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Approach for Meta-Modeling and Sensitivity
Analysis of Computational Codes in the Presence
of Dependent Random Variables.
Application to a design tool for vegetated strips.

Guerlain Lambert¹

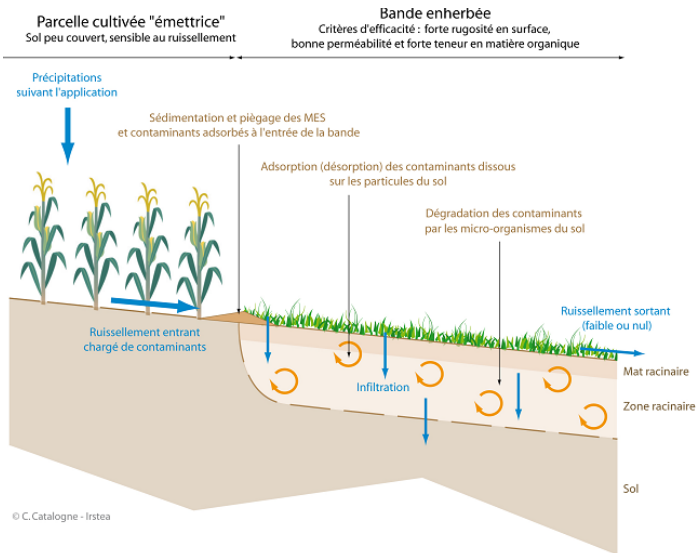
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4 décembre 2023

- 1 Context and motivation
 - A design tool for vegetated strips : BUVARD_MES
 - Group of variables
 - Motivations
- 2 Vectorial Quantization
- 3 Screening step : HSIC measure
- 4 Ranking step : Sobol' indices

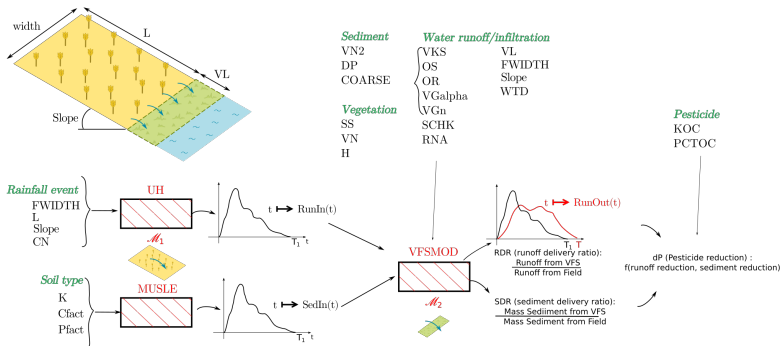
A design tool for vegetated strips : BUVARD_MES



Réf : [Veillon et al., 2022]

A design tool for vegetated strips : BUVARD_MES

Schematic diagram of BUVARD_MES

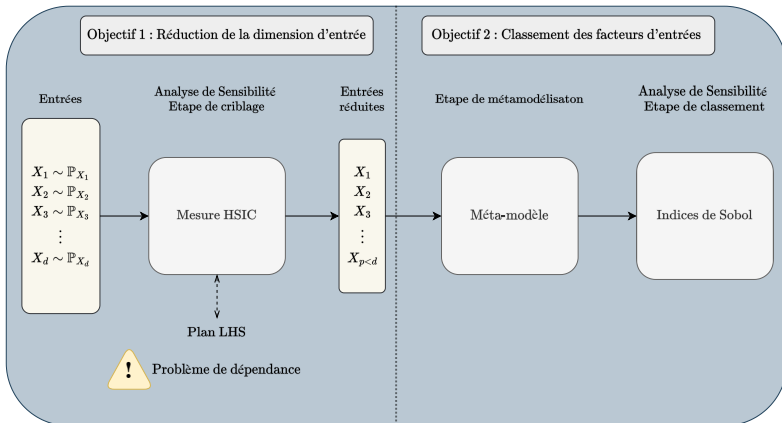


Réf : [Catalogne et al., 2018, Veillon et al., 2022]

General purpose

Goal of this work

Suggesting a global sensitivity analysis of a computationally expensive code: BUVARD_MES applied to Morcille (Beaujolais).



Purpose of this presentation

Significance of using a tailored experimental design for a sensitivity analysis approach in the presence of dependent random variables.

- Using vector quantization to create a design of experiment.
- Comparison with an existing technique : Latin Hypercube Sampling (LHS).

- 1 Context and motivation
- 2 Vectorial Quantization
 - Definition
 - In practice, how can such quantification be achieved?
 - Design of Experiment
 - Application to the BUVARD_MES group of dependent inputs
- 3 Screening step : HSIC measure
- 4 Ranking step : Sobol' indices

Vector quantification in a nutshell : [Pagès, 2018]

Quantization ? Approach a random vector X by a N -quantizer
 $\Gamma = \{x_1, \dots, x_N\} \in (\mathbb{R}^d)^N :$

$$\hat{X} = \text{Proj}(X, \Gamma) = \sum_{i=1}^N x_i 1_{\{X \in C_i(\Gamma)\}} \text{ with } C_i : \text{Voronoi partition}$$

Distorsion and optimal quantization

Let \hat{X} associated to the N -quantizer $\Gamma = \{x_1, \dots, x_N\}$, $N \in \mathbb{N}^*$.

- We call **distorsion** at level N , the mapping from $(\mathbb{R}^d)^N \rightarrow \mathbb{R} :$

$$\mathcal{D}_N^X(\Gamma) = \|X - \hat{X}\|_2^2 = \mathbb{E} \left[\min_{1 \leq i \leq N} |X - x_i|^2 \right]$$

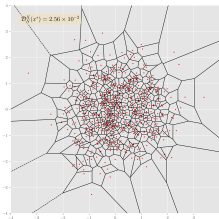
- Any N -quantizer satisfying the following minimization problem is said to be **optimal** :

$$\inf_{\Gamma, \#\Gamma \leq N} \mathcal{D}_N^X(\Gamma) = \inf \left\{ \|X - \hat{X}\|_2^2, \Gamma \subset \mathbb{R}^d, \#\Gamma \leq N \right\}$$

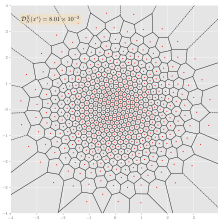
In practice, how can such quantification be achieved?

An example of an optimal quantification application

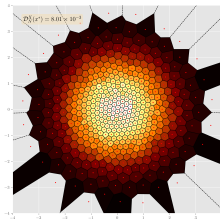
- **Context** : Application to the normal distribution $\mathcal{N}(0, I_2)$
- **Optimal quantization** : difficult to obtain in practice
- Use of a stochastic algorithm : Competitive Learning Vector Quantization (**CLVQ**)



(a) Initial



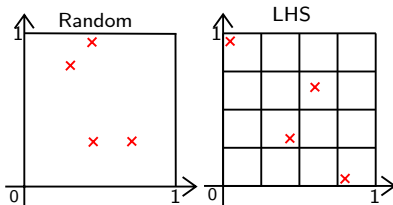
(b) Sans Poids



(c) Avec Poids

Réf : [Pagès, 2015]

LHS: the classic



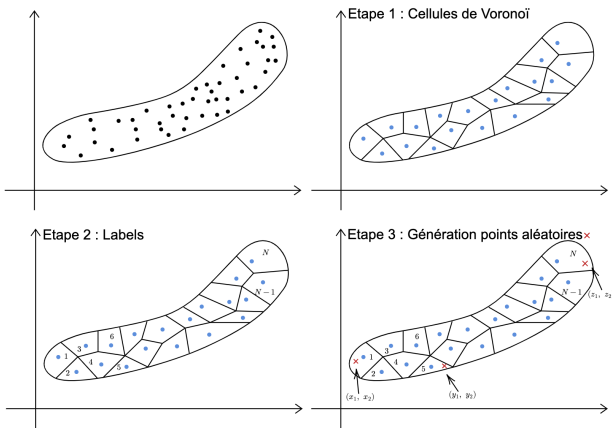
- 1 Divide $[0, 1]^2$ into n^2 squares of equal area.
- 2 Randomly choose n squares so that no pair of squares is equal.
- 3 A point is randomly generated in each selected square.

Formally : $\mathbf{x}_j = \left(\frac{\pi_1^j - u_1^j}{n}, \dots, \frac{\pi_n^j - u_1^j}{n} \right)$

- $(u_i^1, \dots, u_i^j)_{1 \leq i \leq n}$ i.i.d $\mathcal{U}([0, 1])$
- π^1, \dots, π^d permutations of $\{1, \dots, n\}$

Remark : A possible extension for dependence subject to knowledge of the copula: LHSD, see : [Packham and Schmidt, 2008]

RandomQuantif : DoE using vectorial quantization



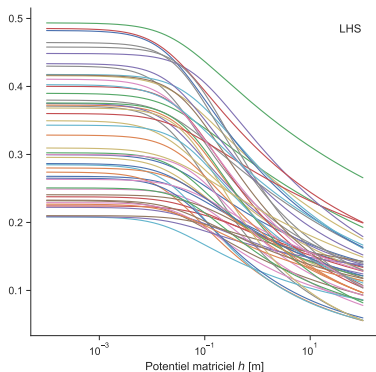
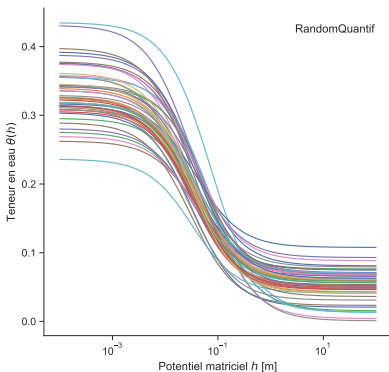
- 1 Generate d permutations π_1, \dots, π_d of $\{1, \dots, N\}$
- 2 Create the design matrix X from these points.

$$\pi = (1, 5, \dots, N)$$

$$X = ((x_1, x_2), (y_1, y_2), \dots, (z_1, z_2))$$

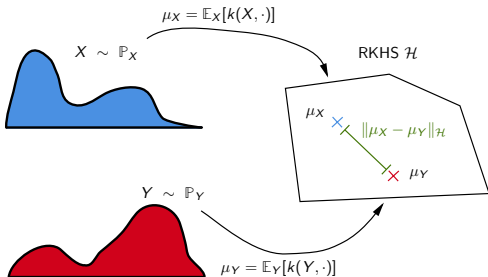
Interest of RandomQuantif on the Van Genuchten group

Water retention curve : $\theta(h) = \theta_s + \frac{\theta_s - \theta_r}{(1 + (\alpha|h|)^n)^{1-1/n}}$



- 1 Context and motivation
- 2 Vectorial Quantization
- 3 Screening step : HSIC measure
 - Sensitivity analysis by kernel
 - Independence test
 - Application to the BUVARD_MES model
- 4 Ranking step : Sobol' indices

HSIC measure



HSIC measure (Réf : [Gretton et al., 2005])

Let \mathcal{H}_i (resp. \mathcal{F}) be an RKHS associated with a kernel k_{X_i} (resp. k_Y). The HSIC measure between two random variables X_i and Y is defined by :

$$\text{HSIC}(X_i, Y) = \|\mu_{P_{X_i, Y}} - \mu_{P_{X_i}} \otimes \mu_{P_Y}\|_{\mathcal{H}_i \times \mathcal{F}}^2$$

with

$$\mu_{P_{X, Y}} = \int_{\mathcal{X}_i \times \mathcal{Y}} k_{X_i}(u, \cdot) k_Y(v, \cdot) dP_{X, Y}(u, v) = \mathbb{E}_{X, Y} [k_{X_i}(X, \cdot) k_Y(Y, \cdot)]$$

Estimation

If k_X and k_Y are characteristic (i.e. *mu* injective), then the following equivalence is true:

$$X_i \perp\!\!\!\perp Y \Leftrightarrow \text{HSIC}(X_i, Y) = 0$$

Fundamental property of HSIC measurements and estimation

Given an i.i.d. copy (X'_i, Y') of (X_i, Y) such that $\mathbb{E}_{X_i, X'_i} [k_{X_i}(X_i, X'_i)] < +\infty$ and $\mathbb{E}_{Y, Y'} [k_Y(Y, Y')] < +\infty$, we obtain that :

$$\begin{aligned} \text{HSIC}(X_i, Y) &= E [k_{X_i}(X_i, X'_i)k_Y(Y, Y')] + E [k_{X_i}(X_i, X'_i)] E [k_Y(Y, Y')] \\ &\quad - 2E [E [k_{X_i}(X_i, X'_i)] E [k_Y(Y, Y')]] \end{aligned}$$

$$\widehat{\text{HSIC}}(X_i, Y) = \frac{1}{n^2} \text{tr}(L_i H L H)$$

with

- L_i and L are Gram matrices.
- $H = (\delta_{ij} - \frac{1}{n})_{1 \leq i, j \leq n}$ where δ_{ij} is the Kronecker symbol.

Independence test based on HSIC measures

Test of independence :

\mathcal{H}_0 : " X_i and Y are independent" \mathcal{H}_0 : $\text{HSIC}(X_i, Y) = 0$
 \mathcal{H}_1 : " X_i and Y are dependent" \mathcal{H}_1 : $\text{HSIC}(X_i, Y) > 0$

equivalent to

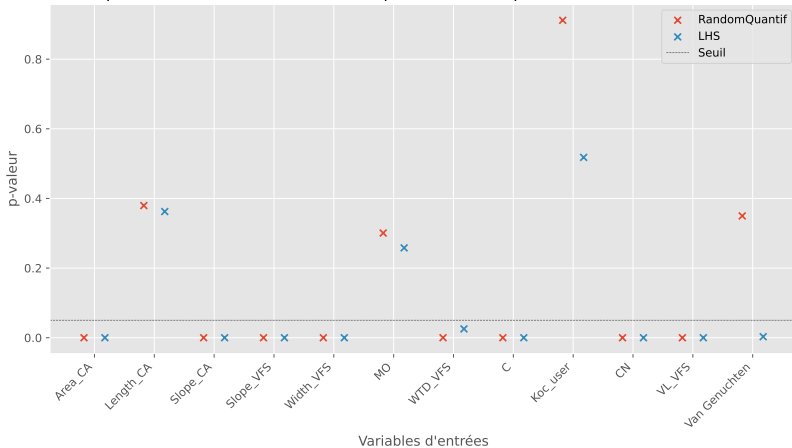
Estimating the test statistic : $\hat{S} = n\widehat{\text{HSIC}}(X_i, Y) \underset{n \rightarrow +\infty}{\sim} \gamma(\alpha, \beta)$

HSIC advantage : Requires a single sample of size $n \in \mathbb{N}^*$. !

Réf : [Gretton et al., 2007]

Application to the BUVARD_MES model

p-valeurs associées au test d'indépendance HSIC pour RandomQuantif et LHS



Results : LHS : Independence of the VG Group ; RandomQuantif :
Dependence on the VG Group

Expert knowledge : Sed_Ratio depends on VG Group

- 1 Context and motivation
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- 3 Screening step : HSIC measure
- 4 Ranking step : Sobol' indices**
 - Sobol indices and estimation
 - Flashback: Gaussian process regression
 - Application to the BUVARD_MES model
 - Conclusion and outlook

Sobol indices and estimation

Sobol' indices, [Sobol, 1993]

Let $\mathcal{M} \in L^2(P_{\mathbf{X}})$, $\mathbf{u} \subset \{1, \dots, d\}$ and $\mathbf{X} = (X_1, \dots, X_d)$ with X_i independent random variables.

- 1 Sobol indices of the first closed order associated with \mathbf{u} :

$$S_{\mathbf{u}} = \sum_{B \subset \mathbf{u}} S_B = \frac{\text{Var}(E[\mathcal{M}(\mathbf{X}) | \mathbf{X}_{\mathbf{u}}])}{V}$$

- 2 Sobol indices of total order associated with \mathbf{u} :

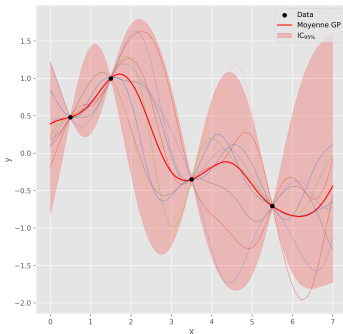
$$S_{\mathbf{u}}^T = 1 - S_{\bar{\mathbf{u}}}$$

Estimation : For Pick-Freeze, see for example [Saltelli et al., 2010]

Watch out! Numerous calls to the calculation code: $N \times (d + 2)$ with N in the range 100 to 1000 (Réf : [Saltelli et al., 2008]) !

Flashback: Gaussian process regression

- $\{\eta(\mathbf{x})\}_{\mathbf{x} \in \mathbb{R}^d} \sim \mathcal{GP}(m, k) \Leftrightarrow$ for any finite set $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ de \mathbb{R}^d , $(\eta(\mathbf{x}_1), \dots, \eta(\mathbf{x}_n))$ is a gaussian vector.
- Optimisation of hyperparameters by max-likelihood.

**RDR_Star**

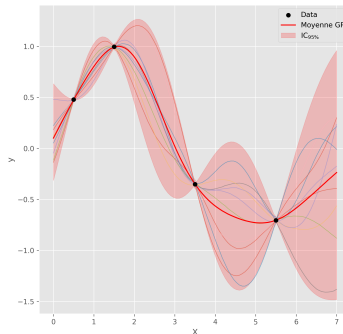
0.990

Sed_Ratio

0.980

dP_100

0.985



Réf : [Rasmussen and Williams, 2005]

Ranking of inputs

Rang	RDR* (RandomQuantif)	RDR* (LHS)
1	WTD_VFS	WTD_VFS
2	CN	CNA
3	Area_CA	Area_CA
4	Width_VFS	Width_VFS
5	Van Genuchten	VL_VFS
6	VL_VFS	Slope_VFS
7	Slope_VFS	Van Genuchten
8	Slope_CA	Slope_CA
9	Length_CA	C
10	MO	MO
11	Koc_user	Koc_user
12	C	Length_CA

Table: Ranking of variables in descending order (from most influential to least influential) of total order index for RDR*.

Conclusion and outlook

What has been done

- 1 Implementation of an adapted metamodeling strategy and sensitivity analysis in the presence of dependent variables.
- 2 The benefits of quantization compared with an LHS plan.

An outlook

- Convergence study for HSIC estimation using vector quantization.



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In 50e congrès du Groupe Français des Pesticides.