

Sequential increase of the input space dimension in Gaussian process regression

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GDR MascotNum meeting, April 28th, 2021

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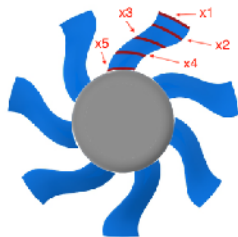
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 - Motivation
 - Model
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Contents

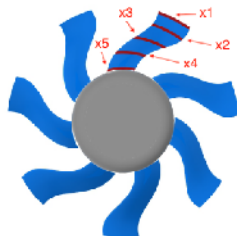
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Industrial motivation

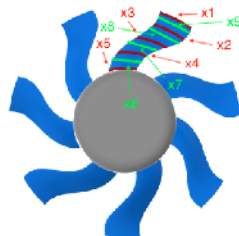


Step 0 : 5 inputs

Industrial motivation

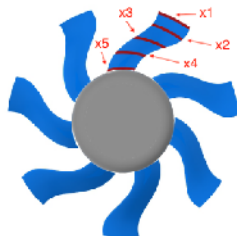


Step 0 : 5 inputs

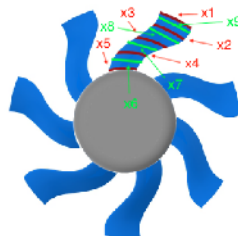


Step 1 : 9 inputs

Industrial motivation



Step 0 : 5 inputs

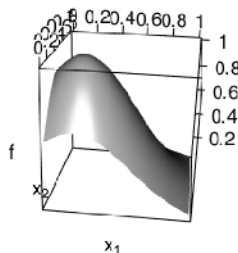


Step 1 : 9 inputs

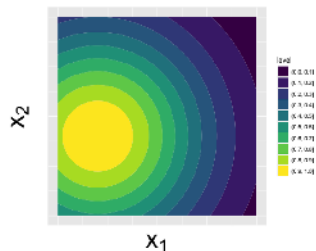
Question : How to take into account the previous information in the new model ? Can we use a multifidelity approach ?

Objective function

$$f : \begin{cases} [0, 1]^2 & \rightarrow \mathbb{R} \\ (x_1, x_2) & \mapsto f(x_1, x_2) \end{cases}$$



3D visualization

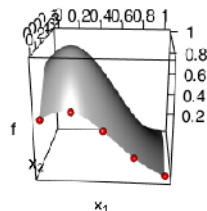
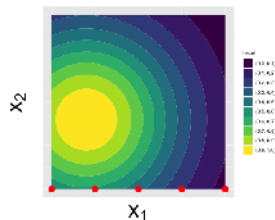
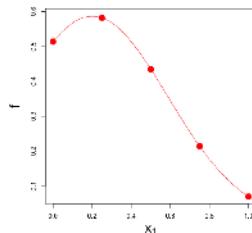


Isocontours

Step 0

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

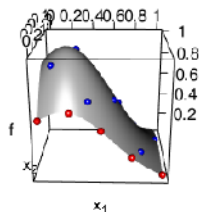
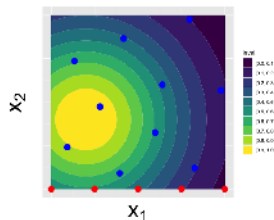
$$\mathbb{X}^0 = \begin{pmatrix} x_1^{(1)} \\ \vdots \\ x_1^{(n_0)} \end{pmatrix} \quad \mathbf{y}^0 = \begin{pmatrix} f(x_1^{(1)}, 0) \\ \vdots \\ f(x_1^{(n_0)}, 0) \end{pmatrix}$$

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 :

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

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

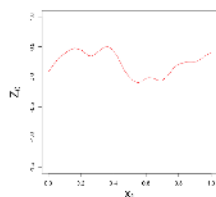
$$\begin{cases} Y_1(x_1, x_2) &= Y_0(x_1) + Z_1(x_1, x_2), & \forall (x_1, x_2) \in [0, 1]^2 \\ Y_1(x_1, 0) &= Y_0(x_1), & \forall x_1 \in [0, 1] \end{cases}$$

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

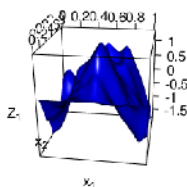
Property verified by the correction process

By construction, Z_1 verifies :

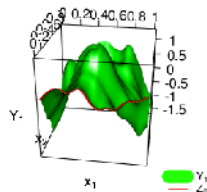
$$\begin{cases} Y_1(x_1, x_2) = Y_0(x_1) + Z_1(x_1, x_2) \\ Y_1(x_1, 0) = Y_0(x_1) \end{cases} \Rightarrow Z_1(x_1, 0) = 0$$

 Y_0

+

 Z_1

=

 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 :

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

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

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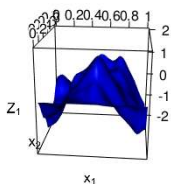
First candidate : Red (Reduced) process

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

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

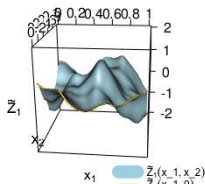
The Red process is defined by

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



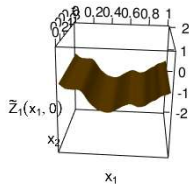
$Z_1^{\text{Red}}(x_1, x_2)$

=



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

-



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First candidate : Red (Reduced) process

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

So

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

with

$$\begin{aligned} \rho((x_1, x_2), (x'_1, x'_2)) &= r((x_1, x_2), (x'_1, x'_2)) + r((x_1, 0), (x'_1, 0)) \\ &\quad - r((x_1, 0), (x'_1, x'_2)) - r((x_1, x_2), (x'_1, 0)) \end{aligned}$$

Second candidate : P (Preconditionned) process

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

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

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

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

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

General formula of the expectation [Gauthier, 2011]

Eigen Problem : $\int_0^1 k((\mathbf{x}_1, \mathbf{0}), (\mathbf{t}_1, \mathbf{0})) \tilde{\phi}_n(\mathbf{t}_1) d\mathbf{t}_1 = \lambda_n \tilde{\phi}_n(\mathbf{x}_1)$

$$\Rightarrow \phi_n(x_1, x_2) = \frac{1}{\lambda_n} \int_0^1 k((x_1, x_2), (\mathbf{t}_1, 0)) \tilde{\phi}_n(\mathbf{t}_1) dt_1$$

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

GP of covariance kernel :

$$k_{H_0}((x_1, x_2), (x'_1, x'_2)) = \sum_{n=1}^{+\infty} \lambda_n \phi_n(x_1, x_2) \phi_n(x'_1, x'_2)$$

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Numerical implementation ?

Tensor product case

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

$$r((x_1, x_2), (x'_1, x'_2)) = r_1(x_1, x'_1)r_2(x_2 - 0, x'_2 - 0), \quad \begin{array}{l} \forall (x_1, x_2) \in [0, 1]^2 \\ \forall (x'_1, x'_2) \in [0, 1]^2 \end{array}$$

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

and

$$k_{H_0}((x_1, x_2), (x'_1, x'_2)) = r_1(x_1, x'_1)r_2(x_2, 0)r_2(x'_2, 0)$$

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So

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

with

$$\rho((x_1, x_2), (x'_1, x'_2)) = r_1(x_1, x'_1) [r_2(x_2, x'_2) - r_2(x_2, 0)r_2(x'_2, 0)]$$

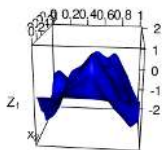
Summary correction process

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

Summary correction process

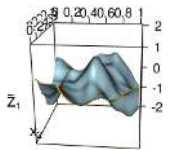
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- Red process :

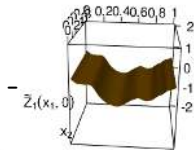


$Z_1^{\text{Red}}(x_1, x_2)$

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

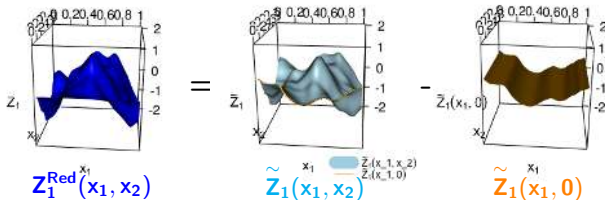


$\tilde{Z}_1(x_1, 0)$

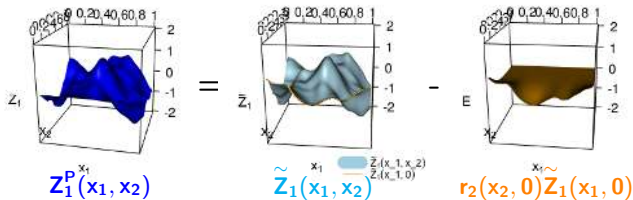
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• P process :



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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 vs complete data

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Observed data :

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

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

Loglikelihood :

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

$\Rightarrow \eta_0$ and η_1 are not separated

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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

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Loglikelihood :

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

\Rightarrow Separation of η_0 and η_1

EM algorithm

Expectation :

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

EM algorithm

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 \end{aligned}$$

Maximization :

We build the sequence $(\eta^{(i)})_i = (\eta_0^{(i)}, \eta_1^{(i)})_i$ 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

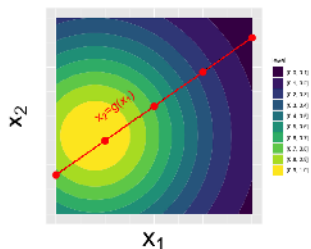
- More steps

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 :

$$r((x_1, x_2), (x'_1, x'_2)) \\ = r_1(x_1, x'_1) r_2(x_2 - g(x_1), x'_2 - g(x'_1))$$

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Test on an analytical function

We consider the function :

$$f : \begin{cases} [0, 1]^2 & \rightarrow \mathbb{R} \\ (x_1, x_2, x_3, x_4) & \mapsto f_1(x_1, x_2) + f_2(x_1, x_2, x_3, x_4) \end{cases}$$

with

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

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with

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

- 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.

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$$f : \begin{cases} [0, 1]^2 & \rightarrow \mathbb{R} \\ (x_1, x_2, x_3, x_4) & \mapsto f_1(x_1, x_2) + f_2(x_1, x_2, x_3, x_4) \end{cases}$$

with

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

- 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

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Methods

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

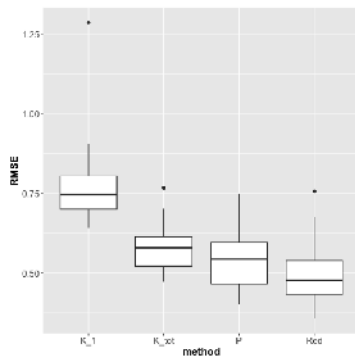
$$\begin{cases} Y_1(x_1, x_2, x_3, x_4) & = Y_0(x_1, x_2) + Z_1(x_1, x_2, x_3, x_4) \\ Z_1(x_1, x_2, \frac{x_1+x_2}{2}, 0.2x_1 + 0.7) & = 0, \end{cases}$$

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

- 1 Introduction
 - Motivation
 - Model
- 2 Correction process
- 3 Estimation of the parameters
- 4 Application
- 5 Conclusion**

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

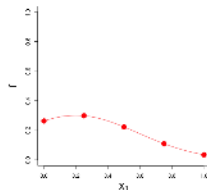
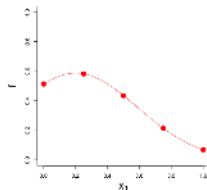
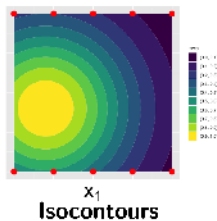
- Auto-regressive model inspired from the multifidelity
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- EM algorithm to jointly estimate the parameters of the processes

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

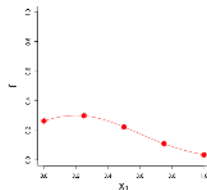
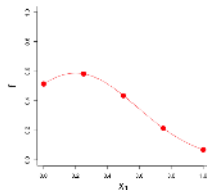
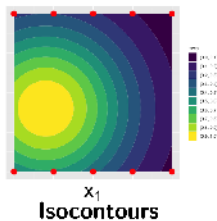
Perspective : Multiple conditioning

• Step 0 x_2

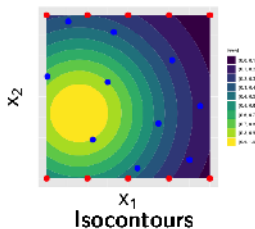


Perspective : Multiple conditioning

• Step 0 x_2



• Step 1



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

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

where

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

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

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

Formula in the tensor product case

- The eigen problem becomes

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

- ϕ_n becomes

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

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

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

Multiple P process

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

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

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

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