Sequential increase of the input space dimension in Gaussian process regression

Thierry Gonon

Ecole Centrale de Lyon, Valeo

GDR MascotNum meeting, April 28th, 2021

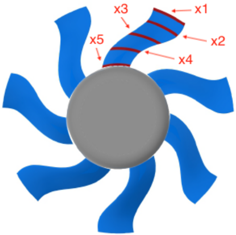
Tutors :

Céline Helbert — Ecole Centrale de Lyon, ICJ
Christophette Blanchet-Scalliet — Ecole Centrale de Lyon, ICJ
Bruno Demory — Valeo

Contents

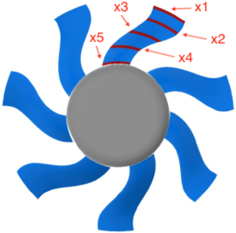
Contents

Industrial motivation

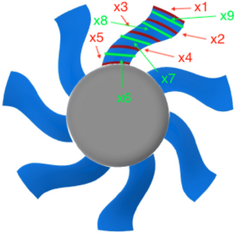


Step 0 : 5 inputs

Industrial motivation

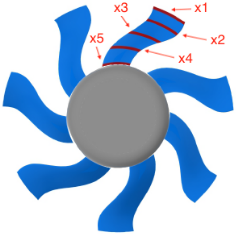


Step 0 : 5 inputs

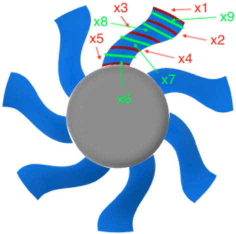


Step 1 : 9 inputs

Industrial motivation



Step 0 : 5 inputs

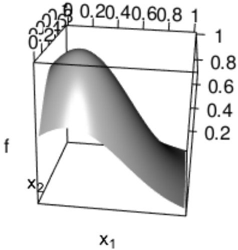


Step 1 : 9 inputs

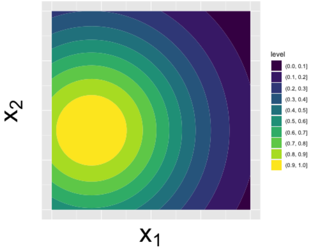
Question : How to take into account the previous information in the new model ? Can we use a multifidelity approach ?

Objective function

$$f : \left| \begin{array}{ccc} [0,1]^2 & \to & \mathbb{R} \\ (x_1, x_2) & \mapsto & f(x_1, x_2) \end{array} \right.$$



3D visualization

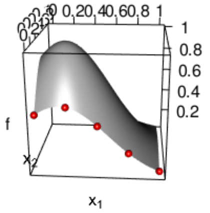


Isocontours

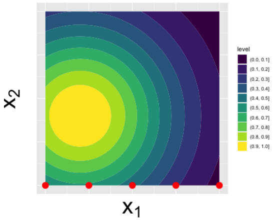
Step 0

We focus on $x_1 \mapsto f(x_1, 0)$. A DoE is generated :

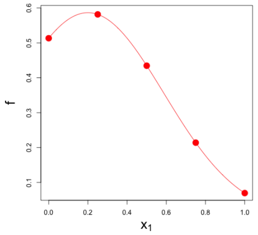
$$\mathbb{X}^0 = \begin{pmatrix} x_1^{(1)} \\ \vdots \\ x_1^{(n_0)} \end{pmatrix} \qquad \mathbf{y}^0 = \begin{pmatrix} f(x_1^{(1)}, 0) \\ \vdots \\ f(x_1^{(n_0)}, 0) \end{pmatrix}$$



3D visualization of f



Isocontours of f

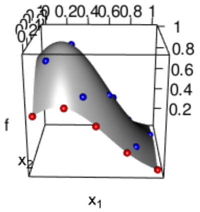


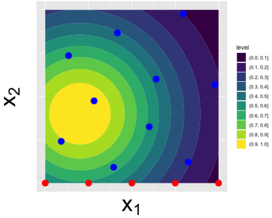
2D visualization of f on the section $x_2 = 0$

Step 1

We focus on the whole function f. A DoE is generated :

$$\mathbb{X}^1 = \begin{pmatrix} x_1^{(n_0+1)} & x_2^{(n_0+1)} \\ \vdots & \\ x_1^{(n_0+n_1)} & x_2^{(n_0+n_1)} \end{pmatrix} \qquad \mathbf{y}^1 = \begin{pmatrix} f(x_1^{(n_0+1)}, x_2^{(n_0+1)}) \\ \vdots \\ f(x_1^{(n_0+n_1)}, x_2^{(n_0+n_1)}) \end{pmatrix}$$





3D visualization of f **Isocontours of f**

Gaussian process regression framework [Santner et al., 2003] [Williams and Rasmussen, 2006]

- **Step 0** : $x_1 \mapsto f(x_1, 0)$ realization of the Gaussian process $Y_0 : [0,1] \times \Omega \rightarrow \mathbb{R}$

Gaussian process regression framework [Santner et al., 2003] [Williams and Rasmussen, 2006]

- **Step 0** : $x_1 \mapsto f(x_1, 0)$ realization of the Gaussian process $Y_0 : [0,1] \times \Omega \to \mathbb{R}$
- **Step 1** : f realization of the Gaussian process $Y_1 : [0,1]^2 \times \Omega \to \mathbb{R}$ such that :

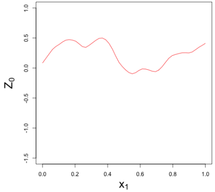
$$\begin{cases} Y_1(x_1, x_2) = Y_0(x_1) + Z_1(x_1, x_2), & \forall (x_1, x_2) \in [0,1]^2 \\ Y_1(x_1, 0) = Y_0(x_1), & \forall x_1 \in [0,1] \end{cases}$$

$Z_1 \perp\!\!\!\perp Y_0$ and Z_1 $\mathcal{GP}$. model inspired from the Multifidelity framework [Kennedy and O'Hagan, 2000]

Property verified by the correction process

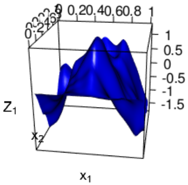
By construction, Z_1 verifies :

$$\begin{cases} Y_1(x_1,x_2) = Y_0(x_1) + Z_1(x_1,x_2) \\ Y_1(x_1,0) = Y_0(x_1) \end{cases} \Rightarrow \quad Z_1(x_1,0) = 0$$



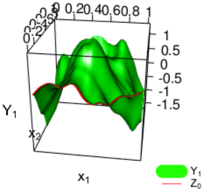
$\mathbf{Y_0}$

+



$\mathbf{Z_1}$

=



$\mathbf{Y_1}$

Problems

- How to build the correction process Z_1 such that :

$$Z_1(x_1, 0) = 0, \quad \forall x_1 \in [0, 1] \ ?$$

Problems

- How to build the correction process Z_1 such that :

$$Z_1(x_1, 0) \quad = \quad 0, \quad \forall x_1 \in [0,1] \ ?$$

- How to jointly estimate the parameters of Y_0 and Z_1 given the DoE $(\mathbb{X}^0, \mathbf{y}^0)$ and $(\mathbb{X}^1, \mathbf{y}^1)$?

Contents

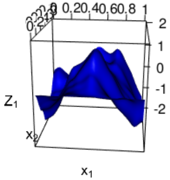
First candidate : Red (Reducted) process

Let $\widetilde{Z}_1 \quad : \quad [0,1]^2 \times \Omega \quad \rightarrow \quad \mathbb{R}$ be a Gaussian process :

$$\widetilde{Z}_1 \quad \sim \quad \mathcal{GP}(0, \sigma_1^2 r)$$

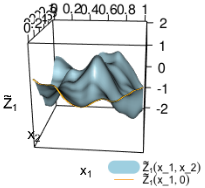
The Red process is defined by

$$Z_1^{Red}(x_1, x_2) \quad = \quad \widetilde{Z}_1(x_1, x_2) - \widetilde{Z}_1(x_1, 0), \quad \forall (x_1, x_2) \in [0,1]^2$$



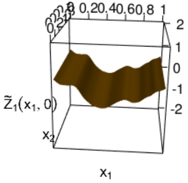
$\mathbf{Z_1^{Red}(x_1, x_2)}$

=



$\mathbf{\widetilde{Z}_1(x_1, x_2)}$

−



$\mathbf{\widetilde{Z}_1(x_1, 0)}$

First candidate : Red (Reducted) process

Let $\widetilde{Z}_1 \quad : \quad [0,1]^2 \times \Omega \quad \to \quad \mathbb{R}$ be a Gaussian process :

$$\widetilde{Z}_1 \quad \sim \quad \mathcal{GP}(0, \sigma_1^2 r)$$

The Red process is defined by

$$Z_1^{Red}(x_1, x_2) \quad = \quad \widetilde{Z}_1(x_1, x_2) - \widetilde{Z}_1(x_1, 0), \quad \forall (x_1, x_2) \in [0,1]^2$$

So

$$Z_1^{Red} \sim \mathcal{GP}(0, \sigma_1^2 \rho)$$

with

$$\begin{aligned} \rho((x_1, x_2), (x_1', x_2')) \quad = \quad & r((x_1, x_2), (x_1', x_2')) + r((x_1, 0), (x_1', 0)) \\ & - r((x_1, 0), (x_1', x_2')) - r((x_1, x_2), (x_1', 0)) \end{aligned}$$

Second candidate : P (Preconditionned) process

Let $\widetilde{Z}_1 \quad : \quad [0,1]^2 \times \Omega \quad \to \quad \mathbb{R}$ be a Gaussian process :

$$\widetilde{Z}_1 \quad \sim \quad \mathcal{GP}(0, \sigma_1^2 r)$$

Second candidate : P (Preconditionned) process

Let $\widetilde{Z}_1 \quad : \quad [0,1]^2 \times \Omega \quad \rightarrow \quad \mathbb{R}$ be a Gaussian process :

$$\widetilde{Z}_1 \quad \sim \quad \mathcal{GP}(0, \sigma_1^2 r)$$

The P process is defined by [Gauthier, 2011] as

$$Z_1^P(x_1, x_2) \quad = \quad \widetilde{Z}_1(x_1, x_2) - \underbrace{\mathbb{E}\left[\widetilde{Z}_1(x_1, x_2) \mid \widetilde{Z}_1(t_1, 0),\ \forall t_1 \in [0,1]\right]}_{p_{H_0}(\widetilde{Z}_1(x_1, x_2))}$$

where $H_0 = \overline{span\left(\widetilde{Z}_1(t_1, 0),\ \forall t_1 \in [0,1]\right)}$

General formula of the expectation [Gauthier, 2011]

Eigen Problem : $\int_0^1 \mathbf{k}((\mathbf{x_1},\mathbf{0}),(\mathbf{t_1},\mathbf{0}))\tilde{\phi}_\mathbf{n}(\mathbf{t_1})\mathbf{dt_1} = \lambda_\mathbf{n}\tilde{\phi}_\mathbf{n}(\mathbf{x_1})$

$$\Rightarrow \phi_n(x_1,x_2) = \frac{1}{\lambda_n}\int_0^1 k((x_1,x_2),(t_1,0))\tilde{\phi}_n(t_1)dt_1$$

$$p_{H_0}(\tilde{Z}_1(x_1,x_2)) = \sum_{n=1}^{+\infty}\phi_n(x_1,x_2)\int_0^1 \tilde{\phi}_n(t_1)\tilde{Z}_1(t_1,0)dt_1$$

GP of covariance kernel :

$$k_{H_0}((x_1,x_2),(x_1',x_2')) = \sum_{n=1}^{+\infty}\lambda_n\phi_n(x_1,x_2)\phi_n(x_1',x_2')$$

General formula of the expectation [Gauthier, 2011]

Eigen Problem : $\int_0^1 \mathbf{k}((\mathbf{x_1},\mathbf{0}),(\mathbf{t_1},\mathbf{0}))\tilde{\phi}_\mathbf{n}(\mathbf{t_1})\mathbf{dt_1} = \lambda_\mathbf{n}\tilde{\phi}_\mathbf{n}(\mathbf{x_1})$

$$\Rightarrow \phi_n(x_1,x_2) = \frac{1}{\lambda_n}\int_0^1 k((x_1,x_2),(t_1,0))\tilde{\phi}_n(t_1)dt_1$$

$$p_{H_0}(\tilde{Z}_1(x_1,x_2)) = \sum_{n=1}^{+\infty}\phi_n(x_1,x_2)\int_0^1 \tilde{\phi}_n(t_1)\tilde{Z}_1(t_1,0)dt_1$$

GP of covariance kernel :

$$k_{H_0}((x_1,x_2),(x_1',x_2')) = \sum_{n=1}^{+\infty}\lambda_n\phi_n(x_1,x_2)\phi_n(x_1',x_2')$$

Numerical implementation ?

Tensor product case

If $\widetilde{Z}_1 \sim \mathcal{GP}(0, \sigma^2 r)$ with :

$$r((x_1,x_2),(x_1',x_2')) \quad = \quad r_1(x_1,x_1')r_2(x_2-0,x_2'-0), \qquad \begin{array}{l}\forall (x_1,x_2)\in[0,1]^2 \\ \forall (x_1',x_2')\in[0,1]^2\end{array}$$

Then $\mathbb{E}\left[\widetilde{Z}_1(x_1,x_2) \mid \widetilde{Z}_1(t_1,0)\ \forall t_1 \in [0,1]\right] \quad = \quad r_2(x_2,0)\widetilde{Z}_1(x_1,0)$

and

$$k_{H_0}((x_1,x_2),(x_1',x_2')) = r_1(x_1,x_1')r_2(x_2,0)r_2(x_2',0)$$

Tensor product case

If $\widetilde{Z}_1 \sim \mathcal{GP}(0, \sigma^2 r)$ with :

$$r((x_1, x_2), (x_1', x_2')) = r_1(x_1, x_1') r_2(x_2 - 0, x_2' - 0), \quad \begin{array}{l} \forall (x_1, x_2) \in [0,1]^2 \\ \forall (x_1', x_2') \in [0,1]^2 \end{array}$$

So

$$\begin{aligned} Z_1^P(x_1, x_2) &= \widetilde{Z}_1(x_1, x_2) - r_2(x_2, 0)\widetilde{Z}_1(x_1, 0) \\ &\sim \mathcal{GP}(0, \sigma_1^2 \rho) \end{aligned}$$

with

$$\rho((x_1, x_2), (x_1', x_2')) = r_1(x_1, x_1') \left[r_2(x_2, x_2') - r_2(x_2, 0) r_2(x_2', 0) \right]$$

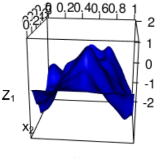
Summary correction process

Let $\widetilde{Z}_1 \sim \mathcal{GP}(0, \sigma^2 r)$

Summary correction process

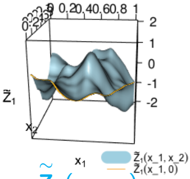
Let $\widetilde{Z}_1 \sim \mathcal{GP}(0, \sigma^2 r)$

- Red process :



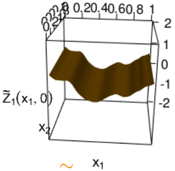
$Z_1^{Red}(x_1, x_2)$

=



$\widetilde{Z}_1(x_1, x_2)$

-

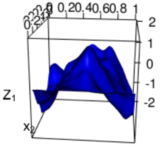


$\widetilde{Z}_1(x_1, 0)$

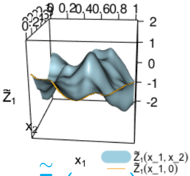
Summary correction process

Let $\widetilde{Z}_1 \sim \mathcal{GP}(0, \sigma^2 r)$

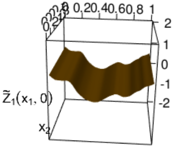
- Red process :



$Z_1^{Red}(x_1, x_2)$ =

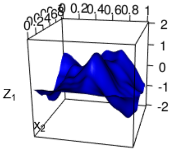


$\widetilde{Z}_1(x_1, x_2)$ -

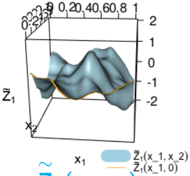


$\widetilde{Z}_1(x_1, 0)$

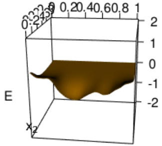
- P process :



$Z_1^{P}(x_1, x_2)$ =



$\widetilde{Z}_1(x_1, x_2)$ -



$r_2(x_2, 0)\widetilde{Z}_1(x_1, 0)$

Contents

Observed data vs complete data

We need to estimate $\eta = (\eta_0, \eta_1)$ with η_0 parameters of Y_0, η_1 parameters of $\widetilde{Z}_1$:

Observed data vs complete data

We need to estimate $\eta = (\eta_0, \eta_1)$ with η_0 parameters of Y_0, η_1 parameters of $\tilde{Z}_1$:

Observed data :

- $Y_0(\mathbb{X}^0) = \mathbf{y^0}$
- $Y_1(\mathbb{X}^1) = \mathbf{y^1}$

Observed data vs complete data

We need to estimate $\eta = (\eta_0, \eta_1)$ with η_0 parameters of Y_0, η_1 parameters of $\tilde{Z}_1$:

Observed data :

- $Y_0(\mathbb{X}^0) = \mathbf{y^0}$
- $Y_1(\mathbb{X}^1) = \mathbf{y^1}$

Loglikelihood :

$$l(\eta_0, \eta_1; \mathbf{y^0}, \mathbf{z^0}, \mathbf{z^1}) \quad = \quad \log h_{Y_0(\mathbb{X}^0), Y_1(\mathbb{X}^1)} \left(\mathbf{y^0}, \mathbf{y^1}\right)$$

$\Rightarrow \eta_0$ and η_1 are not separated

Observed data vs complete data

We need to estimate $\eta = (\eta_0, \eta_1)$ with η_0 parameters of Y_0, η_1 parameters of $\widetilde{Z}_1$:

Observed data :

- $Y_0(\mathbb{X}^0) = \mathbf{y^0}$
- $Y_1(\mathbb{X}^1) = \mathbf{y^1}$

Loglikelihood :

$$l(\eta_0, \eta_1; \mathbf{y^0}, \mathbf{z^0}, \mathbf{z^1}) = \log h_{Y_0(\mathbb{X}^0), Y_1(\mathbb{X}^1)}\left(\mathbf{y^0}, \mathbf{y^1}\right)$$

$\Rightarrow \eta_0$ and η_1 are not separated

Complete data :

- $Y_0(\mathbb{X}^0) = \mathbf{y^0}$
- $Y_0(\mathbb{X}^1) = \mathbf{z^0}$
- $Z_1(\mathbb{X}^1) = \mathbf{z^1}$

Observed data vs complete data

We need to estimate $\eta = (\eta_0, \eta_1)$ with η_0 parameters of Y_0, η_1 parameters of $\tilde{Z}_1$:

Observed data :

- $Y_0(\mathbb{X}^0) = \mathbf{y^0}$
- $Y_1(\mathbb{X}^1) = \mathbf{y^1}$

Loglikelihood :

$$l(\eta_0, \eta_1; \mathbf{y^0}, \mathbf{z^0}, \mathbf{z^1}) = \log h_{Y_0(\mathbb{X}^0), Y_1(\mathbb{X}^1)}\left(\mathbf{y^0}, \mathbf{y^1}\right)$$

$\Rightarrow$ η_0 and η_1 are not separated

Complete data :

- $Y_0(\mathbb{X}^0) = \mathbf{y^0}$
- $Y_0(\mathbb{X}^1) = \mathbf{z^0}$
- $Z_1(\mathbb{X}^1) = \mathbf{z^1}$

Loglikelihood :

$$\begin{aligned} l_c(\eta_0, \eta_1; \mathbf{y^0}, \mathbf{z^0}, \mathbf{z^1}) &= \log h_{Y_0(\mathbb{X}^0), Y_0(\mathbb{X}^1), Z_1(\mathbb{X}^1)}\left(\mathbf{y^0}, \mathbf{z^0}, \mathbf{z^1}\right) \\ &= l_0\left(\eta_0; \mathbf{y^0}, \mathbf{z^0}\right) + l_1\left(\eta_1; \mathbf{y^1}\right) \end{aligned}$$

$\Rightarrow$ Separation of η_0 and η_1

EM algorithm

Expectation :

$$
\begin{aligned}
Q(\eta,\eta') &= \mathbb{E}_{\eta'}\left[l_c(\eta_0,\eta_1; Y_0(\mathbb{X}^0), Y_0(\mathbb{X}^1), Z_1(\mathbb{X}^1)) \mid Y_0(\mathbb{X}^0)=\mathbf{y^0}, Y_1(\mathbb{X}^1)=\mathbf{y^1}\right] \\
&= \mathbb{E}_{\eta'}\left[l_0(\eta_0; Y_0(\mathbb{X}^0), Y_0(\mathbb{X}^1) \mid Y_0(\mathbb{X}^0)=\mathbf{y^0}, Y_1(\mathbb{X}^1)=\mathbf{y^1}\right] \\
&+ \mathbb{E}_{\eta'}\left[l_1(\eta_1; Z_1(\mathbb{X}^1) \mid Y_0(\mathbb{X}^0)=\mathbf{y^0}, Y_1(\mathbb{X}^1)=\mathbf{y^1}\right] \\
&= Q_0(\eta_0,\eta') + Q_1(\eta_1,\eta')
\end{aligned}
$$

EM algorithm

Expectation :

$$\begin{aligned} Q(\eta,\eta') &= \mathbb{E}_{\eta'}\left[l_c(\eta_0,\eta_1;Y_0(\mathbb{X}^0),Y_0(\mathbb{X}^1),Z_1(\mathbb{X}^1)) \mid Y_0(\mathbb{X}^0)=\mathbf{y^0},\,Y_1(\mathbb{X}^1)=\mathbf{y^1}\right] \\ &= \mathbb{E}_{\eta'}\left[l_0(\eta_0;Y_0(\mathbb{X}^0),Y_0(\mathbb{X}^1) \mid Y_0(\mathbb{X}^0)=\mathbf{y^0},\,Y_1(\mathbb{X}^1)=\mathbf{y^1}\right] \\ &+ \mathbb{E}_{\eta'}\left[l_1(\eta_1;Z_1(\mathbb{X}^1) \mid Y_0(\mathbb{X}^0)=\mathbf{y^0},\,Y_1(\mathbb{X}^1)=\mathbf{y^1}\right] \\ &= Q_0(\eta_0,\eta')+Q_1(\eta_1,\eta') \end{aligned}$$

Maximization :
We build the sequence $\left(\eta^{(i)}\right)_i = \left(\eta_0^{(i)},\eta_1^{(i)}\right)_i$ such that :

- $\eta_0^{(i+1)}$ solution of $\max_{\eta_0} Q_0(\eta_0,\eta^{(i)})$
- $\eta_1^{(i+1)}$ solution of $\max_{\eta_1} Q_1(\eta_1,\eta^{(i)})$

Remark

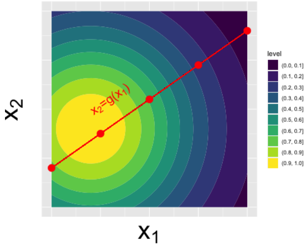
- More steps

Remark

- More steps
- More input variables by step

Remark

- More steps
- More input variables by step
- Fixed input variables not necessarily constant equal to 0 but function of the free input variables



Z_1^P based on $\tilde{Z}_1$ of kernel :

$$r((x_1, x_2), (x_1', x_2')) = r_1(x_1, x_1') r_2(x_2 - g(x_1), x_2' - g(x_1'))$$

Contents

Test on an analytical function

We consider the function :

$$f \quad : \left| \begin{array}{ccc} [0,1]^2 & \to & \mathbb{R} \\ (x_1, x_2, x_3, x_4) & \mapsto & f_1(x_1, x_2) + f_2(x_1, x_2, x_3, x_4) \end{array} \right.$$

with

$$\left\{ \begin{array}{lcl} f_1(x_1, x_2) & = & \left[4 - 2.1(4x_1 - 2)^2 + \frac{(4x_1 - 2)^4}{3}\right](4x_1 - 2)^2 \\ & + & (4x_1 - 2)(2x_2 - 1) + \left[-4 + 4(2x_2 - 1)^2\right](2x_2 - 1)^2 \\ f_2(x_1, x_2, x_3, x_4) & = & 4 \exp\left(- \|x - 0.3\|^2\right) \end{array} \right.$$

Test on an analytical function

We consider the function :

$$f \quad : \left| \begin{array}{ccc} [0,1]^2 & \rightarrow & \mathbb{R} \\ (x_1, x_2, x_3, x_4) & \mapsto & f_1(x_1, x_2) + f_2(x_1, x_2, x_3, x_4) \end{array} \right.$$

with

$$\left\{ \begin{array}{rcl} f_1(x_1, x_2) & = & \left[4 - 2.1(4x_1 - 2)^2 + \frac{(4x_1 - 2)^4}{3}\right](4x_1 - 2)^2 \\ & + & (4x_1 - 2)(2x_2 - 1) + \left[-4 + 4(2x_2 - 1)^2\right](2x_2 - 1)^2 \\ f_2(x_1, x_2, x_3, x_4) & = & 4 \exp\left(-\|x - 0.3\|^2\right) \end{array} \right.$$

- At step 0, we focus on $(x_1, x_2) \mapsto f(x_1, x_2, \frac{x_1 + x_2}{2}, 0.2x_1 + 0.7)$. We dispose of a DoE $(\mathbb{X}^0, \mathbf{y^0})$ of size 10.

Test on an analytical function

We consider the function :

$$f \quad : \left| \begin{array}{lcl} [0,1]^2 & \to & \mathbb{R} \\ (x_1, x_2, x_3, x_4) & \mapsto & f_1(x_1, x_2) + f_2(x_1, x_2, x_3, x_4) \end{array} \right.$$

with

$$\left\{ \begin{array}{lcl} f_1(x_1, x_2) & = & \left[4 - 2.1(4x_1 - 2)^2 + \frac{(4x_1-2)^4}{3}\right](4x_1 - 2)^2 \\ & + & (4x_1 - 2)(2x_2 - 1) + \left[-4 + 4(2x_2 - 1)^2\right](2x_2 - 1)^2 \\ f_2(x_1, x_2, x_3, x_4) & = & 4 \exp\left(-\left\|x - 0.3\right\|^2\right) \end{array} \right.$$

- At step 0, we focus on $(x_1, x_2) \mapsto f(x_1, x_2, \frac{x_1+x_2}{2}, 0.2x_1 + 0.7)$. We dispose of a DoE $(\mathbb{X}^0, \mathbf{y^0})$ of size 10.
- At step 1, we focus on f. We dispose of a DoE $(\mathbb{X}^1, \mathbf{y^1})$ of size 20.

Methods

- **K_1** : kriging model trained on $(\mathbb{X}^1, \mathbf{y}^1)$ with a covariance kernel stationary tensor product Matern $\frac{5}{2}$.

Methods

- **K_1** : kriging model trained on $(\mathbb{X}^1, \mathbf{y^1})$ with a covariance kernel stationary tensor product Matern $\frac{5}{2}$.
- **K_tot** : kriging model trained on $(\mathbb{X}^0, \mathbf{y^0})$ and $(\mathbb{X}^1, \mathbf{y^1})$ with a covariance kernel stationary tensor product Matern $\frac{5}{2}$.

Methods

- **K_1** : kriging model trained on $(\mathbb{X}^1, \mathbf{y^1})$ with a covariance kernel stationary tensor product Matern $\frac{5}{2}$.
- **K_tot** : kriging model trained on $(\mathbb{X}^0, \mathbf{y^0})$ and $(\mathbb{X}^1, \mathbf{y^1})$ with a covariance kernel stationary tensor product Matern $\frac{5}{2}$.
- Our method :

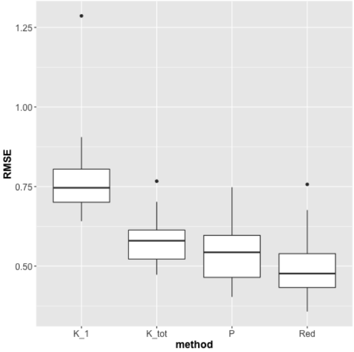
$$\begin{cases} Y_1(x_1, x_2, x_3, x_4) & = & Y_0(x_1, x_2) + Z_1(x_1, x_2, x_3, x_4) \\ Z_1(x_1, x_2, \frac{x_1+x_2}{2}, 0.2x_1 + 0.7) & = & 0, \end{cases}$$

trained on $(\mathbb{X}^0, \mathbf{y^0})$ and $(\mathbb{X}^1, \mathbf{y^1})$.

  - Y_0 with a covariance kernel stationary tensor product Matern $\frac{5}{2}$
  - $\tilde{Z}_1$ with a covariance kernel stationary tensor product Matern $\frac{5}{2}$ robustified (of covariance parameters $(\theta_1, \theta_1, \theta_2, \theta_2)$)
  - Z_1 a **Red** or **P** process build on $\tilde{Z}_1$.

Results

RMSE's on a sobol sequence of size 10000. Boxplots over 30 different training samples $(\mathbb{X}^0, \mathbf{y^0})$, $(\mathbb{X}^1, \mathbf{y^1})$. **Red** is better.



Boxplots of RMSE's

Contents

Conclusion

- Auto-regressive model inspired from the multifidelity

Conclusion

- Auto-regressive model inspired from the multifidelity
- Additional property of the correction term : two candidates that verify it

Conclusion

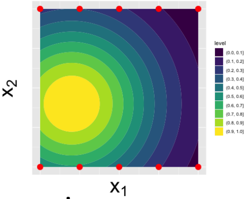
- Auto-regressive model inspired from the multifidelity
- Additional property of the correction term : two candidates that verify it
- EM algorithm to jointly estimate the parameters of the processes

Conclusion

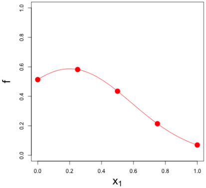
- Auto-regressive model inspired from the multifidelity
- Additional property of the correction term : two candidates that verify it
- EM algorithm to jointly estimate the parameters of the processes
- Comforting results on a toy case

Perspective : Multiple conditionning

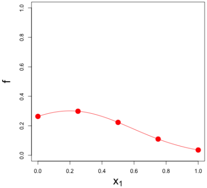
- Step 0



Isocontours



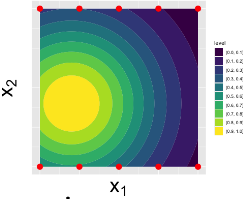
$x_2 = 0$



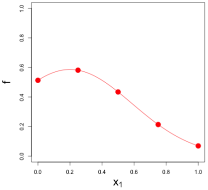
$x_2 = 1$

Perspective : Multiple conditionning

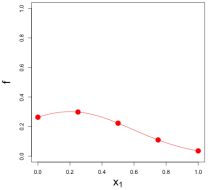
- Step 0



Isocontours

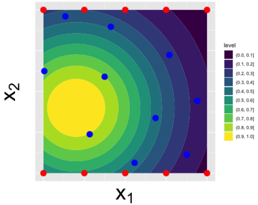


$x_2 = 0$



$x_2 = 1$

- Step 1



Isocontours

Other perspectives

- Industrial case

Other perspectives

- Industrial case
- Enrichment of the samples

Other perspectives

- Industrial case
- Enrichment of the samples
- Noise (no interpolation)

References

Gauthier, B. (2011).
Approche spectrale pour l'interpolation à noyaux et positivité conditionnelle.
PhD thesis, Ecole Nationale Supérieure des Mines de Saint-Etienne.

Kennedy, M. C. and O'Hagan, A. (2000).
Predicting the output from a complex computer code when fast approximations are available.
Biometrika, 87(1) :1–13.

Santner, T. J., Williams, B. J., Notz, W., and Williams, B. J. (2003).
The design and analysis of computer experiments, volume 1.
Springer.

Williams, C. K. and Rasmussen, C. E. (2006).
Gaussian processes for machine learning, volume 2.
MIT press Cambridge, MA.

General formula of the P process [Gauthier, 2011]

Let $\widetilde{Z}_1 \sim \mathcal{GP}(0, k)$ be a stationary GP. Then

$$\mathbb{E}\left[\widetilde{Z}_1(x_1, x_2) \mid \widetilde{Z}_1(t_1, 0),\ \forall t_1 \in [0,1]\right] = \sum_{n=1}^{+\infty} \phi_n(x_1, x_2) \int_0^1 \widetilde{\phi}_n(t_1) \widetilde{Z}_1(t_1, 0) dt_1$$

where

$$\phi_n(x_1, x_2) = \frac{1}{\lambda_n} \int_0^1 k((x_1, x_2), (t_1, 0)) \widetilde{\phi}_n(t_1) dt_1$$

and $(\lambda_n, \widetilde{\phi}_n)_n$ solutions of

$$\int_0^1 k((x_1, 0), (t_1, 0)) \widetilde{\phi}_n(t_1) dt_1 = \lambda_n \widetilde{\phi}_n(x_1)$$

Formula in the tensor product case

- The eigen problem becomes

$$\int_0^1 r_1(x_1, t_1)\widetilde{\phi}_n(t_1)dt_1 = \lambda_n \widetilde{\phi}_n(x_1)$$

- ϕ_n becomes

$$\phi_n(x_1, x_2) = r_2(x_2, 0)\widetilde{\phi}_n(x_1)$$

- $\mathbb{E}\left[\widetilde{Z}_1(x_1, x_2) \mid \widetilde{Z}_1(t_1, 0),\ \forall t_1 \in [0, 1]\right]$ becomes

$$\underbrace{\sum_{n=1}^{+\infty} \widetilde{\phi}_n(x_1) \int_0^1 \widetilde{\phi}_n(t_1)\widetilde{Z}_1(t_1, 0)dt_1}_{=\widetilde{Z}_{\mathbf{1}}(x_{\mathbf{1}}, 0)} r_2(x_2, 0)$$

Multiple P process

Let $\widetilde{Z}_1 \sim \mathcal{GP}(0, k)$ be a stationary GP. The multiple P process conditionned on $x_2 = 0$ and $x_2 = 1$ is defined as :

$$Z_1^P(x_1, x_2) = \widetilde{Z}_1(x_1, x_2) - \mathbb{E}\left[\widetilde{Z}_1(x_1, x_2) \mid \begin{array}{ccc} \widetilde{Z}_1(t_1, 0) & = & 0 \\ \widetilde{Z}_1(t_1, 1) & = & 0 \end{array} \forall t_1 \in [0, 1]\right]$$

If $k = r_1 r_2$ then $\mathbb{E}\left[\widetilde{Z}_1(x_1, x_2) \mid \begin{array}{ccc} \widetilde{Z}_1(t_1, 0) & = & 0 \\ \widetilde{Z}_1(t_1, 1) & = & 0 \end{array} \forall t_1 \in [0, 1]\right]$ is equal to

$$\begin{pmatrix} r_2(x_2, 0) & r_2(x_2, 1) \end{pmatrix} \begin{pmatrix} r_2(0, 0) & r_2(0, 1) \\ r_2(1, 0) & r_2(1, 1) \end{pmatrix}^{-1} \begin{pmatrix} \widetilde{Z}_1(x_1, 0) \\ \widetilde{Z}_1(x_1, 1) \end{pmatrix}$$