Uncertainty quantification and visualization for functional random variables

MascotNum Workshop 2014

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April 23rd 2014

Introduction

- Identify/characterize the statistical properties of functional random variables.
- The variables are dependent and linked to a scalar (or vectorial) covariate.
- Propose a methodology of uncertainty characterization in order to:
  - get an estimate of the joint probability density function of the variables,
  - simulate new samples according to the estimated distribution,
  - adapt visualization tools to identify uncertainty characteristics of dependent functional variables.

Problem description

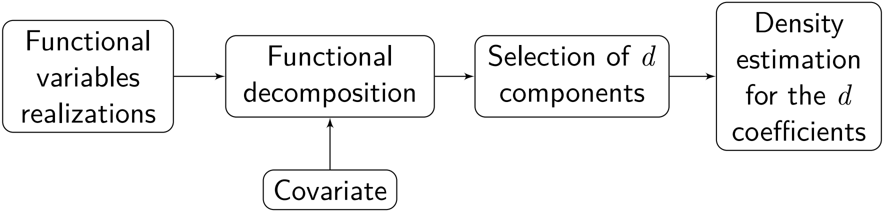
- Let $f_1, \ldots, f_m : I \times \Omega \to \mathbb{R}$ be dependent functional random variables.
- Let Y be a random variable, called covariate.
- Let $\mathcal{M}$ be a computer code/simulator such that

$$Y = \mathcal{M}(f_1, \ldots, f_m).$$

- Let f_j^i be the i^{th} realization of the j^{th} functional random variable, for $1 \leq i \leq n,\ 1 \leq j \leq m$.

Proposed methodology

- Two main steps:
  1. Decomposition on a reduced functional basis, taking into account the covariate
  2. Modeling of the probability density function of the decomposition coefficients



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Decomposition on a functional basis

Definition

Let $f : I \to \mathbb{R}$, $x \in I$.

$$f(x) = \sum_{k=1}^{+\infty} \alpha_k \phi_k(x)$$

- α_k coefficients,
- ϕ_k basis functions

Decomposition on a functional basis

Definition

Let $f : I \to \mathbb{R}$, $x \in I$.

$$\hat{f}(x) = \sum_{k=1}^{d} \alpha_k \phi_k(x)$$

- α_k coefficients,
- ϕ_k basis functions,
- d basis size

Partial Least Squares regression

- Let X $(n \times p)$ and Y $(n \times q)$ data matrices of respectively observable and predicted variables.
- X and Y are centered and standardized.
- Principle: linear regression between the projections of X and Y in a new space, called latent variables, whose correlation is maximal.

Algorithm of PLS regression [Wold, 1975]

- Initialization: $X_0 = X, \ Y_0 = Y$
- At each step h, we are seeking for the latent variables $\alpha_h = X_{h-1}u_h$ and $\omega_h = Y_{h-1}v_h$ solutions of

$$\max_{\|u_h\|=\|v_h\|=1} \mathrm{cov}(X_{h-1}u_h, Y_{h-1}v_h).$$

- "Deflation": $X_h = X_{h-1} - \alpha_h \phi_h^T$, with $\phi_h = X_{h-1}\alpha_h / (\alpha_h^T \alpha_h)$

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Partial Least Squares decomposition

- It can be deduced from the deflation step that X can be written as follows:

$$X = A\Phi^T + \epsilon$$

where the column vectors of A and Φ are respectively α_h and ϕ_h and ϵ are the residuals.

- Let the column vectors of X be functions discretized on p points and Y be the covariate.
  - $\Rightarrow$ A is the matrix of coefficients of the decomposition.
  - $\Rightarrow$ Φ is the matrix of basis functions.

- Basis functions are fitted to data, and
- adjusted to maximize the correlation between the functions and the covariate.

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Simultaneous PLS decomposition

- Objective: extend PLS decomposition to deal with multiple functional dependent variables simultaneously
- We suppose that functions $f_1 \dots f_m$ are correlated and have common reduction directions.
- Let $t_1 < \dots < t_p \in I$
- Let $\mathbf{f}_i = (f_i(t_1), \dots, f_i(t_p))$ be the discretized version of f_i, $i = 1, \dots, m$.
- Let each column vector of X be:

$$(\mathbf{f}_1, \dots, \mathbf{f}_m) \in \mathbb{R}^{dm}$$

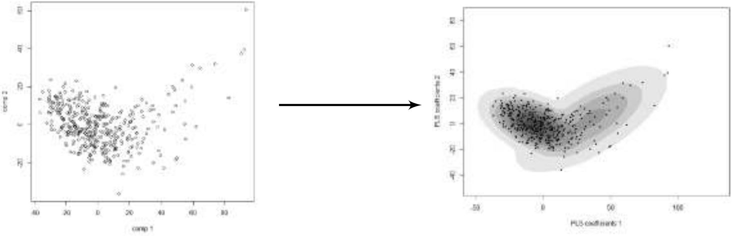
- Simultaneous PLS decomposition consists in applying the PLS decomposition to the previously defined matrix X.
  $\rightarrow$ **SPLS decomposition**

Objectives

- Estimate the probability density function (pdf) of d coefficients from SPLS decomposition
- High dimension: $d > 10$

  $\Rightarrow$ kernel density estimation not adapted

$\rightarrow$ Solution: **Gaussian mixture model**



Gaussian Mixture

- Probability density function of a Gaussian mixture:

$$g(\alpha|\mu_1, \Sigma_1, \dots, \mu_G, \Sigma_G) = \sum_{k=1}^{G} \tau_k \phi(\alpha|\mu_k, \Sigma_k), \ \forall \alpha \in \mathbb{R}^d$$

  - G clusters
  - n sample points
  - ϕ: Gaussian probability density function
  - $\tau_k, \ \mu_k, \ \Sigma_k$: proportion, mean and covariance matrix of cluster k

- Advantages / drawbacks
  - Fast algorithm for parameter estimation
  - Very fast simulation of a new realization
  - Can be used in dimension $d > 10$
  - parametric model: modeling hypothesis
  - Number of clusters to be determined

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EM algorithm

- Expectation-Maximization algorithm (EM) [Dempster et al., 1977] estimates the parameters of the Gaussian mixture model.
- Let us introduce z_{ik}, the probability of the i^{th} point to be in the k^{th} cluster.

Expectation Minimization algorithm:

1. Initialize parameters $\tau_k^{(0)}$, $\mu_k^{(0)}$ et $\Sigma_k^{(0)}$
2. Expectation Step: Compute $z_{ik}^{(j)}$
3. Maximization Step: Compute $\tau_k^{(j+1)}$, $\mu_k^{(j+1)}$, $\Sigma_k^{(j+1)}$
4. Repeat steps $2-3$ until convergence

Number of parameters reduction

- Total number of Gaussian mixture parameters:
  $N_T = G - 1 + Gd + G\frac{d(d+1)}{2}$
- G: number of clusters in the model
- N_T increases quickly with the dimension d

$\rightarrow$ Solution: **sparse covariance matrices estimation**

Two methods

- sEM method: penalizing the inverses of covariance matrices [Krishnamurthy, 2011]
- sEM2 method: penalizing the covariance matrices

sEM method

Penalizing the inverses of covariance matrices

- A **lasso penalization** on the inverses of the covariance matrices is added in the maximization step:

$$\hat{\Sigma}_k = \text{argmax}_{\Sigma_k} (\ell) \quad \dashrightarrow \quad \hat{\Sigma}_k = \text{argmax}_{\Sigma_k} \left(\ell - \lambda \|\Sigma_k^{-1}\|_1 \right)$$

- $\|M\|_1 = \sum_{i,j=1}^{p} M_{i,j}$.
- The penalization parameter λ is chosen bycross-validation.
- The penalized maximization is solved by [Friedman et al., 2008] coordinate descent-based algorithm.

sEM method

Penalizing the inverses of covariance matrices

sEM algorithm [Krishnamurthy, 2011]

1. Initialize parameters $\tau_k^{(0)}$, $\mu_k^{(0)}$ et $\Sigma_k^{(0)}$
2. Expectation Step: Compute $z_{ik}^{(j)}$
3. Maximization Step: Compute $\tau_k^{(j+1)}$, $\mu_k^{(j+1)}$
4. $\Sigma_k^{(j+1)} \leftarrow \text{argmax}_\Sigma \left(\ell - \lambda \left\|\Sigma^{-1}\right\|_1\right)$
5. Repeat steps $2-4$ until convergence

sEM2 method

Penalizing the covariance matrices

- A **lasso** penalization on the covariance matrices is added in the maximization step:

$$\hat{\Sigma}_k = \text{argmax}_{\Sigma_k} \left(\ell - \lambda \| P * \Sigma_k \|_1 \right)$$

- $*$ stands for Hadamard product.
- P: penalization matrix.
- The penalization parameter λ is chosen by cross-validation.
- The penalized maximization is solved by [Wang, 2013] coordinate descent-based algorithm.

sEM2 method

Penalizing the covariance matrices

- Several proposed matrices P:
  - **sEM2.1**: Equal weights to all matrix elements. All elements are penalized in the same way.

$$P_{ij} = 1$$

  - **sEM2.2**: Diagonal elements are not penalized. All others are penalized equally.

$$P_{ij} = \begin{cases} 1 & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}$$

  - **sEM2.3**: The lower the off-diagonal element, the more penalized. Diagonal elements are not penalized.

$$P_{ij} = \begin{cases} \frac{1}{\Sigma_{ij}} & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}$$

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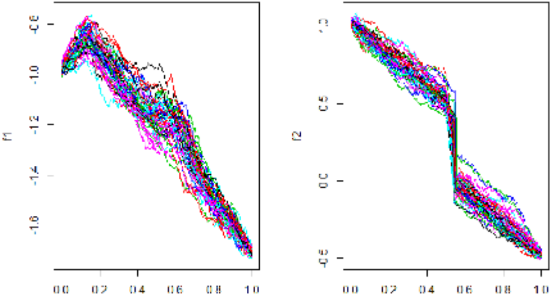
Illustration on an analytical example



- 2 temporal functional random variables f_1 et f_2 depending on three random variables a_1, a_2, a_3.
- a_1, a_2, a_3 have uniform distributions.
- Let define the covariate

$$Y(a_1, a_2, a_3) = \int_0^1 \left(f_1(t, a_1, a_2, a_3) + f_2(t, a_1, a_2, a_3)\right) dt.$$

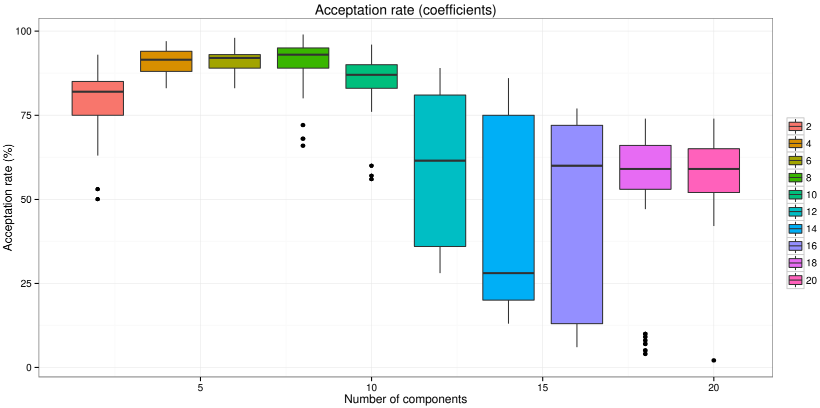
Illustration on an analytical example

- Hypothesis
  - Learning dataset: 600 curves
  - Test dataset: 1000 curves
  - SPLS decomposition + Gaussian mixture model
  - Optimal number G^* of clusters chosen with Bayesian Information Criterion (BIC)
- Proposed criteria to select the basis size d and assess the quality of the characterization method:
  - **Criterion C1**: Goodness-of-fit of estimated coefficients pdf and the real pdf with1 [Fromont et al., 2012] test.
  - **Criterion C2**: Goodness-of-fit of estimated covariate pdf and the pdf computed with known covariates with Kolmogorov-Smirnov (KS) test.
  - **Criterion C3**: Relative mean square between correlation on estimated functions and realizations of the variables.

$\rightarrow$ First step: use of EM algorithm

Illustration on an analytical example

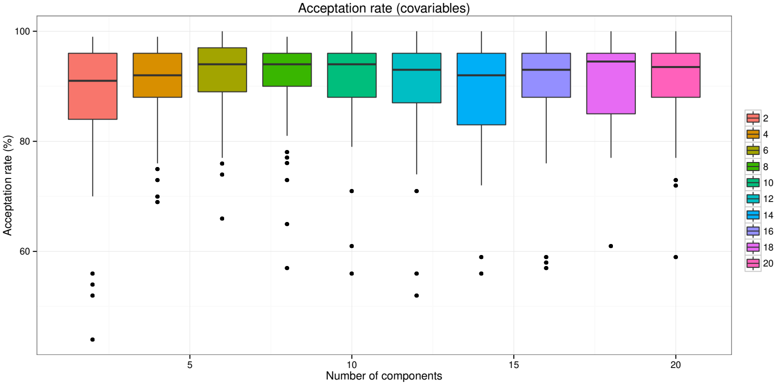
Criterion C1: Comparison of coefficients densities



- Maximal median at $d = 8$ components.
- After $d = 8$, model quality decreases.

Illustration on an analytical example

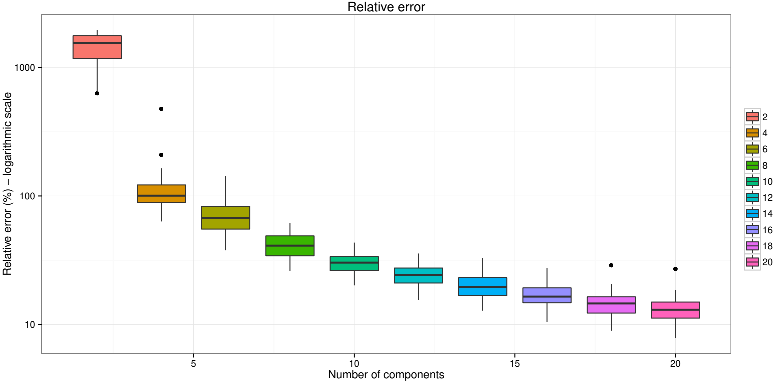
Criterion C2: Comparison of covariates densities



- Maximal median at $d = 6, 8, 10, 18$ components.
- Low variance for $d = 8$.
- Very close acceptance rates for all basis sizes.

Illustration on an analytical example

Criterion C3: Comparison of correlations between variables



- The correlation decrease is very even.
- Relative error is about 40% for $d = 8$.

Illustration on an analytical example: conclusions

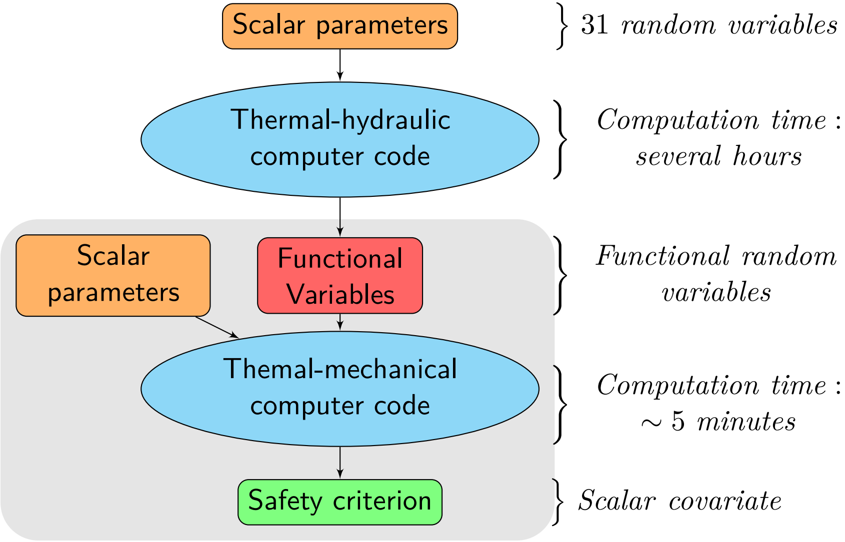
- Based on the three criteria → optimal basis size $d^* = 8$:
  - Good acceptance rates are obtained with EM algorithm.
  - The relative errors on correlation are still quite high.

- The same criteria have been computed for other estimation algorithms → similar results obtained (same d^* and criteria values).

- For the analytical example, the EM algorithm seems to be the best choice (efficient, easy and fast): as the number of parameters is quite low in this example ($n = 89$ for $d = 8$), the use of sparse algorithms does not improve the estimation.

- In practice, if no test basis is available, criteria C1, C2 and C3 are computed by cross-validation.

A nuclear safety test case (1)



A nuclear safety test case (2)

Dataset:

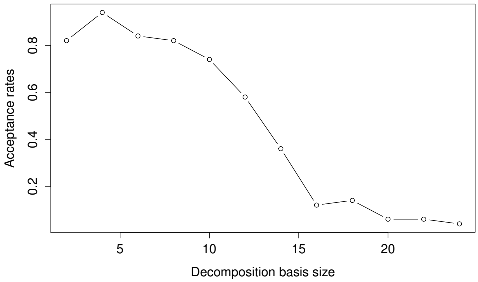
- 3 functional random variables depending on time
- Scalar covariate: a safety criterion
- Learning sample: 400 samples
- Logarithmic transformation of the sample (positivity constraint)

Methodology:

- SPLS decomposition + Gaussian mixture model + EM algorithm
- Optimal G^* determined by BIC
- Criteria C1, C2 and C3 computed by cross-validation
- Optimal d^* chosen by the analysis of the three criteria

A nuclear safety test case (3)

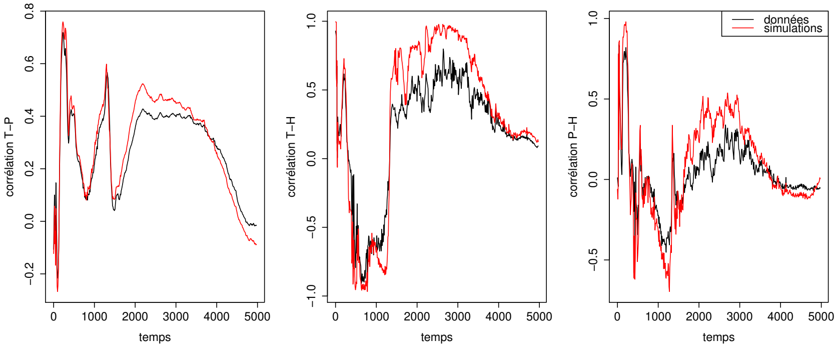
- Criterion 1:
  - optimal $d^* = 4$
  - acceptance rates under 80% for $d > 8$
  - fast decrease of acceptance rates for $d \geqslant 10$



- Criterion 2: low acceptance rates for all basis sizes

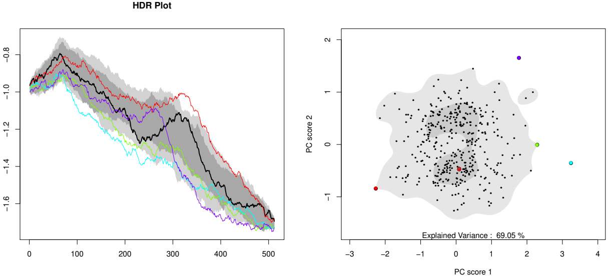
A nuclear safety test case (4)

- Criterion 3: quite good approximation of functional variable correlations for $d^* = 4$.



Visualization: High Density Region boxplot (HDR)

- Proposed by [Hyndman and Shang, 2010] and based on
  - Principal Component Analysis
  - First two basis functions selected
  - Kernel density estimation

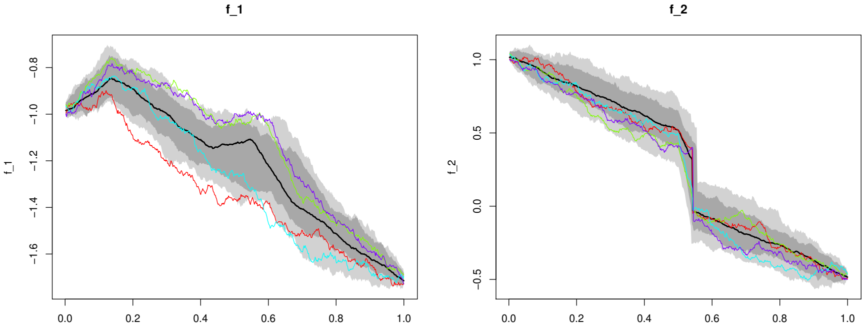


- Application on the analytical example:
  - Black curve: functional median
  - Colored curves: outliers
  - Dark (resp. light) gray zone: 50% (resp. 95%) highest density region

Visualization: Modified HDR boxplot

- Combination of the HDR boxplot and our proposed characterization methodology (SPLS + Gaussian mixture model)
  - ⇒ Simultaneous visualization of multiple functions
  - ⇒ Taking into account a covariate
  - ⇒ Decomposition on higher basis

- Illustration on the analytical example:



Conclusion and perspectives

- Development of a global methodology to simultaneously characterize dependent functional random variables linked to a covariate.

$\rightarrow$ **Simultaneous PLS decomposition + Gaussian mixture with sparse covariance matrices**

  - $\Rightarrow$ Estimation of probabilities for the variables to exceed a threshold.
  - $\Rightarrow$ Simulation according to the estimated pdf.
  - $\Rightarrow$ Visualization of the uncertainty of the variables.

- Different proposed criteria to assess the methodology efficiency:
  - Application on an analytical example: good results
  - Application on a nuclear safety test case: functions and correlations quite well reproduced but the covariate pdf not well fitted

Perspectives:

- Computing probabilities and quantiles to exceed a threshold.
- Using this methodology to run uncertainty propagation and sensitivity analysis studies.

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Appendix

Analytical example definition

$$
\begin{aligned}
f_1(t, a_1, a_2, a_3) &= 0.8 a_2 BB(t) + a_1 + c_1(t) + h(t) \\
f_2(t, a_1, a_2, a_3) &= a_2 BB(t) + a_1 + c_2(t)
\end{aligned}
$$

with

$$a_1 \sim \mathcal{U}(0, 0.05)\ ;\ a_2 \sim \mathcal{U}(0.05, 0.2)\ ;\ a_3 \sim \mathcal{U}(2, 3)$$

$$
\begin{aligned}
c_1(t) &= \begin{cases} t-1 & \text{if } t < \frac{70}{512} \\ \frac{372}{512} - t & \text{otherwise} \end{cases} \\
c_2(t) &= \begin{cases} 1-t & \text{if } t < 0.5 \\ \frac{64}{5a_3} - 0.5t & \text{if } 0.5 < t < 0.5 + \frac{10a_3}{512} \\ 0.5 - t & \text{otherwise} \end{cases} \\
h(t) &= 0.15\left(1 - \left|\frac{t - 100a_3}{60}\right|\right)
\end{aligned}
$$