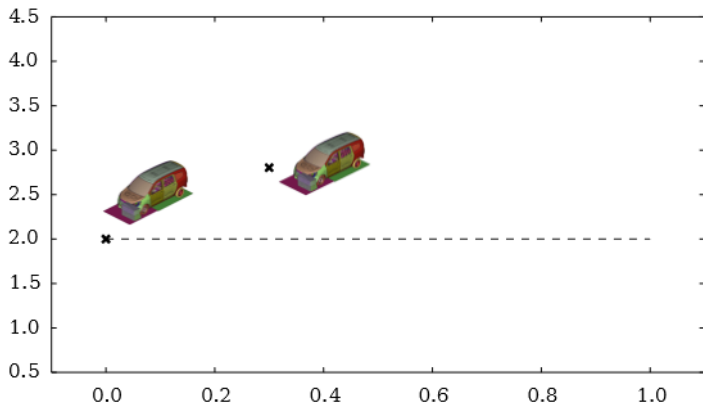
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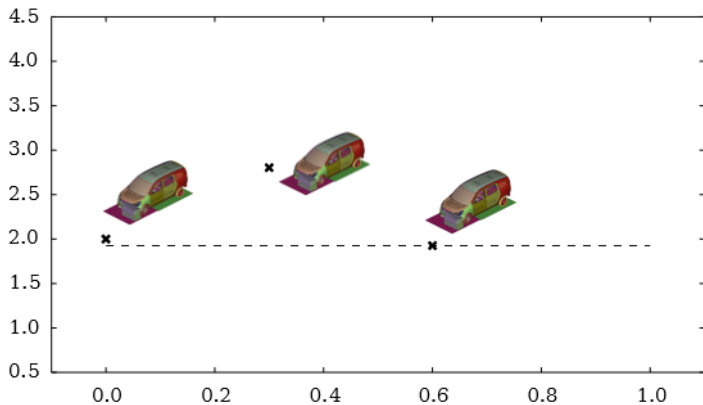
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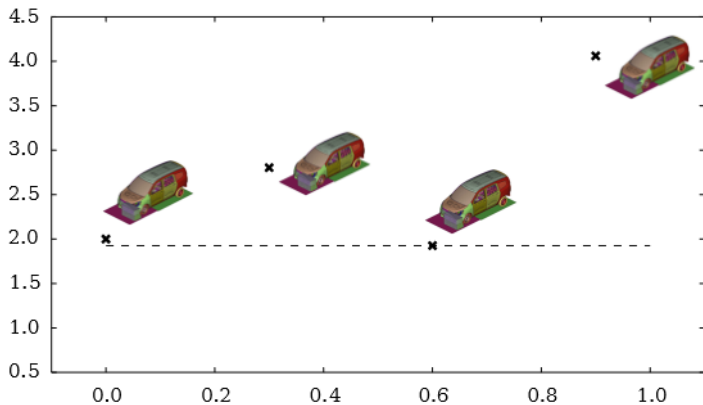
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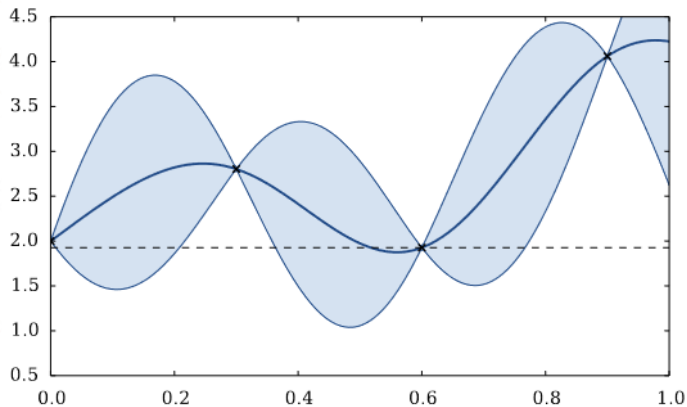
How to find the global minimum of a function... when each evaluation is costly ?



Bayesian optimization

A solution : **Bayesian optimization (BO)** [Moćkus, 1975, Jones et al., 1998]

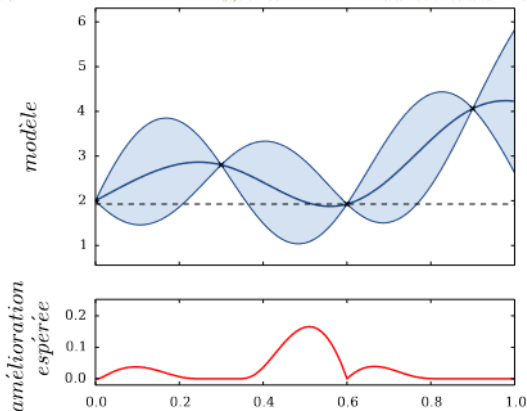
First ingredient : a GP model Y



Bayesian optimization

Second ingredient : an **easy-to-compute** criterion **accounting for uncertainty at unknown regions**, e.g. here “expected improvement”

$$EI(x) = \mathbb{E}([y_0 - Y(x)]^+ | Y(x_1), \dots, Y(x_n)) \quad y_0 : \text{current minimum}$$



Bayesian optimization

Notice that the expected improvement is indeed **easy-to-compute**.

Denote m_k, s_k the so-called **conditional mean & standard deviation**, i.e.

$$Y(x) | Y(x_1), \dots, Y(x_n) \sim \mathcal{N}(m_k(x), s_k(x)^2)$$

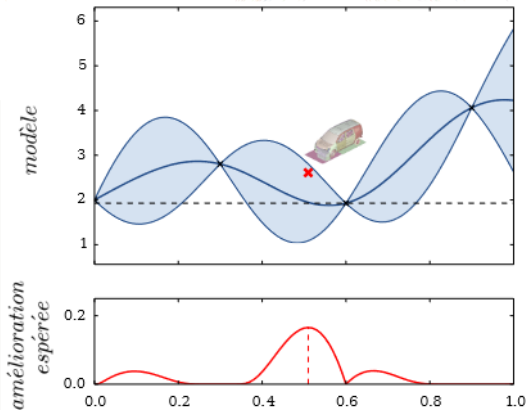
Then, we have the closed-form expression :

$$EI(x) = s_k(x)(z_0\Phi(z_0) + \phi(z_0))$$

with $z_0 = \frac{y_0 - m_k(x)}{s_k(x)}$ and ϕ, Φ the pdf, cdf of the $\mathcal{N}(0, 1)$ distribution.

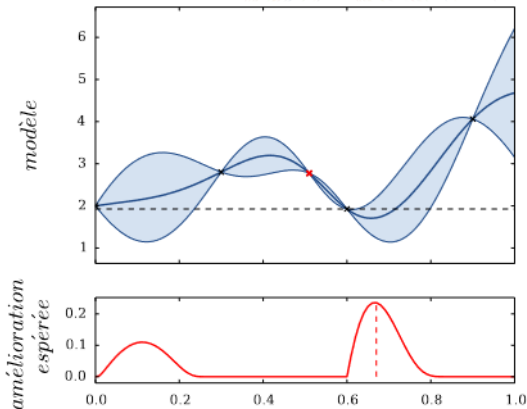
Bayesian optimization

The algorithm (here “EGO”) : (1) Find the next point by maximizing the criterion
→ (2) Evaluate the function → (3) Update the GP model ↑



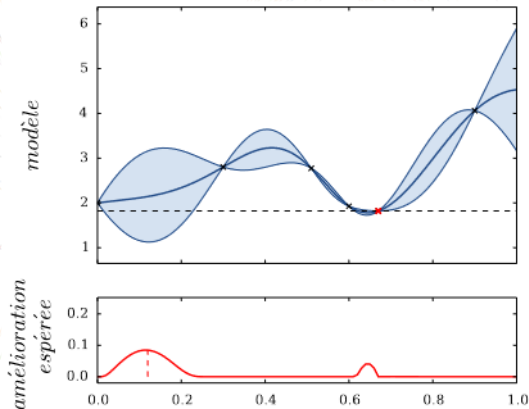
Bayesian optimization

Iteration 2 :



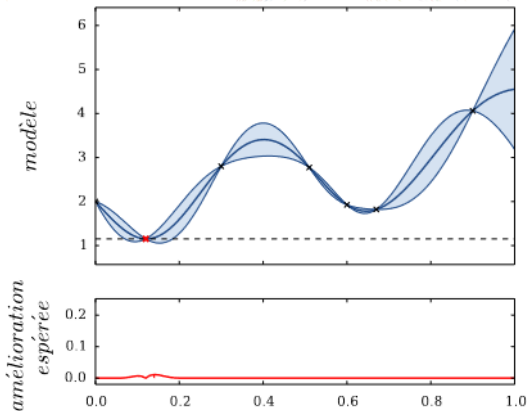
Bayesian optimization

Iteration 3 :



Bayesian optimization

Theory shows that **EGO algorithm** provides a dense sequence of points, up to a slight condition on the kernel used for GPs [[Vazquez and Bect, 2010](#)].



Application to algorithm tuning in machine learning

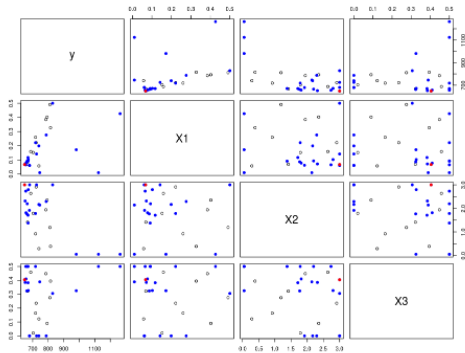
In machine learning, an algorithm can be a (time-consuming) black-box.

Example on ozone data (from computer lab) :

- output : k-fold cross validation error (fixed folds)
- inputs : kernel parameter, cost (regulariz. param.), epsilon (tube size)

With a small 30-point budget, BO outperforms a grid search and default tuning. Observe the tradeoff between exploration/exploitation.

Default tuning	678.8
Grid search	678.4
Marginal optim.	655.4
Bayesian optim.	647.9

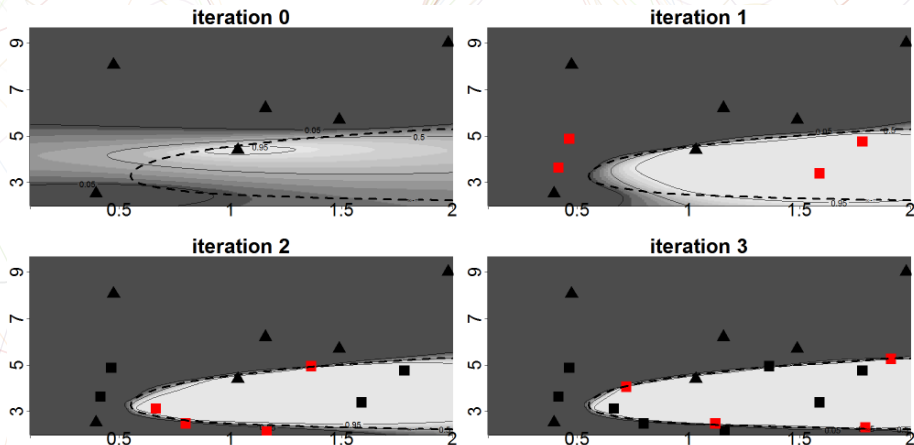


GP-based inversion

Same receipt for estimating a probability of failure (“SUR” strategy).

See [Chevalier et al., 2014] for details and [Bect et al., 2017] for a convergence analysis with supermartingales.

Illustration : Estimation of the nuclear criticality region $k_{\text{eff}} > 0.95$



Adaptation of EGO to noisy observations : the EQI criterion

For noisy observations, we assume that

$$Y_i = Y(x_i) + \varepsilon_i \quad i = 1, \dots, n$$

where $Y \sim GP(0, k)$ and the ε_i 's are $N(0, \tau_i^2)$ independent mutually and of Y .
The aim is to predict $Y(x)$ given $Y_1, \dots, Y_n \rightarrow$ **filtering**.

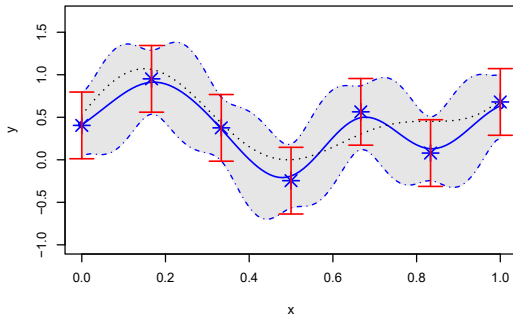


Figure – Illustration of Kriging with noisy observations.

Adaptation of EGO to noisy observations : the EQI criterion

For noisy observations, the improvement is replaced by [the quantile improvement](#), this is the Expected Quantile Improvement criterion (EQI) [[Picheny et al., 2013](#)].

Conditionally on $\mathcal{F}_n = \{Y_1, \dots, Y_n\}$, given an order β (e.g. 0.9),

$$EQI(x) = \mathbb{E}([q_0 - Q(x)]^+) \quad q_0 : \text{current minimum quantile}$$

where q_0 is the minimum of the quantiles (at order β) of the laws of $Y(x_i)$, and $Q(x)$ is the quantile of $Y(x)$ knowing the *unobserved* $Y_{n+1} = Y(x) + \varepsilon_{n+1}$, where $\varepsilon_{n+1} \sim N(0, \tau_{n+1}^2)$ for a given τ_{n+1} .

Although Y_{n+1} is unobserved, the law of $Q(x)$ can be computed as a normal distribution, leading to an analytical expression for EQI .

Adaptation of EGO to noisy observations : the EQI criterion

Exercise (Gaussian filtering)

Let (Z, ε) a centered Gaussian vector with Z, ε independent. Then $Z|\{Z + \varepsilon\}$ is normally distributed with mean $\frac{\sigma_Z^2}{\sigma_Z^2 + \sigma_\varepsilon^2}(Z + \varepsilon)$ and variance $\frac{\sigma_Z^2 \sigma_\varepsilon^2}{\sigma_Z^2 + \sigma_\varepsilon^2}$.

Exercise (EQI expression)

Conditionally on \mathcal{F}_n :

- 1 The law of $Y(x)|Y_{n+1} \sim \mathcal{N}(M_{n+1}(x), S_{n+1}(x)^2)$ with

$$M_{n+1}(x) = m_k(x) + \frac{s_k(x)^2}{s_k(x)^2 + \tau_{n+1}^2}(Y_{n+1} - m_k(x)), \quad S_{n+1}(x)^2 = \frac{s_k(x)^2 \tau_{n+1}^2}{s_k(x)^2 + \tau_{n+1}^2}$$

- 2 Thus $Q(x) = M_{n+1}(x) + \Phi^{-1}(\beta)S_{n+1}(x)$.
- 3 Moreover $Q(x) \sim \mathcal{N}(m_Q(x), s_Q(x)^2)$ with

$$m_Q = m_k(x) + \Phi_{-1}(\beta) \frac{s_k(x)\tau_{n+1}}{\sqrt{s_k(x)^2 + \tau_{n+1}^2}}, \quad s_Q^2 = \frac{s_k(x)^4}{s_k(x)^2 + \tau_{n+1}^2}$$

Finally, the EQI criterion has the same analytical expression as EI criterion, replacing y_0, m_k, s_k by q_0, m_Q, s_Q .

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From geostatistics to GP regression models

Time line

- 1951 : Spatial interpolation in geosciences [[Kriging, 1951](#)]
→ "Kriging"
- 1963 : Foundations of geostatistics [[Matheron, 1963](#)]
- 1989 : Computer experiments, metamodelling [[Sacks et al., 1989](#)]
→ Application to dimensions ≥ 4

From geostatistics to GP regression models

Geostatistical approach for spatial interpolation, Simple Kriging

Let Y be a centered stochastic process (or with known mean).

In geostatistics, the prediction of $Y(x)$ knowing $Y(x^{(1)}), \dots, Y(x^{(n)})$ is computed by the **Best Linear Unbiased Predictor (BLUP)**. It means, to find w_1, \dots, w_n s.t.

$$\hat{Y}(x) := w_0 + w_1 Y(x^{(1)}) + \dots + w_n Y(x^{(n)})$$

minimizes $\text{MSE} := \mathbb{E}([Y(x) - \hat{Y}(x)]^2)$ under $\mathbb{E}(\hat{Y}(x)) = \mathbb{E}(Y(x))$.

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Link between Simple Kriging and Gaussian process interpolation

- If Y is Gaussian, the conditional expectation coincides with the orthogonal projection onto a linear space
 → **BLUP = conditional expectation** and **$\min(\text{MSE}) = \text{conditional variance}$**
- If Y is not Gaussian, the two approaches are different in general
 → Advantage of BLUP : closed-form expressions

Gaussian processes, splines and RKHS

The 3 faces of a kernel

$GP(0, k(x, x')) \Leftrightarrow$ p.s.d. functions $k \Leftrightarrow$ RKHS : $\mathcal{H} = \overline{\text{span}\{k(., x), x \in D\}}$

where \mathcal{H} is a "Reproducing Kernel" Hilbert Space with dot product :

$$\langle k(x, .), k(x', .) \rangle = k(x, x') \quad (*)$$

RKHS can be also defined as Hilbert spaces of functions such that evaluations $f \rightarrow f(x)$ are continuous : By Riesz theorem, there exists a unique $k(., x)$ s.t.

$$f(x) = \langle f, k(., x) \rangle$$

Choosing $f = k(., x')$ gives the reproducing identity ().*

Ref : [[Aronszajn, 1950](#)], [[Berlinet and Thomas-Agnan, 2011](#)].

Gaussian processes, splines and RKHS

Correspondence between interpolation spline and GP conditional mean

[Kimeldorf and Wahba, 1971]

The interpolation spline is defined by the functional problem

$$(*) \quad \min_{h \in \mathcal{H}} \|h\| \quad \text{s.t.} \quad h(x^{(i)}) = y_i, \quad i = 1, \dots, n$$

If \mathcal{H} is the RKHS of kernel k , and if $k(X, X) = (k(x^{(i)}, x^{(j)}))_{1 \leq i, j \leq n}$ is invertible, $(*)$ has a unique solution in the finite dimensional space spanned by the $k(\cdot, x^{(i)})$:

$$\begin{aligned} h_{\text{opt}}(x) &= \mathbb{E} \left[Y(x) \mid Y(x^{(i)}) = y_i, \quad i = 1, \dots, n \right] \\ &= k(X, x)^\top k(X, X)^{-1} y \end{aligned}$$

where $Y \sim GP(0, k)$, $k(X, x) = (k(x, x^{(i)}))_{1 \leq i \leq n}$ and $y = (y_i)_{1 \leq i \leq n}$.

→ In this sense, GPs are generalizing interpolation splines.

The first part (reduction to finite dimension) is known as *Representer theorem*.

Gaussian processes, splines and RKHS

Correspondence between **approximation spline** and **GP conditional mean for noisy observations** [Kimeldorf and Wahba, 1971]

The **approximation spline** is defined by the **regression** problem with a **ridge penalty**

$$(*) \quad \min_{h \in \mathcal{H}} \sum_{i=1}^n (h(x^{(i)}) - y_i)^2 + \lambda \|h\|^2$$

If \mathcal{H} is the RKHS of kernel k , and if $k(X, X) + \lambda I_n$ is invertible, then $(*)$ has a unique solution in the finite dimensional space spanned by the $k(\cdot, x^{(i)})$:

$$\begin{aligned} h_{\text{opt}}(x) &= \mathbb{E} \left[Y(x) \mid Y(x^{(i)} + \varepsilon_i) = y_i, i = 1, \dots, n \right] \\ &= k(X, x)^\top (k(X, X) + \lambda I_n)^{-1} y \end{aligned}$$

where $\varepsilon_1, \dots, \varepsilon_n$ are independent $\mathcal{N}(0, \lambda)$, and indep. of the GP Y .

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Some valid operations on kernels

A lot of flexibility can be obtained with kernels !

Building a kernel from other ones (basic examples)

Sum, tensor sum	$k_1 + k_2, k_1 \oplus k_2$
Product, tensor product	$k_1 \times k_2, k_1 \otimes k_2$
ANOVA	$(1 + k_1) \otimes (1 + k_2)$
Warping	$k(x, x') = k_1(f(x), f(x'))$
...	...

See examples in [[Rasmussen and Williams, 2006](#)]

Kernels of stationary processes

A centered GP is (second order) stationary iff $k(x, x')$ depend on $x - x'$.
 → we denote $k(h) = k(x, x + h)$ (abuse of notation)

Bochner's theorem (see e.g. [Rasmussen and Williams, 2006])

The kernel of a real-valued stationary process on \mathbb{R}^d is the Fourier transform of a probability distribution

$$k(h) = \int_{\mathbb{R}^d} \cos(2\pi \langle h, t \rangle) d\mu(t) \quad (1)$$

where $\langle ., . \rangle$ is the usual scalar product on \mathbb{R}^d .

The probability measure μ is called **spectral measure**.

Exercise. Using the definition of positive semidefinite functions, prove that k defined by (1) is a valid kernel.

Kernels of stationary processes

Kernel name	Kernel form	Spectral measure
cosine	$\cos(2\pi h)$	Dirac δ_1
sinc	$\frac{\sin(\pi h)}{\pi h}$	Uniform
Squared exponential	$k(h) = \exp\left(-\frac{1}{2} \frac{h^2}{\ell^2}\right)$	Gaussian
Exponential	$\exp\left(-\frac{ h }{\ell}\right)$	Student $t_{1/2}$
Matérn 3/2	$\left(1 + \sqrt{3} \frac{ h }{\ell}\right) \exp\left(-\sqrt{3} \frac{ h }{\ell}\right)$	Student $t_{3/2}$
Matérn 5/2	$\left(1 + \sqrt{5} \frac{ h }{\ell} + \frac{5}{3} \frac{h^2}{\ell^2}\right) \exp\left(-\sqrt{5} \frac{ h }{\ell}\right)$	Student $t_{5/2}$

Table – Examples of kernels of 1-dimensional stationary processes

Remark : Characteristic length

The parameter ℓ in the previous slide is called "**range**" in geostatistics or "**characteristic length**" in machine learning. It is a **scale parameter** for x .

More precisely, if Y_ℓ is a centered GP with kernel of the forme

$$k_\ell(x, x') = k_1(x/\ell, x'/\ell)$$

then for all x, x' , we have

$$\text{Cov}(Y_\ell(x), Y_\ell(x')) = \text{Cov}(Y_1(x/\ell), Y_1(x'/\ell))$$

meaning that two Gaussian processes $(Y_\ell(x))$ and $(Y_1(x/\ell))$ have the same finite dimensional distributions.

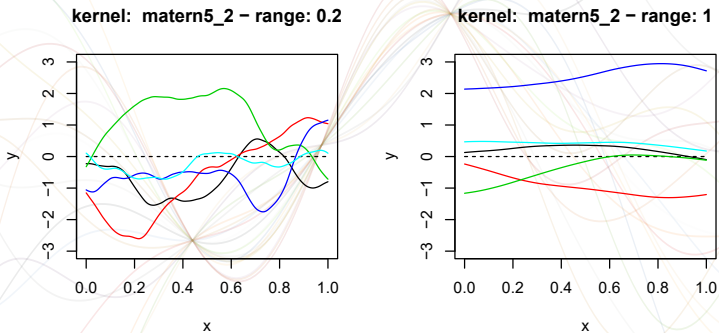


Figure – Sample paths of a GP with a Matérn 5/2 kernel for $\ell = 0.2$ and $\ell = 1$. Zooming 5 times on the first graph is equivalent to the second, in distribution.

Kernels for discrete data

- A kernel for a discrete input with L levels is a **positive semi-definite matrix** (p.s.d.) of size L
- The general p.s.d. matrix has $L(L + 1)/2$ parameters. More **parcimonious parameterizations** are useful, such as exchangeable covariance matrices

$$\begin{pmatrix} v & c & \dots & c \\ c & v & \ddots & \vdots \\ \vdots & \ddots & \ddots & c \\ c & \dots & c & v \end{pmatrix}, \quad \text{with} \quad -\frac{1}{L-1} \leq \frac{c}{v} \leq 1.$$

- If the variable is **ordinal**, with “1” < ... < “L”, one can use a continuous stationary kernel, up to an increasing real-valued function

$$k(\text{“i”}, \text{“j”}) = k_{\text{cont}}(|f(\text{“i”}) - f(\text{“j”})|)$$

→ $h = f(\text{“i”}) - f(\text{“j”})$ represents the distance between levels “i” and “j”

Gaussian processes and linear operations

Proposition (GP and linearity)

If $Y \sim GP(0, k(s, t))$ and L is linear (acting on the sample paths of Y), then

$$LY \sim GP(0, L_s L_t k(s, t))$$

The notation L_s (resp. L_t) means that we apply L on $s \mapsto f(s, t)$ (resp. $t \mapsto k(s, t)$) when f is a function of two inputs s, t .

Formal proof

- Gaussian : Since L is linear, a linear combination from LY can be rewritten as a linear combination from Y .
- Using the bilinearity of covariance,

$$\text{Cov}(LY(s), LY(t)) = L_t \text{Cov}(LY(s), Y(t)) = L_s L_t \text{Cov}(Y(s), Y(t))$$

Playing with kernels

Example (A kernel for even functions).

$$Lf(x) = f(x) + f(-x), \quad LY(x) = Y(x) + Y(-x)$$

- Why LY is a GP ?
 - ▶ For any x_1, \dots, x_n , the linear combination of $LY(x_1), \dots, LY(x_n)$ is a linear combination of Y values at $x_1, -x_1, \dots, x_n, -x_n$.
 - ▶ Since Y is a GP, this linear combination is Normal. Hence LY is a GP.
- Compute the kernel of LY , and observe that $x \mapsto k(x, x')$ is even for all x' :

$$\begin{aligned} \text{Cov}(LY(s), LY(t)) &= L_s L_t k(s, t) = L_s(k(s, t) + k(s, -t)) \\ &= [k(s, t) + k(s, -t)] + [k(-s, t) + k(-s, -t)] \end{aligned}$$
- Conversely, if $x \mapsto k(x, x')$ is even for all x' , then LY has even sample paths
 - ▶ Check that $\text{var}(Y(x) - Y(-x)) = 0$, which implies that $Y(x) = Y(-x)$ a.s.

→ This result can be generalized for a large class of linear operators
[Ginsbourger et al., 2016].

Playing with kernels

Example (Derivatives, integrals).

Assume that Y is a centered GP with kernel k . Then, under technical conditions :

- The derivative process $(Y'(x))_x$ is a centered GP with kernel

$$k_{Y'}(s, t) = \frac{\partial^2 k}{\partial s \partial t}(s, t)$$

Moreover, we have $\text{Cov}(Y(s), Y'(t)) = \frac{\partial k}{\partial t}(s, t)$.

- The integral $\int Y(x)dx$ is a centered random variable with variance

$$\iint k(s, t) ds dt$$

and we have for instance $\text{Cov}(Y(s), \int_t Y(t)dt) = \int k(s, t)dt$.

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A trended GP model

A common form of GP model is to use a linear trend

$$Y(x) = m(x) + Z(x)$$

with :

- $m(x) = \beta_1 f_1(x) + \dots + \beta_p f_p(x)$ a linear trend (the f_i 's are known functions)
- Z a centered GP with kernel $k(x, y; \Theta)$.

Here β and Θ are vectors of **unknown parameters**.

Model inference

Parameter estimation can be done with two classes of methods :

- **Maximum likelihood**. The likelihood is the pdf value at $y = (y_1; \dots; y_n)$ of $(Y(x^{(1)}); \dots; Y(x^{(n)})) \sim \mathcal{N}(F\beta; k(X, X; \Theta))$:

$$L(\beta, \Theta) = \frac{1}{(2\pi)^{n/2} |k(X, X; \Theta)|^{1/2}} \exp \left(-\frac{1}{2} (y - F\beta)^\top k(X, X; \Theta)^{-1} (y - F\beta) \right)$$

where F is the $n \times p$ matrix whose row i contains $f_1(x^{(i)}), \dots, f_p(x^{(i)})$.

- **Cross validation**. For instance, leave-one-out criterion

$$LOO(\beta, \Theta) = \sum_{i=1}^n (\hat{y}_{-i}(x^{(i)}) - y_i)^2$$

Notice that update formula express $k(X_{-i}, X_{-i}; \Theta)$ with known expressions.

In both cases, there are no closed-form expression, the criterions are not convex and may have several local optima \rightarrow **optimization is done numerically**.

Bayesian inference, Ordinary and Universal Kriging

- Uncertainty measured by GP variance (Simple Kriging formula) assumes that the parameters are known.
- It can be adapted to the case of **unknown parameters in a Bayesian framework**, i.e. assuming that **the parameters themselves are random**
- Prediction is obtained by integrating out the parameter distributions :

$$\begin{aligned} & \mathbb{E} \left(g(Y(x)) | Y(x^{(1)}), \dots, Y(x^{(n)}) \right) \\ &= \int \mathbb{E} \left(g(Y(x)) | Y(x^{(1)}), \dots, Y(x^{(n)}), \beta, \Theta \right) f_{\beta, \Theta}(\beta, \theta) d\beta d\Theta \end{aligned}$$

(Use $g = Id$ for the Kriging mean, $g(y) = y^2$ for the Kriging variance)

Bayesian inference, Ordinary and Universal Kriging

Unfortunately, Bayesian inference does not provide closed-form expressions, except for special cases. The most famous one is reported below :

Universal Kriging (UK) formula, [Cressie, 1992, Helbert et al., 2008]

Assume that Θ is known, but β is unknown. Then,

- ① The BLUP has the same form as for Simple Kriging, replacing β by its GLS estimate $\hat{\beta} = (F^\top K^{-1} F)^{-1} F^\top y$, with $K = k(X, X)$.
- ② The UK variance is greater than SK variance, with additional term :

$$\begin{aligned} s_{UK}^2(x) &= s_{SK}^2(x) \\ &+ (f(x)^\top - k(x, X)K^{-1}F)^\top (F^\top K^{-1}F)^{-1} (f(x)^\top - k(x, X)K^{-1}F) \end{aligned}$$

- ③ These formula coincide with the Bayesian approach when choosing the improper prior for $\beta \sim \mathcal{N}(\mu, \lambda k(X, X))$, with $\lambda \rightarrow \infty$.

Vocabulary : If the trend is a constant, UK is also called Ordinary Kriging (OK)

Model validation

- Aim : Check that (y_1, \dots, y_n) is drawn from a multivariate normal dist.
- At least, we check graphically that the leave-one-out (LOO) predictions of $Y(x^{(i)})$ are normal (removing $x^{(i)}$ from the learning set)

$$Y(x^{(i)}) | \{Y(x^{(j)}) = y_j, \forall j \neq i\} \sim \mathcal{N}\left(m_{k,-i}(x^{(i)}), s_{k,-i}^2(x^{(i)})\right)$$

Diagnostic : plot the standardized LOO residuals

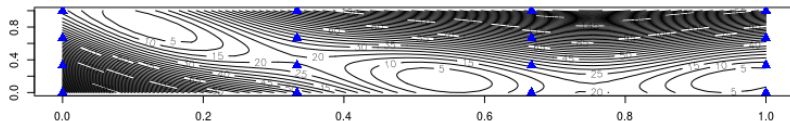
$$\frac{y_i - m_{k,-i}(x^{(i)})}{s_{k,-i}(x^{(i)})}$$

Under the GP assumption, they are drawn from a $N(0, 1)$ distribution.
Notice that they are correlated.

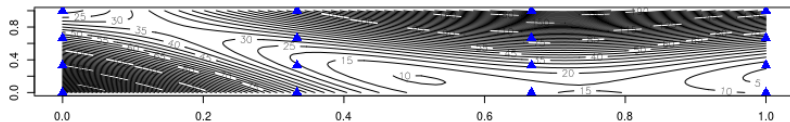
Remark. *This is true if all parameters are known.*

Illustration, with the DiceKriging R package [Roustant et al., 2012]

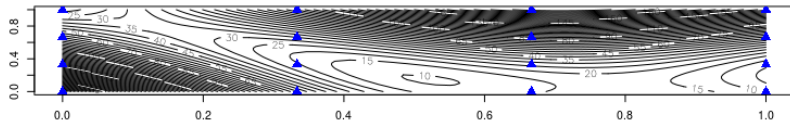
Branin



Ordinary Kriging



Universal Kriging



Call:

```
km(formula = ~.^2, design = design, response = y, multistart = 100)
```

Trend coeff.:

	Estimate
(Intercept)	195.1009
x1	-310.9559
x2	-210.3665
x1:x2	514.2816

Covar. type : matern5_2

Covar. coeff.:

	Estimate
theta(x1)	0.2141
theta(x2)	0.4025

Variance estimate: 1197.468

Figure – Details of parameter estimation for the UK Kriging model

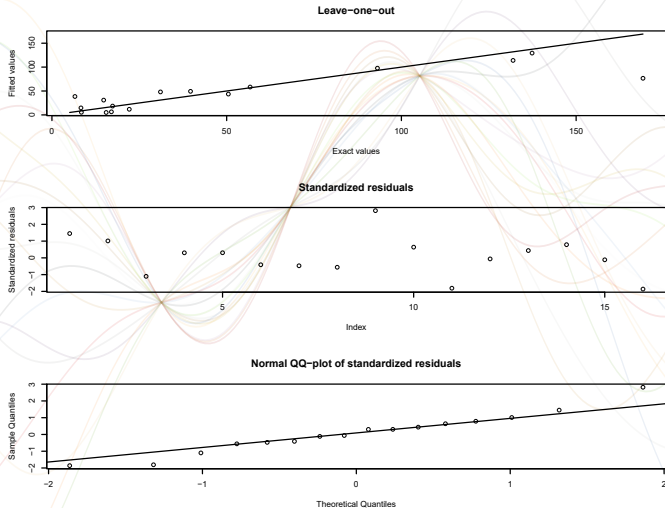


Figure – Leave-one-out validation for the UK Kriging model

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