Multi-fidelity modeling for time-series output

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Outline

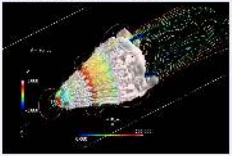
Model

Input parameters x

Physical system

$\approx$

Computer code

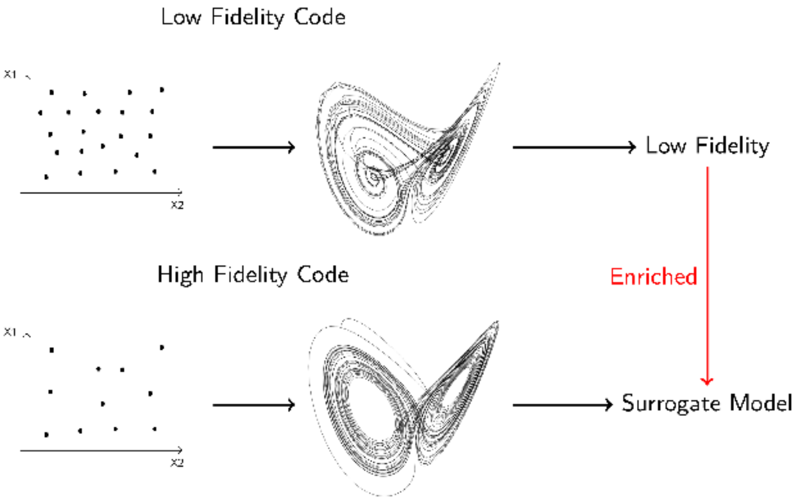


$\approx$

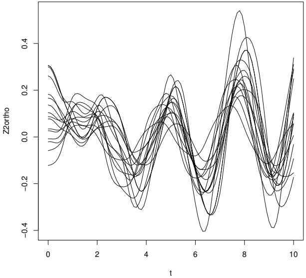
Surrogate model

$g_{\mathrm{exp}}(x)$ | $g_{\mathrm{num}}(x)$ | $\hat{g}(x)$

Multi-fidelity surrogate model



Time dependent outputs, definition and use



- Functional output of dimension 1
- Each realization of the code gives a 1D curve
- $Z(x, t_u)$ is known for t_u with $u = 1, \cdots, N_t$ but only for some $x \in \mathbb{R}^d$.

Multi-fidelity time-series outputs model

- Objective : model a multi-fidelity and time-series outputs system
- Idea : Combine the tensorized covariance method and Multifidelity CoKriging.

- Decomposition of the problem into two parts :

$$Z_L(x,t_u) = \sum_{i=1}^{N} A_{i,L}(x)\Gamma_i(t_u) + Z_L^{\perp}(x,t_u)$$

$$Z_H(x,t_u) = \underbrace{\sum_{i=1}^{N} \overbrace{A_{i,H}(x)}^{\text{coefficients}}\overbrace{\Gamma_i(t_u)}^{\text{basis}}}_{\text{dimension reduction}} + \underbrace{Z_H^{\perp}(x,t_u)}_{\text{orthogonal part}}$$

Method in 3 steps

1. Dimension reduction, definition of the basis Γ expression onto Γ.
2. Multi-fidelity CoKriging for $A_{i,H}(x)$ and $A_{i,L}(x)$.
3. Gaussian process regression with tensorized covariance for $Z_H^{\perp}(x, t_u)$.

- The value of N is chosen by cross-validation.

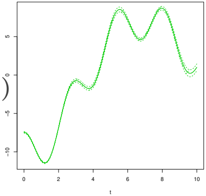
Dimension Reduction, step 1

We try to reduce the size of the outputs so we express :

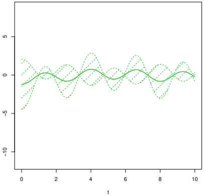
$$Z(x,t) = \sum_{i=1}^{N} A_i(x)\Gamma_i(t) + Z^{\perp}(x,t)$$

So we have $A_i(\boldsymbol{x})$ that we can use to do our regression. We are back to the previous regression problem.

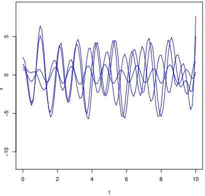
$Z(x,t) = A_1(x)$



$+A_2(x)$



$+$



The not so easy choice of basis

We propose different basis distributions for Γ :

Dirac

- We can give ourselves a basis a priori thanks to an expert judgement.
- The other solution is to carry out the SVD on the low fidelity data set.

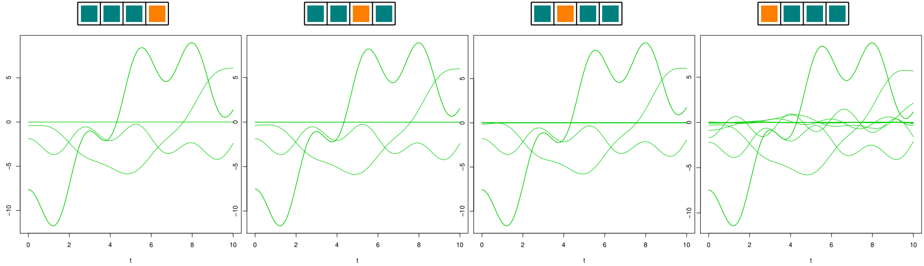
Empirical

- The method is inspired by K-fold cross-validation :
  - First define a learning set out of the available low fidelity output set.
  - Second generate the basis with the SVD on the learning set.
  - Finally compute the first two moments of the basis elements.

→ allows to compute the predictive mean and variance for $Z_H(x, t_u)$.

Definition of the empirical basis

Illustration of the construction of the bases taking into account the subset data used :



Multi-fidelity Gaussian process regression, step 2

- The quantities of interest : $a_H(x) \in \mathbb{R}$, respectively $a_L(x)$ with $x \in \mathbb{R}^d$.
- Hypothesis : $(a_H(x), a_L(x))$ **realization of GP** $(A_H(x), A_L(x))$
- Autoregressive CoKriging model from Kennedy et O'Hagan 2000 ; Le Gratiet et Garnier 2014 :

$$A_H(x) = \rho(x) A_L(x) + \delta(x),$$

where $\delta(x)$ GP independent of $A_L(x)$ and $\rho(x)$ ajustment linear form.

- Prediction : when the hyperparameters of the model are known,

$$[A_H(x)|\text{data}] \sim \mathcal{GP}(m_{A_H}(x), \sigma^2_{A_H}(x)),$$

the quantities $m_{A_H}(x)$ and $\sigma^2_{A_H}(x)$ have **analytical expressions**.

Tensorisation of the covariance, step 3

- Assumption : $z_H^{\perp}(x,t)$ **realization of a Gaussian process** $Z_H^{\perp}(x,t)$ with values in $\text{Span}\left\{\Gamma_{N+1}(t_u)\cdots\Gamma_{N_t}(t_u)\right\}$.

- Proposed approach PERRIN 2019 : the **covariance function** is **separable** in time and space. The covariance function $R_x(x,x')$ in x is Matèrn kernel. The covariance matrix in t_u is estimated by maximum likelihood.

- We keep the stationarity for x, but the **non-stationarity** in t is used.

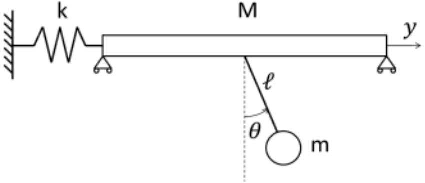
- The process $Z_H^{\perp}(x,t_u)$: $\left[Z_H^{\perp}(x,t_u)|\text{data}, \text{hyperparameters}\right] \sim \mathcal{GP}\left(\mu_\star(x), R_\star(x,x',t_u)\right)$ $\mu_\star(x)$ and $R_\star(x,x',t_u,t_u')$ have **analytical expressions** PERRIN 2019.

- **Estimation of R_x hyperparameters** : Leave One Out-Cross validation :

$$l_{c\,\mathbf{LOO}} = \underset{l\in(\mathbb{R}^+)^{n_x}}{\arg\min} \sum_{k=1}^{n_x} \left\| \mu_\star^{(-k)}\left(x^{(k)}, l_c\right) - z^{\perp(k)} \right\|^2,$$

The double pendulum

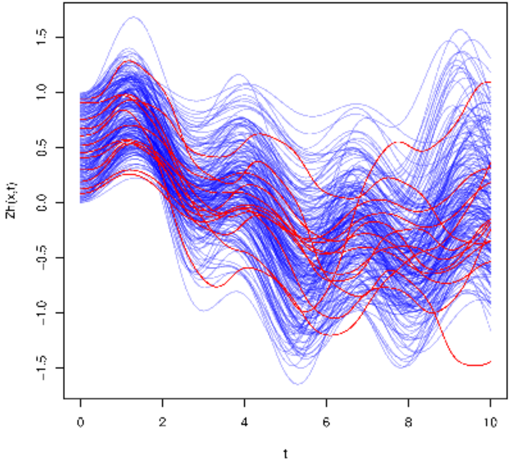
We use the outputs of a calculation code that models the system with two levels of fidelity :



	inputs
k	spring stiffness
M	mobile mass
l	pendulum length
y	mobile position
θ	pendulum angle
m	pendulum mass
	output
z	pendulum position

The difference between high and low fidelity is that the for low fidelity we assume that the angle θ is small.

Examples of Outputs

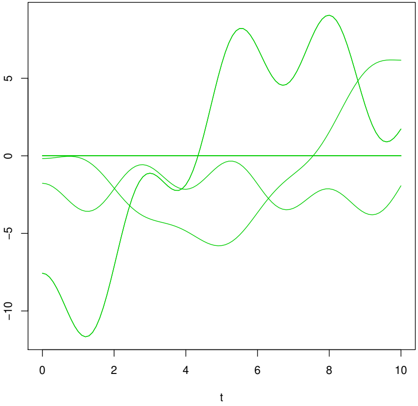


M	$[3; 8]$
k	$[0.1; 2.1]$
θ_0	$\left[\frac{\pi}{4}; \frac{\pi}{2}\right]$
$\dot{\theta}_0$	$\left[0; \frac{1}{6}\right]$
y_0	$[0; 0.2]$
$\dot{y}_0$	0
l	2
m	0.5
g	9.81

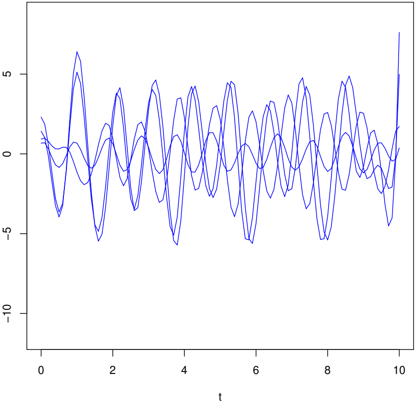
TABLE – Range of variation of the different system parameters.

For $N_H = 10$ (red), $N_L = 100$ (blue) and $N_t = 101$

Basis and orthogonal part of the example

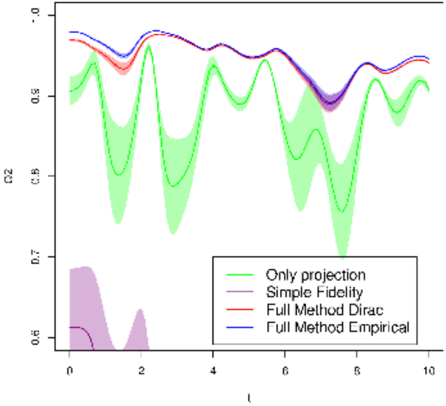


First 4 elements of the basis



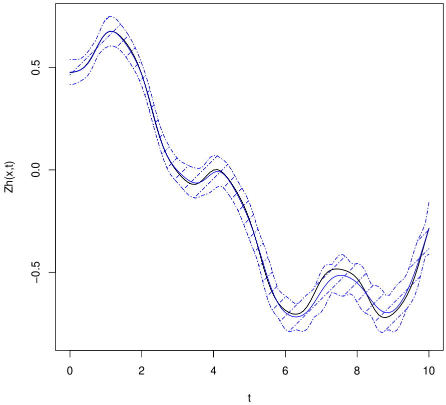
Orthogonal realisations for 5 different values of x

The result in Q^2 :

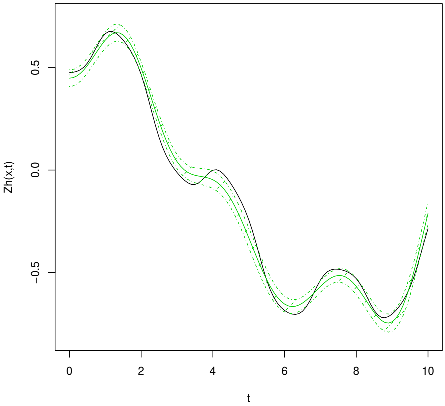


Optimise in N different for each method and each data set

Example of prediction with and without orthogonal part



with



without

Conclusion

- About this method :
  - Uncertainty is fully estimated even for the orthogonal part.
  - Our method is always better than the simple fidelity. The adavantages of coKriging and tensorisation approaches are exploited.
  - We are able to reduce the dimension and to exploit the orthogonal part.
- Perspectives :
  - The sequential learning
  - Image output
  - Non linear multi-fidelity approach

References

Kennedy, M. C. et A. O'Hagan (2000). "Predicting the Output from a Complex Computer Code When Fast Approximations Are Available". In : *Biometrika* 87.1, p. 1-13.

Le Gratiet, Loic et Josselin Garnier (2014). "Recursive co-kriging model for design of computer experiments with multiple levels of fidelity". In : *International Journal for Uncertainty Quantification* 4.5.

Perrin, Guillaume (2019). "Adaptive calibration of a computer code with time-series output". In : *Reliability Enginering and System Safety.*

Questions ?