Electronic Journal of Statistics
Vol. 6 (2012) 2420–2448
ISSN: 1935-7524
DOI: 10.1214/12-EJS749

Generalized Hoeffding-Sobol decomposition for dependent variables - application to sensitivity analysis

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Abstract: In this paper, we consider a regression model built on dependent variables. This regression modelizes an input output relationship. Under boundedness type assumptions on the joint density function of the input variables, we show that a generalized Hoeffding-Sobol decomposition is available. This leads to new indices measuring the sensitivity of the output with respect to the input variables. We also study and discuss the estimation of these new indices.

Keywords and phrases: Sensitivity index, Hoeffding decomposition, dependent variables, Sobol decomposition.

Received March 2012.

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1. Introduction

Sensitivity analysis (SA) aims to identify the variables that most contribute to the variability into a non linear regression model. Global SA is a stochatic approach whose objective is to determine a global criterion based on the density of the joint probability distribution function of the output and the inputs of the regression model. The most usual quantification is the variance-based method, widely studied in SA literature. Hoeffding decomposition [13] (see also Owen [30]) states that the variance of the output can be uniquely decomposed into summands of increasing dimensions under orthogonality constraints. Following this approach, Sobol [35] introduces variability measures, the so called *Sobol sensitivity indices*. These indices quantify the contribution of each input on the system.

Different methods have been exploited to estimate Sobol indices. The Monte Carlo algorithm was proposed by Sobol [36], and has been later improved by the Quasi Monte Carlo technique, performed by Owen [31]. FAST methods are also widely used to estimate Sobol indices. Introduced earlier by Cukier *et al.* [3] [4], they are well known to reduce the computational cost of multidimensional integrals thanks to Fourier transformations. Later, Tarantola *et al.* [38] adapted the Random Balance Designs (RBD) to FAST method for SA (see also recent advances on the subject by Tissot *et al.* [40]).

However, these indices are constructed on the hypothesis that the input variables are independent, which seems unrealistic for many real life phenomena. In the literature, only a few methods and estimation procedures have been proposed to handle models with dependent inputs. Several authors have proposed sampling techniques to compute marginal contribution of inputs to the outcome variance (see the introduction in Mara and references therein [27]). As underlined in Mara *et al.* [27], if inputs are not independent, the amount of the response variance due to a given factor may be influenced by its dependence to other inputs. Therefore, classical Sobol indices and FAST approaches for dependent variables are difficult to interpret (see, for example, Da Veiga's illustration [5] p.133). Xu and Gertner [42] proposed to decompose the partial variance of an input into a correlated part and an uncorrelated one. Such an approach allows to exhibit inputs that have an impact on the output only through their strong correlation with other incomes. However, they only investigated linear models with linear dependences.

Later, Li *et al.* [24] extended this approach to more general models, using the concept of High Dimensional Model Representation (HDMR [23]). HDMR is based on a hierarchy of component functions of increasing dimensions (truncation of Sobol decomposition in the case of independent variables). The component functions are then approximated by expansions in terms of some suitable basis functions (e.g., polynomials, splines, ...). This meta-modeling approach allows the splitting of the response variance into a correlative contribution and a structural one of a set of inputs. Mara *et al.* [27] proposed to decorrelate the inputs with the Gram-Schmidt procedure, and then to perform the ANOVA-HDMR of Li *et al.* [24] on these new inputs. The obtained indices can be interpreted as fully, partially correlated and independent contributions of the inputs to the output. Nevertheless, this method does not provide a unique orthogonal set of inputs as it depends on the order of the inputs in the original set. Thus, a large number of sets has to be generated for the interpretation of resulting indices. As a different approach, Borgonovo *et al.* [1, 2] initiated the construction of a new generalized moment free sensitivity index. Based on geometrical consideration, these indices measure the shift area between the outcome density and this same density conditionally to a parameter. Thanks to the properties of these new indices, a methodology is given to obtain them analytically through test cases. Recently, Kucherenko *et al.* [19] proposed to use first order and total sensitivity indices based on the classical decomposition of total variance. These new indices are estimated by crude Monte Carlo method on conditional expectation through several numerical examples.

Notice that none of these works has given an exact and unambiguous definition of the functional ANOVA for correlated inputs as the one provided by Hoeffding-Sobol decomposition when inputs are independent. Consequently, the exact form of the model has neither been exploited to provide a general variance-based sensitivity measures in the dependent frame.

In a pionnering work, Hooker [14], inspired by Stone [37], shed new lights on hierarchically orthogonal function decomposition.

We revisit here the work of Hooker and Stone. We obtain hierarchical functional decomposition under a general assumption on the inputs distribution. Furthermore, we also show the uniqueness of the decomposition leading to the definition of new sensitivity indices. Under suitable conditions on the joint distribution function of the input variables, we give a hierarchically orthogonal functional decomposition (HOFD) of the model. The summands of this decomposition are functions depending only on a subset of input variables and are hierarchically uncorrelated. This means that two of these components are orthogonal whenever all the variables involved in one of the summands also appear in the other. This decomposition leads to the construction of generalized sensitivity indices well tailored to perform global SA when the input variables are dependent. In the case of independent inputs, this decomposition is nothing more than the Hoeffding one. Furthermore, our generalized sensitivity indices are in this case the classical Sobol ones.

Recently, Li *et al.* [22] proposed a numerical method to compute the decomposition components given by Hooker. Using a constrainted minimization of the squared error, the variational counterpart of the decomposition also given in [14], they estimate the decomposition with an extended basis by using a continuous descent technique.

Here, we propose an estimation method performed by solving linear system involving suitable projection operators. We will focus on the particular case where the inputs are independent pairs of dependent variables (IPDV). Firstly, in the simplest case of a single pair of dependent variables, the HOFD may be obtained by solving a functional linear system of equations (see Procedure 1). In the more general IPDV case, the HOFD is then obtained in two steps (see Procedure 2). The first step is a classical Hoeffding-Sobol decomposition of the output on the input pairs, as developped in Jacques *et al.* [16]. The second step is the HOFDs of all the pairs. In practical situations, the non parametric regression function of the model is generally not exactly known. In this case, one can only have at hand some realizations of the model and have to estimate, with this information, the HOFD. Here, we study this statistical problem in the IPDV case. We build estimators of the generalized sensitivity indices and study numerically their properties. One of the main conclusion is that the generalized indices have a total normalized sum. This is not true for classical Sobol indices in the frame of dependent variables.

The paper is organized as follows. In Section 2, we give and discuss general results on the HOFD. The main result is Theorem 1. We show here that a HOFD is available under a boundedness type assumption (C.2) on the density of the joint distribution function of the inputs. Further, we introduce the generalized indices. In Section 3, we give examples of multivariate distributions to which Theorem 1 applies. We also state a sufficient condition for (C.2) and necessary and sufficient conditions in the IDPV case. Section 4 is devoted to the estimation procedures of the components of the HOFD and of the new sensitivity indices. Section 5 presents numerical applications. Through three toy functions, we estimate generalized indices and compare their performances with the analytical values. In the first two examples, we compare the sensitivity indices estimations to the true values to show the relevance of our new indices. The last example is a more realistic model. To prevent an industrial site from inundation, the overflow of a river is modelized by a set of eight inputs, in which some pairs are linearly correlated. The goal of this last application is to detect the most influential variables taking into account the dependence of the variables in the physical model. In Section 6, we give conclusions and discuss future work. Technical proofs and further details are postponed to the Appendix.

2. Generalized Hoeffding decomposition-application to SA

To begin with, let introduce some notation. We briefly recall the usual functional ANOVA decomposition, and Sobol indices. We then state a generalization of this decomposition, allowing to deal with correlated inputs.

2.1. Notation and first assumptions

We denote by $\subset$ the strict inclusion, that is $A \subset B \Rightarrow A \cap B \neq B$, whereas we use $\subseteq$ when equality is possible.

Let $(\Omega, \mathcal{A}, P)$ be a probability space and let Y be the output of a deterministic model η. Suppose that η is a measurable function of a random vector $\mathbf{X} = (X_1, \dots, X_p) \in \mathbb{R}^p$, $p \geq 1$ and let $P_{\mathbf{X}}$ be the pushforward measure of P by $\mathbf{X}$,

$$Y : \begin{array}{ccccc} (\Omega, \mathcal{A}, P) & \rightarrow & (\mathbb{R}^p, \mathcal{B}(\mathbb{R}^p), P_{\mathbf{X}}) & \rightarrow & (\mathbb{R}, \mathcal{B}(\mathbb{R})) \\ \omega & \mapsto & \mathbf{X}(\omega) & \mapsto & \eta(\mathbf{X}(\omega)) \end{array}$$

Let ν be a σ–finite measure on $(\mathbb{R}^p, \mathcal{B}(\mathbb{R}^p))$. Assume that $P_{\mathbf{X}} << \nu$ and let $p_{\mathbf{X}}$ be the density of $P_{\mathbf{X}}$ with respect to ν, that is $p_{\mathbf{X}} = \frac{dP_{\mathbf{X}}}{d\nu}$.

Also, assume that $\eta \in L^2_{\mathbb{R}}(\mathbb{R}^p, \mathcal{B}(\mathbb{R}^p), P_{\mathbf{X}})$. The associated inner product of this Hilbert space is:

$$\langle h_1, h_2 \rangle = \int h_1(\mathbf{x}) h_2(\mathbf{x}) p_{\mathbf{X}} d\nu(\mathbf{x}) = \mathbb{E}(h_1(\mathbf{X}) h_2(\mathbf{X}))$$

Here $\mathbb{E}(\cdot)$ denotes the expectation. The corresponding norm will be classically denoted by $\|\cdot\|$. Further, $V(\cdot) = \mathbb{E}[(\cdot - \mathbb{E}(\cdot))^2]$ denotes the variance, and $\mathrm{Cov}(\cdot, *) = \mathbb{E}[(\cdot - \mathbb{E}(\cdot))(* - \mathbb{E}(*))]$ the covariance.
Let $\mathcal{P}_p := \{1, \dots, p\}$ and S be the collection of all subsets of $\mathcal{P}_p$. Define $S^- := S \setminus \mathcal{P}_p$ as the collection of all subsets of $\mathcal{P}_p$ except $\mathcal{P}_p$ itself. The cardinality of a set u is denoted by $\#(u)$ or $|u|$ according to the context.

Further, let $\mathbf{X_u} := (X_l)_{l \in u}$, $u \in S \setminus \{\emptyset\}$. We introduce the subspaces of $L^2_{\mathbb{R}}(\mathbb{R}^p, \mathcal{B}(\mathbb{R}^p), P_{\mathbf{X}})$ $(H_u)_{u \in S}$, $(H_u^0)_{u \in S}$ and H^0. H_u is the set of all measurable and square integrable functions depending only on $\mathbf{X_u}$. $H_\emptyset$ is the set of constants and is identical to $H_\emptyset^0$. H_u^0, $u \in S \setminus \emptyset$, and H^0 are defined as follows:

$$H_u^0 = \left\{ h_u(\mathbf{X_u}) \in H_u,\ \langle h_u, h_v \rangle = 0, \forall\ v \subset u, \forall\ h_v \in H_v^0 \right\}$$

$$H^0 = \left\{ h(\mathbf{X}) = \sum_{u \in S} h_u(\mathbf{X_u}), h_u \in H_u^0 \right\}$$

At this stage, we do not make assumptions on the support of $\mathbf{X}$.

2.2. Sobol sensitivity indices

In this section, we recall the classical Hoeffding-Sobol decomposition, and the Sobol sensitivity indices if the inputs are independent, that is when $P_{\mathbf{X}} = P_{X_1} \otimes \cdots \otimes P_{X_p}$.

The usual presentation is done when $\mathbf{X} \sim \mathcal{U}([0,1]^p)$ [35], but the Hoeffding decomposition remains true in the more general case of independent variables [41].

Let $\mathbf{x} = (x_1, \ldots, x_p) \in \mathbb{R}^p$. The decomposition consists in writting $\eta(\mathbf{x}) = \eta(x_1, \ldots, x_p)$ as the sum of increasing dimension functions:

$$\begin{aligned}
\eta(\mathbf{x}) &= \eta_0 + \sum_{i=1}^{p} \eta_i(x_i) + \sum_{1 \leq i < j \leq p} \eta_{i,j}(x_i, x_j) + \cdots + \eta_{1,\ldots,p}(\mathbf{x}) \\
&= \sum_{u \subseteq \{1 \cdots p\}} \eta_u(\mathbf{x_u}) \qquad (1)
\end{aligned}$$

The expansion (1) exists and is unique under the assumption

$$\int \eta_u(\mathbf{x_u}) dP_{X_i} = 0 \quad \forall\ i \in u, \forall\ u \subseteq \{1 \cdots p\}$$

Equation (1) tells us that the model function $Y = \eta(\mathbf{X})$ can be expanded in a functional ANOVA. The independence of the inputs and the orthogonality properties ensure the global variance decomposition of the output as $V(Y) = \sum_{u \in S \setminus \emptyset} V(\eta_u(\mathbf{X_u}))$. Moreover, by integration,

$$\eta_0 = \mathbb{E}(Y), \quad \eta_u = \mathbb{E}(Y|\mathbf{X_u}) - \sum_{v \subset u} \eta_v,\ |u| \geq 1 \qquad (2)$$

Hence, the contribution of a group of variables $\mathbf{X_u}$ in the model can be quantified in the fluctuations of Y. The Sobol indices are defined by:

$$S_u = \frac{V(\eta_u)}{V(Y)} = \frac{V[\mathbb{E}(Y|\mathbf{X_u})] - \sum_{v \subset u} (-1)^{|u|-|v|} V[\mathbb{E}(Y|\mathbf{X_v})]}{V(Y)}, \quad u \subseteq \mathcal{P}_p \qquad (3)$$

Furthermore, Sobol indices are summed to 1.

However, the main assumption is that the input parameters are independent. This is unrealistic in many cases. The use of the previous expressions is not excluded in case of inputs' dependence, but could lead to an unobvious or a wrong interpretation. Moreover, used methods to estimate them may mislead final results because most of these methods are built on the assumption of independence. For these reasons, the objective of the upcoming work is to show that the construction of sensitivity indices under dependence condition can be done into a mathematical frame.

In the next section, we propose a generalization of the Hoeffding decomposition under suitable conditions on the joint distribution function of the inputs. This decomposition consists of summands of increasing dimension, like in Hoeffding one. But this time, the components are hierarchically orthogonal instead of being mutually orthogonal. The hierarchical orthogonality will be mathematically defined further, and the obtained decomposition will be denoted by HOFD, as mentioned in the introduction. Thus, the global variance of the output could be decomposed as a sum of covariance terms depending on the summands of the HOFD. It leads to the construction of generalized sensitivity indices summed to 1 to perform well tailored SA in case of dependence.

2.3. Generalized decomposition for dependent inputs

We no more assume that $P_{\mathbf{X}}$ is a product measure. Nevertheless, we assume:

$$\boxed{\begin{array}{c} P_{\mathbf{X}} << \nu \\ \textit{where} \\ \nu(dx) = \nu_1(dx_1) \otimes \cdots \otimes \nu_p(dx_p) \end{array}} \tag{C.1}$$

Our main assumption is:

$$\boxed{\exists\ 0 < M \leq 1,\ \forall\ u \subseteq \mathcal{P}_p, \quad p_{\mathbf{X}} \geq M \cdot p_{\mathbf{X_u}} p_{\mathbf{X_{u^c}}} \quad \nu\text{-}a.e.} \tag{C.2}$$

where u^c denotes the complement set of u in $\mathcal{P}_p$. $p_{\mathbf{X_u}}$ and $p_{\mathbf{X_{u^c}}}$ are respectively the marginal densities of $\mathbf{X_u}$ and $\mathbf{X_{u^c}}$.

A sufficient condition for (C.2) will be given later in Proposition 2. It will give a better understanding of (C.2). However, (C.2) may pave the way for another type of dependence. Indeed, for $p = 2$ and $M = 1$, it implies the positive quadrant dependence given by Lehmann [21]. Furthermore, the reinterpretation with copulas, given in Proposition 3, shows that (C.2), despite its unobvious form, holds for a wide class of copulas.

The section is organized as follows: a preliminary lemma gives the main result to show that H^0 is a complete space. This is a reminder of Lemma 3.1 studied in [37]. It ensures the existence and the uniqueness of the projection of η onto H^0, as given in Theorem 3.1 of [37]. The generalized decomposition of η is finally obtained by adding a residual orthogonal to every summand, as suggested in [14].

To begin with, let us state some definitions. In the usual ANOVA context, a model is said to be hierarchical if for every term involving some inputs, all lower-order terms involving a subset of these inputs also appear in the model. Correspondingly, a hierarchical collection T of subsets of $\mathcal{P}_p$ is defined as follows:

Definition 1. A collection $T \subset S$ is hierarchical if for $u \in T$ and v a subset of u, one has $v \in T$.

Using this definition, let state the following result:

Lemma 1. *Let $T \subset S$ be hierarchical. Suppose that (C.1) and (C.2) hold. Set $\delta = 1 - \sqrt{1-M} \in]0,1]$. Then, for any $h_u \in H_u^0$, $u \in T$, we have:*

$$\mathbb{E}[(\sum_{u \in T} h_u(\mathbf{X}))^2] \geq \delta^{\#(T)-1} \sum_{u \in T} \mathbb{E}[h_u^2(\mathbf{X})] \tag{4}$$

Lemma 1 is one of the key tool to show the hierarchical decomposition given in Theorem 1. To be self-contained, we give the proofs of Lemma 1 and Theorem 1 in the Appendix.

Theorem 1. *Let η be any function in $L^2_{\mathbb{R}}(\mathbb{R}^p, \mathcal{B}(\mathbb{R}^p), P_{\mathbf{X}})$. Then, under (C.1) and (C.2), there exist functions $\eta_0, \eta_1, \ldots, \eta_{\mathcal{P}_p} \in H_\emptyset \times H_1^0 \times \cdots H_{\mathcal{P}_p}^0$ such that the following equality holds:*

$$\begin{aligned}\eta(X_1, \ldots, X_p) &= \eta_0 + \sum_i \eta_i(X_i) + \sum_{i,j} \eta_{ij}(X_i, X_j) + \cdots + \eta_{\mathcal{P}_p}(X_1, \ldots, X_p) \\ &= \sum_{u \in S} \eta_u(\mathbf{X_u}) \end{aligned} \tag{5}$$

Moreover, this decomposition is unique.

Notice that in the case where the input variables $X_1, \ldots, X_p$ are independent, $\delta = 1$ and Inequality (4) of Lemma 1 becomes an equality. Indeed, in this case, this equality is directly obtained by orthogonality of the summands, and the HOFD turns out to be the classical Sobol decomposition.

2.4. Generalized sensitivity indices

As stated in Theorem 1, under (C.1) and (C.2), the output Y of the model can be uniquely decomposed as a sum of hierarchically orthogonal terms. Thus, the global variance has a simplified decomposition into a sum of covariance terms. From this fact, we can define generalized sensitivity indices.

Definition 2. The sensitivity index S_u of order $|u|$ measuring the contribution of $\mathbf{X_u}$ into the model is given by:

$$\boxed{S_u = \frac{V(\eta_u(\mathbf{X_u})) + \sum_{u \cap v \neq u, v} Cov(\eta_u(\mathbf{X_u}), \eta_v(\mathbf{X_v}))}{V(Y)}} \tag{6}$$

More specifically, the first order sensitivity index S_i is given by:

$$\boxed{S_i = \frac{V(\eta_i(X_i)) + \sum_{\substack{v \neq \emptyset \\ i \notin v}} Cov(\eta_i(X_i), \eta_v(\mathbf{X_v}))}{V(Y)}} \tag{7}$$

An obvious consequence is given in Proposition 1 (see proof in the Appendix):

Proposition 1. *Under (C.1) and (C.2), the sensitivity indices S_u defined previously sums to 1, i.e.*

$$\sum_{u \in S \setminus \{\emptyset\}} S_u = 1 \tag{8}$$

Discussion

First, we note that these indices are very similar to the ones proposed in Li *et al.* [24]. Nevertheless, their approach is different as they are mainly interested with the estimation of these quantities. For this purpose, they first approximate the model output by component functions. Further, they deduce a decomposition of the global variance. Here, indices originate from the HOFD of any regular function, but the assumptions (C.1) and (C.2) are required. Although the problem takes another route here, it should be noted that there exist other several methods to evaluate the importance of variables. Among them, the PLS [11], the Lasso regression [39], or, more generally, the LARS method [9] are performed for shrinkage and variable selection. More closely related, the COSSO regression [25] is a Lasso on SS-ANOVA [12] components to select a sparse number of effects. In [20], the prediction quality of linear models after parameters selection by sensitivity analysis is compared to Lasso regression. It highlights the complex relationship between sensitivity analysis and the prediction mean squared error.

In terms of interpretation, we notice that the covariance terms included in these indices allow to take into account the input dependence. Thus, they allow to measure the influence of a variable on the model, especially when a part of its variability is embedded into the one of other dependent terms. The form of the sensitivity indices allows for distinguishing the full contribution of a variable and its contribution into another correlated income. Also, if inputs are independent, the summands η_u are mutually orthogonal, so $\mathrm{Cov}(\eta_u, \eta_v) = 0$, $u \neq v$, and we recover the well known Sobol indices. Hence, these new sensitivity indices can be seen as a generalization of Sobol indices.

3. Examples of distribution function

This section is devoted to examples of distribution function satisfying (C.1) and (C.2). The first hypothesis only implies that the reference measure is a product measure, whereas the second is trickier to obtain.

In the first part, we give a sufficient condition to get (C.2) for any number p of input variables. The second part deals with the case $p = 2$, for which we give equivalences of (C.2) in terms of copulas.

3.1. Boundedness of the inputs density function

The difficulty of Condition (C.2) is that the inequality has to be true for any splitting of the set $(X_1, \dots, X_p)$ into two disjoint blocks. We give a sufficient condition for (C.2) to hold in Proposition 2. This proposition is basically the condition given by Stone in the case of the Lebesgue measure on a compact rectangle. The proof can be found in [37] page 132.

Proposition 2. *Assume that there exist M_1,$M_2 > 0$ with*

$$\boxed{M_1 \leq p_{\mathbf{X}} \leq M_2} \qquad (C.3)$$

Then, Condition (C.2) holds.

Let give now an example where (C.3) is satisfied.

Example 1. Let ν be the multidimensional gaussian distribution $N_p(m,\Sigma)$ with

$$m = \begin{pmatrix} m_1 \\ \vdots \\ m_p \end{pmatrix}, \quad \Sigma = \begin{pmatrix} \sigma_1^2 & \cdots & 0 \\ & \ddots & \\ 0 & \cdots & \sigma_p^2 \end{pmatrix}$$

Assume that $P_{\mathbf{X}}$ is the Gaussian mixture $\alpha \cdot N_p(m,\Sigma) + (1-\alpha) \cdot N_p(\mu,\Omega)$, $\alpha \in]0,1[$ with

$$\mu = \begin{pmatrix} \mu_1 \\ \vdots \\ \mu_p \end{pmatrix}, \quad \Omega = \begin{pmatrix} \varphi_1^2 & \rho_{12} & \cdots & \rho_{1p} \\ & \cdots & & \\ \rho_{1p} & \cdots & \cdots & \varphi_p^2 \end{pmatrix}$$

Then, (C.3) holds iff the matrix $(\Omega^{-1} - \Sigma^{-1})$ is positive definite.

In the next section, we will see that (C.2) has a copula version when $p = 2$. Thus, we establish two equivalent conditions to (C.2). We will give some examples of distribution satisfying one of these conditions.

3.2. Examples of distribution of two inputs

Here, we consider the simpler case $p = 2$. Also, until Section 4, we will assume that ν is absolutely continuous with respect to Lebesgue measure. The structure of dependence of X_1 and X_2 can be modelized by copulas. Copulas [29] give a relationship between a joint distribution and its marginals. Sklar's theorem [34] ensures that for any distribution function $F(x_1,x_2)$ with marginal distributions $F_1(x_1)$ and $F_2(x_2)$, F has the copula representation,

$$F(x_1,x_2) = C(F_1(x_1), F_2(x_2))$$

where the measurable function C is unique whenever F_1 and F_2 are absolutely continuous.

The next corollary gives in the absolutely continuous case the relationship between a joint density and its marginal:

Corollary 1. *In terms of copulas, the joint density of* $\mathbf{X}$ *is given by:*

$$p_X(x_1,x_2) = c(F_1(x_1), F_2(x_2)) p_{X_1}(x_1) p_{X_2}(x_2) \tag{9}$$

Furthermore,

$$c(u,v) = \frac{\partial^2 C}{\partial u \partial v}(u,v), \quad (u,v) \in [0,1]^2 \tag{10}$$

Now, Condition (C.2) may be rephrased in terms of copulas:

Proposition 3. *For a two-dimensional model, the three following conditions are equivalent:*

1. $\boxed{\exists\, 0 < M < 1,\ p_X \geq M \cdot p_{X_1} p_{X_2} \quad \nu\text{-a.e.}}$ *(C.4)*

2. $\boxed{\exists\, 0 < M < 1,\ c(u,v) \geq M, \quad \forall\ (u,v) \in [0,1]^2}$ *(C.5)*

3. $\boxed{\exists\, 0 < M < 1,\ C(u,v) = Muv + (1-M)\tilde{C}(u,v),\ \textit{for some copula}\ \tilde{C}}$ *(C.6)*

The proof of Proposition 3 is postponed to the Appendix. Hence, the generalized Hoeffding decomposition holds for a wide class of examples. The Morgenstern [28] and the Frank copulas belong to this class.

Example 2.

- The Morgenstern copulas satisfies (C.6) with

$$C_\theta(u,v) = uv[1 + \theta(1-u)(1-v)], \quad \theta \in]-1,1[$$

- The Frank copula is a Archimedian copula, and satisfies (C.5). It is characterized by the generator:

$$\varphi(x) = \log\left(\frac{e^{-\theta x} - 1}{e^{-\theta} - 1}\right), \quad \theta \in \mathbb{R} \setminus \{0\}$$

and

$$C(u,v) = \varphi^{-1}[\varphi(u) + \varphi(v)], \quad u, v \in [0,1] \tag{11}$$

Here, $c(u,v) \geq -\theta(e^{-\theta} - 1)e^{-2\theta}$ if $\theta > 0$, $c(u,v) \geq -\theta(e^{-\theta} - 1)$ elsewhere.

Other examples of copulas from the Archimedian class also satisfy (C.4)-(C.6) by an intermediate proposition. Details are given in Appendix. Leaving the class of copulas, we now directly work with the joint density function. Proposition 4 gives a general form of distribution for our framework:

Proposition 4. *If $p_{\mathbf{X}}$ has the form*

$$p_X(x_1,x_2) = \alpha \cdot f_{X_1}(x_1) f_{X_2}(x_2) + (1-\alpha) \cdot g_X(x_1,x_2), \quad \alpha \in]0,1[\tag{12}$$

where f_{X_1}, f_{X_2} are univariate density functions, and g_X is any density function (with respect to ν) with marginals f_{X_1} and f_{X_2}, then $p_{\mathbf{X}}$ satisfies (C.5).

The proof is straightforward.

The remaining part of the paper is devoted to the estimation of the HOFD components. In the next section, we will assume that the set of inputs is an independent pairs of dependent variables (abbreviated in IPDV).

The simplest case of a single pair of dependent variables is first discussed. Then, the more general IPDV case is studied. In all cases, first and second order indices are defined to measure the contribution of each pair of dependent variables and each of its components in the model. Indices of order greater than one involving variables from different pairs will not be studied here.

4. Estimation

Here, we investigate a different approach from [22]. The method relies on the property of hierarchical orthogonality ($H_u^0 \perp H_v^0,\ \forall\ v \subset u$), and on projection operator onto H_u^0, denoted by $P_{H_u^0}$, for $u \in S$. The idea is to project the output onto $H_u^0,\ \forall\ u$, to get the HOFD components $(\eta_u)_u$ as a solution of a functional linear system. It then consists in solving the system numerically. This section is first devoted to the HOFD terms computation with this method in two dimensional models. At last, we extend the procedure to the more general IPDV case.

4.1. Models of $p = 2$ input variables

This part is devoted to the simple case of bidimensional models $Y = \eta(X_1, X_2)$.

Assuming that Conditions (C.1) and (C.2) both hold, we proceed as follows:

Procedure 1

1. *HOFD of the output:*

$$Y = \eta_0 + \eta_1(X_1) + \eta_2(X_2) + \eta_{12}(X_1, X_2) \tag{13}$$

2. *Projection of $Y = \eta(\mathbf{X})$ on $H_u^0,\ \forall\ u \subseteq \{1, 2\}$. As $H_u^0 \perp H_v^0,\ \forall\ v \subset u$, we obtain:*

$$\begin{pmatrix} Id & 0 & 0 & 0 \\ 0 & Id & P_{H_1^0} & 0 \\ 0 & P_{H_2^0} & Id & 0 \\ 0 & 0 & 0 & Id \end{pmatrix} \begin{pmatrix} \eta_0 \\ \eta_1 \\ \eta_2 \\ \eta_{12} \end{pmatrix} = \begin{pmatrix} P_{H_\emptyset}(\eta) \\ P_{H_1^0}(\eta) \\ P_{H_2^0}(\eta) \\ P_{H_{12}^0}(\eta) \end{pmatrix} \tag{14}$$

3. *Computation of the right-hand side vector of (14):*

$$\begin{pmatrix} P_{H_\emptyset}(\eta) \\ P_{H_1^0}(\eta) \\ P_{H_2^0}(\eta) \\ P_{H_{12}^0}(\eta) \end{pmatrix} = \begin{pmatrix} \mathbb{E}(\eta) \\ \mathbb{E}(\eta|X_1) - \mathbb{E}(\eta) \\ \mathbb{E}(\eta|X_2) - \mathbb{E}(\eta) \\ \eta - \mathbb{E}(\eta|X_1) - \mathbb{E}(\eta|X_2) + \mathbb{E}(\eta) \end{pmatrix} \tag{15}$$

In this frame, we have:

Proposition 5. *Let η be any function of $L^2_{\mathbb{R}}(\mathbb{R}^p, \mathcal{B}(\mathbb{R}^p), P_{\mathbf{X}})$. Then, under (C.1) and (C.2), the linear system*

$$(\mathcal{S}) \begin{pmatrix} Id & 0 & 0 & 0 \\ 0 & Id & P_{H_1^0} & 0 \\ 0 & P_{H_2^0} & Id & 0 \\ 0 & 0 & 0 & Id \end{pmatrix} \begin{pmatrix} h_0 \\ h_1 \\ h_2 \\ h_{12} \end{pmatrix} = \begin{pmatrix} P_{H_\emptyset}(\eta) \\ P_{H_1^0}(\eta) \\ P_{H_2^0}(\eta) \\ P_{H_{12}^0}(\eta) \end{pmatrix} \tag{16}$$

admits in $h = (h_0, \dots, h_{12}) \in H_\emptyset \times \cdots \times H_{12}^0$ the unique solution $h^* = (\eta_0, \eta_1, \eta_2, \eta_{12})$.

4. *Reduction of the system (14). As the constant term corresponds to the mean value of η, and the last term η_{12} can be deduced from the others, the dimension of the system (16) can even be reduced to:*

$$\begin{pmatrix} Id & P_{H_1^0} \\ P_{H_2^0} & Id \end{pmatrix} \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} = \begin{pmatrix} \mathbb{E}(\eta|X_1) - \mathbb{E}(\eta) \\ \mathbb{E}(\eta|X_2) - \mathbb{E}(\eta) \end{pmatrix} \tag{17}$$

For the next step, we will denote by $A_2\Delta = B$ the system (17), where A_2 is the left-hand side matrix of projection operators of (17), $\Delta = {}^t\begin{pmatrix} \eta_1 & \eta_2 \end{pmatrix}$, and B is the right-hand side vector of (17).

5. *Estimation procedure: Suppose that we get a sample of n observations $(Y_l, \mathbf{X}_l)_{l=1,\dots,n}$.*
   - *The numerical resolution of (17) is achieved by an iterative Gauss Seidel algorithm [18] which consists first in decomposing A_2 as a sum of lower triangular (L_2) and strictly upper triangular (U_2) matrices. Further, the technique uses an iterative scheme to compute Δ. At step $k+1$, we have:*

   $$\Delta^{(k+1)} := \begin{pmatrix} \Delta_1^{(k+1)} \\ \Delta_2^{(k+1)} \end{pmatrix} = L_2^{-1}(B - U_2 \cdot \Delta^{(k)}) \tag{18}$$

   Using expression of A_2, we get:

   $$\Delta^{(k+1)} = \begin{pmatrix} \mathbb{E}(Y - \Delta_2^{(k)}|X_1) - \mathbb{E}(Y - \Delta_2^{(k)}) \\ \mathbb{E}(Y - \Delta_1^{(k+1)}|X_2) - \mathbb{E}(Y - \Delta_1^{(k+1)}) \end{pmatrix} \tag{19}$$

   The iterative scheme (19) requires to estimate conditional expectations. As studied in Da Veiga et al [6], we propose to estimate these quantities by local polynomial regression at each point of observation $(Y_l, \mathbf{X}_l)$. Then, we use the leave-one-out technique to set the learning sample and the test sample. Moreover, as the local polynomial method can be summed up to a generalized least squares (see Fan and Gijbels [10]), the Sherman-Morrison formula [33] is applied to reduce the computational time.

   We stop the procedure when $\|\Delta^{(k+1)} - \Delta^{(k)}\| \le \varepsilon$, for a small positive ε.

   Once (η_1, η_2) have been estimated, we deduce an estimation of η_{12} by substraction.
   - *We use empirical variance and covariance estimation to estimate sensitivity indices S_1, S_2 and S_{12}.*
6. *Convergence of the algorithm: now, we hope that the Gauss Seidel algorithm converges to the true solution. Looking back at (14), we see that we only have to consider $P_{H_1^0}$ (respectively $P_{H_2^0}$) restricted to H_2^0 (respectively to H_1^0).*

Under this restriction, let us define the associated norm operator as:

$$\|P_{H_i^0}\|^2 := \sup_{\substack{\mathbb{E}(U^2)=1\\ U\in H_j^0}} \mathbb{E}[P_{H_i^0}(U)^2], \quad i,j=1,2,\ j\neq i$$

As explained in [7], Gauss Seidel algorithm converges to the true solution Δ if A_2 is stricltly diagonally dominant, which is implied by:

$$\|P_{H_i^0}\| < \|Id\| = 1, \quad i=1,2 \tag{20}$$

As $P_{H_i^0}(U) = \mathbb{E}(U|X_i) - \mathbb{E}(U)$ by (15), the Jensen inequality [17] is applied. Take $U \in H_1^0$:

$$\begin{array}{rcl} \|P_{H_2^0}\| & = & \sup_{\substack{\mathbb{E}(U^2)=1\\ U\in H_1^0}} \mathbb{E}[(\mathbb{E}(U|X_2) - \mathbb{E}(U))^2] \\ & \leq & \sup_{\substack{\mathbb{E}(U^2)=1\\ U\in H_1^0}} \mathbb{E}[\mathbb{E}(U^2|X_2)] = 1 \quad \textit{as} \quad U\in H_1^0 \end{array}$$

The same holds for $\|P_{H_2^0}\|$. Thus $\|P_{H_2^0}\| < 1$ holds if U (function of X_j) is not X_i-measurable. Hence, the condition of convergence holds if X_1 is not a measurable function of X_2.

4.2. Generalized IPDV models

Assume that the number of inputs is even, so $p = 2k$, $k \geq 2$. We note each group of dependent variables as $\mathbf{X}^{(i)} := (X_1^{(i)}, X_2^{(i)})$, $i = 1, \dots, k$. By rearrangement, we may assume that:

$$\mathbf{X} = (\underbrace{X_1, X_2}_{\mathbf{X}^{(1)}}, \dots, \underbrace{X_{2k-1}, X_{2k}}_{\mathbf{X}^{(k)}})$$

If p is odd, one of the pairs is reduced to a single input. SA for IPDV models has already been treated in [16]. Indeed, they proposed therein to estimate usual sensitivity indices on groups of variables via a Monte Carlo method. Thus, they have interpreted the influence of every group of variables on the global variance. Here, we will go further by trying to measure the influence of each variable on the output, but also the effets of the independent pairs.

To begin with, as a slight generalization of [35] and used in [16], let apply the Sobol decomposition on independent groups of dependent variables,

$$\eta(\mathbf{X}) = \eta_0 + \eta_1(\mathbf{X}^{(1)}) + \cdots + \eta_k(\mathbf{X}^{(k)}) + \sum_{|u|=2}^{k} \eta_u(\mathbf{X}^{(u)})$$

where for $u = \{u_1, \dots, u_t\}$ and $t = |u|$, we set $\mathbf{X}^{(u)} = (\mathbf{X}^{(u_1)}, \dots, \mathbf{X}^{(u_t)})$. Furthermore, $\langle \eta_u, \eta_v \rangle = 0$, $\forall\ u \neq v$.

Under the assumptions discussed in the previous section, we can apply the HOFD on each component η_i, that is,

$$\eta_i(\mathbf{X}^{(i)}) = \eta_i(X_1^{(i)}, X_2^{(i)}) = \varphi_{i0} + \varphi_{i,1}(X_1^{(i)}) + \varphi_{i,2}(X_2^{(i)}) + \varphi_{i,12}(\mathbf{X}^{(i)})$$

with $\langle \varphi_{i,u}, \varphi_{i,v} \rangle = 0$, $\forall\ v \subset u \subseteq \{1,2\}$. In this way, let define some new generalized indices for IPDV models:

Definition 3. For $i = 1, \ldots, k$, the sensitivity index measuring the respective contribution of $X_j^{(i)}$ $(j = 1,2)$ and $(X_1^{(i)}, X_2^{(i)})$ on the output is:

$$S_{i,j} = \frac{V(\varphi_{i,j}) + \mathrm{Cov}(\varphi_{i,j}, \varphi_{i,k})}{V(Y)}, k = 2 \text{ if } j = 1 \quad S_{i,12} = \frac{V(\varphi_{i,12})}{V(Y)} \tag{21}$$

The estimation procedure of these indices is quite similar to Procedure 1:

Procedure 2

1. *Estimation of $(\eta_i)_{i=1,\ldots,k}$: as reminded in Part 2.2 with Equations (2), $\eta_i = \mathbb{E}(Y|\mathbf{X}^{(i)}) - \mathbb{E}(Y)$. We use the non parametric estimation reminded in step 5 of Procedure 1 to get $\hat{\eta}_i$.*
2. *For $i = 1, \ldots, k$, we apply step 2 to step 5 of Procedure 1, considering $\hat{\eta}_i$ as the new output.*

If p is odd, the procedure is the same except that the influence of the independent variable is measured by a Sobol index, as it is independent from all the others. The next part is devoted to numerical examples.

5. Numerical examples

In this section, we study three examples with dependent input variables. For the first two illustrations, we consider IPDV models and a Gaussian mixture distribution on the input variables. The covariance matrices of the mixture satisfy conditions of Example 1.

We give estimations of our new indices, and compare these estimations to the true values, computed from expressions (6). We also compute dispersions of the estimators.

In [6], Da Veiga *et al.* proposed to estimate the classical Sobol indices as defined in (3) by nonparametric tools. Indeed, the local polynomial regression were used to estimate conditional moments $\mathbb{E}(Y|\mathbf{X_u}), u \subseteq \mathcal{P}_p$. This method, used further, will be called Da Veiga procedure (DVP). Results given by DVP are compared with our method. We show that the usual sensitivity indices are not appropriate in the dependence frame, even if a relevant estimation method is used.

The last example is devoted to a more realistic case. The study case concerns the river flood inundation of an industrial site. In this example, input variables have different distributions, and some pairs are linearly correlated. We represent dispersions of the estimation of our new indices, and give some physical interpretations.

5.1. *Two-dimensional IPDV model*

Let consider the model

$$Y = \exp X_1 + X_1 + X_2$$

Here, ν and $P_{\mathbf{X}}$ are of the form given by Example 1, with $m = \mu = 0$.

Thus, the analytical decomposition of Y is

$$\eta_0 = \mathbb{E}(\exp X_1), \quad \eta_1 = \exp X_1 + X_1 - \mathbb{E}(\exp X_1), \quad \eta_2 = X_2$$

For the application, we implement Procedure 1 in Matlab software. We proceed to $L = 50$ simulations and $n = 1000$ observations. Parameters were fixed at $\sigma_1 = \sigma_2 = 1$, $\varphi_1^2 = \varphi_2^2 = 0.5$, $\rho_{12} = 0.4$ and $\alpha = 0.2$.

In Table 1, we give the estimation of our indices and their standard deviation (indicated by $\pm\cdot$) on L simulations. In comparison, we give the analytical value of each index. We also give estimators of the classical Sobol indices with DVP.

Notice that we obtain a quite good estimation of S_1 with our estimation procedure. $\hat{S}_2$ is lightly lower than expected, and, consequently, the estimation error of the interaction term η_{12} is bigger than 0. In comparison, the DVP badly scales S_2, even if for both methods, the inputs hierarchy is the same.

In our method, it would be relevant to separate the variance part to the covariance one in the first order indices. Indeed, in this way, we would be able to get the part of variability explained by X_i alone in S_i, and its contribution hidden in the dependence with X_j. We note S_i^v the variance contribution alone, and S_i^c the covariance contribution, that is

$$S_i = \underbrace{\frac{V(X_i)}{V(Y)}}_{S_i^v} + \underbrace{\frac{\mathrm{Cov}(X_i, X_j)}{V(Y)}}_{S_i^c}, \quad i = 1, 2,\ j \neq i$$

The new indices estimations given in Table 1 are decomposed in Table 2.

For each index, the covariate X_1 explains 65% (in estimation, 61% in reality) of the part of the total variability. However, the contribution embedded in the

Table 1
Estimation of the new and DVP indices with $\rho_{12} = 0.4$

		S_1	S_2	S_{12}	$\sum_u S_u$
New indices	Estimation	0.7449 ± 0.0159	0.2187 ± 0.0151	0.0455 ± 0.0123	1
	Analytical	0.7497	0.2503	0	1
DVP indices	Estimation	0.7774	0.1792	0.043	1.00

Table 2
Estimation of S_i^v and S_i^c with $\rho_{12} = 0.4$

		S_i^v	S_i^c	S_i
Estimated	X_1	0.6531	0.0918	0.7449
	X_2	0.1049	0.1138	0.2187
Analytical	X_1	0.6122	0.1375	0.7497
	X_2	0.1129	0.1375	0.2504

correlation is not negligible as it represents between 9% and 11% (13.75% analytically)of the total variance. Considering the shape of the model, it is quite natural to get a higher contribution of X_1. Also, as their dependence is quite important, with a covariance term equals to 0.4, we are not surprised by the relatively high value of S_1^c (resp. S_2^c).

5.2. Linear four-dimensional model

The test model is

$$Y = 5X_1 + 4X_2 + 3X_3 + 2X_4$$

Let consider the case of two blocks $\mathbf{X}^{(1)} = (X_1, X_3)$ and $\mathbf{X}^{(2)} = (X_2, X_4)$ of correlated variables. $\mathbf{X}^{(i)}$, $i = 1, 2$ follows the Gaussian mixture. The analytical sensitivity indices are given by (21). For $L = 50$ simulations and $n = 1000$ observations, we took $\varphi_1^{2(1)} = \varphi_2^{2(1)} = 0.5$, $\varphi_1^{2(2)} = 0.7$, $\varphi_2^{2(2)} = 0.3$, $\rho_{13}^{(1)} = 0.4$, $\rho_{24}^{(2)} = 0.37$, $\alpha_1 = \alpha_2 = 0.2$ and $\Sigma^{(1)} = \Sigma^{(2)} = \mathrm{I}_2$.

Figure 1 displays the dispersion of indices of first order for all variables and second order for grouped variables. The true values and the estimators of classical Sobol indices with DVP are also represented.

On Figure 1, we see that X_1 has the biggest contribution, whereas the influence of X_4 is very low. It reflects well the model if we look at the coefficients of X_i, $i = 1, \ldots, 4$. Notice that the interaction terms are well estimated, as they are closed to 0. For each case, the dispersion on 50 simulations is very low.

Furthermore, the DVP estimators are once again very high compared with the true indices values.

5.3. River flood inundation

Several SA methods have been studied on the simplified model of river flood inundation. A brief description of the model is given here, but more details can be found in [15, 8]. The study case concerns an industrial site located near a river, and protected from it by a dyke. The goal is to study the water level with respect to the dyke height to prevent from inundation. The model has the following form

$$S = \underbrace{Z_v + h}_{Z_c} - H_d - C_b, \quad h = \left(\frac{Q}{BK_s \sqrt{\frac{Z_m - Z_v}{L}}} \right)^{0.6}$$

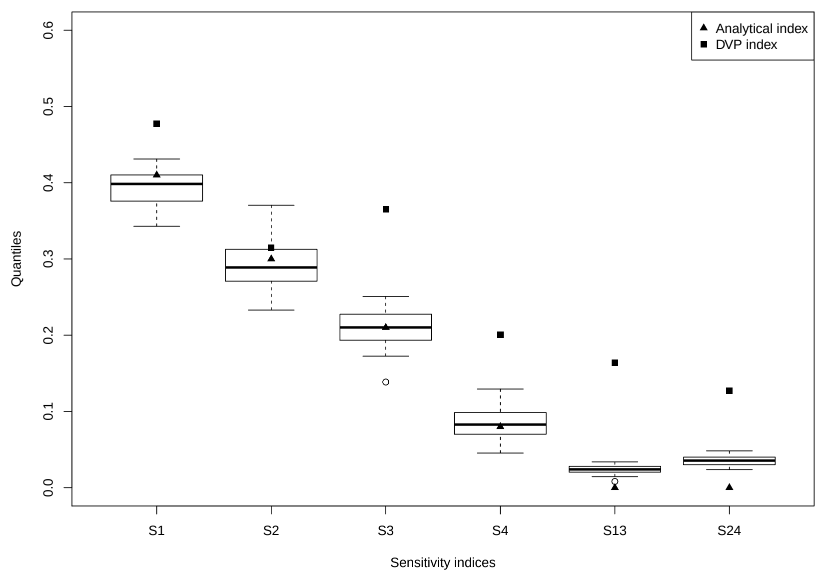

FIG 1. *Boxplots representation of new indices-Comparison with analytical and DVP indices*

TABLE 3
Description of inputs-output of the river flood model

Variables	Meaning	Distribution
h	maximal annual water level	-
Q	maximal annual flow rate	Gumbel $G(1013, 558)$ truncated to $[500; 3000]$
K_s	Strickler coefficient	Normal $N(30, 8)$ truncated to $[15, +\infty[$
Z_v	river downstream level	Triangular $T(49, 50, 51)$
Z_m	river upstream level	Triangular $T(54, 55, 56)$
H_d	dyke height	Uniform $\mathcal{U}([7, 9])$
C_b	bank level	Triangular $T(55, 55.5, 56)$
L	length of the river stretch	Triangular $T(4990, 5000, 5010)$
B	river width	Triangular $T(295, 300, 305)$

This model is a crude simplification of the 1-D Saint Venant equations, when uniform and constant flow rate is assumed. The model output S is the maximal overflow that depends on eight random variables. H_d is a design parameter. The randomness of other inputs is due to their spatio-temporal variability, or some inaccuracies of their estimation. Table 3 gives the meaning of each input variable, and how they are distributed. The river flow is represented in Figure 2.

Here, we suppose that (Q, K_s) is a correlated pair, with correlation coefficient $\rho = 0.5$. This correlation is admitted in real case, as we consider that the

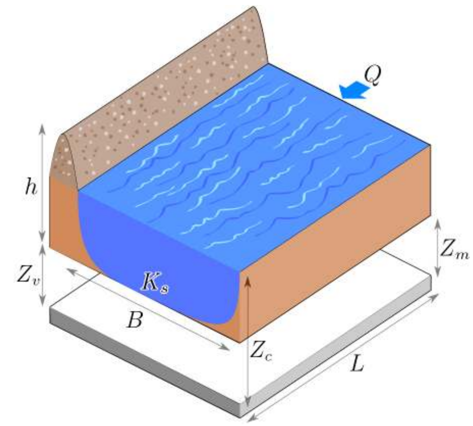

FIG 2. *The river flood model*

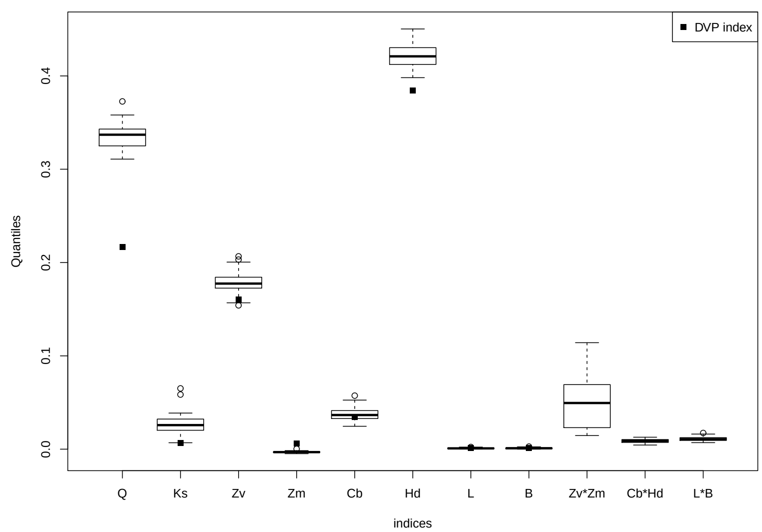

FIG 3. *Boxplots of new indices for the river flood model*

friction coefficient increases with the flow rate. Also, (Z_v, Z_m) and (L, B) are assumed to be dependent with the same Pearson coefficient $\rho = 0.3$, because data are supposed to be simultaneously collected by the same measuring device. Correlated variables are simulated according to the algorithm given in [32]. A theoretical background can be found in [29]. We made $n = 1000$ model evaluations repeated $L = 50$ times. The dispersion of estimated indices is represented in Figure 3.

The most influential parameters are the flow rate Q, the downstream level Z_v, and the dyke height H_d. Q and H_d's strong contribution makes sense here, as they represent the most important parameters to limit river flood.

6. Conclusions and perspectives

This paper gives a rigorous frame for general Hoeffding-Sobol decomposition in the case of dependent input variables. In the statistical procedure, we only consider the restricted case of IPDV models. Thus, for more general models, the mathematical properties of the statistical estimation of this decomposition remains a challenging open problem.

Appendix A: Generalized Hoeffding decomposition

A.1. Generalized decomposition for dependent inputs

The upcoming proof follows the guideline of the proof of Lemma 3.1 in Stone [37].

Proof of Lemma 1.

By induction on the cardinal of T, let show that

$$\mathcal{H}(n): \quad \forall\, T|\#(T)=n, \quad \mathbb{E}[(\sum_{u\in T} h_u(\mathbf{X}))^2] \geq \delta^{\#(T)-1} \sum_{u\in T} \mathbb{E}[h_u^2(\mathbf{X})]$$

- $\mathcal{H}(1)$ is obviously true, as T is reduced to a singleton
- Let $n \in \mathbb{N}^*$. Suppose that $\mathcal{H}(n')$ is true for all $1 \leq n' \leq n$. Let T such that $\#(T) = n+1$. We want to prove $\mathcal{H}(n+1)$.
  Choose a maximal set r of T, i.e. r is not a proper subset of any set u in T. We show first that

$$\mathbb{E}[(\sum_{u\in T} h_u(\mathbf{X}))^2] \geq M \cdot \mathbb{E}(h_r^2(\mathbf{X})) \tag{22}$$

  - If $\#(r) = p$, by definition of H_r^0, we get $\mathbb{E}[(\sum_{u\in T} h_u(\mathbf{X}))^2] \geq \mathbb{E}(h_r^2(\mathbf{X})) \geq M\mathbb{E}(h_r^2(\mathbf{X}))$ as $M \leq 1$.
  - If $1 \leq \#(r) \leq p-1$, set $\mathbf{X} = (X_1, X_2)$, where $X_1 = (X_l)_{l\notin r}$ and $X_2 = (X_l)_{l\in r}$. By Condition (C.2), it follows that

$$p_{\mathbf{X}} \geq M \cdot p_{X_1} p_{X_2}$$

  As a consequence,

$$\begin{aligned}
\mathbb{E}[(\sum_{u\in T} h_u(\mathbf{X}))^2] &= \int_{\mathcal{X}_1}\int_{\mathcal{X}_2} [h_r(x_2) + \sum_{u\neq r} h_u(x_1,x_2)]^2 p_{\mathbf{X}} \nu(dx_1, dx_2) \\
&\geq M \int_{\mathcal{X}_1}\int_{\mathcal{X}_2} [h_r(x_2) \\
&\quad + \sum_{u\neq r} h_u(x_1,x_2)]^2 p_{X_1} p_{X_2} \nu_1(dx_1)\nu_2(dx_2) \\
&\geq M \int_{\mathcal{X}_1} \mathbb{E}[(h_r(X_2) + \sum_{u\neq r} h_u(x_1, X_2))^2] p_{X_1} \nu_1(dx_1)
\end{aligned}$$

  when $\mathcal{X}_i$ denotes the support of X_i, $i = 1, 2$. By maximality of r and by definition of H_r^0,

* If $u \subset r$, h_u only depends on X_2 and by orthogonality,

$$\mathbb{E}(h_u(X_2)h_r(X_2)) = 0$$

* If $u \not\subset r$, h_u depends on X_1 fixed at x_1, and $X_2^u = (X_l)_{l \in r \cap u}$, so $h_u(x_1, \cdot) \in H^0_{r \cap u}$, with $r \cap u \subset r$, it comes then

$$\mathbb{E}(h_u(x_1, X_2)h_r(X_2)) = 0$$

Thus,

$$\begin{aligned} \mathbb{E}[(\sum_{u \in T} h_u(\mathbf{X}))^2] &\geq M \int_{\mathcal{X}_1} \mathbb{E}(h_r^2(X_2)) p_{X_1} \nu_1(dx_1) \\ &= M \cdot \mathbb{E}(h_r^2(\mathbf{X})) \end{aligned}$$

So (22) holds for any size of any maximal sets of T.

By using (22) with $\tilde{h}_r = h_r$ and $\tilde{h}_u = -\beta h_u$, $\forall\ u \neq r$, we get

$$\mathbb{E}[(h_r(\mathbf{X}) - \beta \sum_{u \neq r} h_u(\mathbf{X}))^2] \geq M\mathbb{E}(h_r^2(\mathbf{X})) \tag{23}$$

Taking $\beta = \dfrac{\mathbb{E}[h_r(\mathbf{X}) \sum_{u \neq r} h_u(\mathbf{X})]}{\mathbb{E}[(\sum_{u \neq r} h_u(\mathbf{X}))^2]}$, it follows that:

$$\begin{aligned} &\mathbb{E}[(h_r(\mathbf{X}) - \beta \sum_{u \neq r} h_u(\mathbf{X}))^2] &\geq M\mathbb{E}(h_r^2(\mathbf{X})) \\ \text{that is} \quad &\mathbb{E}[h_r^2(\mathbf{X})] - \frac{[\mathbb{E}(h_r(\mathbf{X}) \sum_{u \neq r} h_u(\mathbf{X}))]^2}{\mathbb{E}[(\sum_{u \neq r} h_u(\mathbf{X}))^2]} &\geq M\mathbb{E}(h_r^2(\mathbf{X})) \end{aligned}$$

Hence,

$$[E(h_r(\mathbf{X}) \sum_{u \neq r} h_u(\mathbf{X}))]^2 \leq (1 - M) \cdot \mathbb{E}(h_r^2(\mathbf{X})) \cdot \mathbb{E}[(\sum_{u \neq r} h_u(\mathbf{X}))^2] \tag{24}$$

This implies

$$\mathbb{E}[(\sum_{u} h_u(\mathbf{X}))^2] \geq (1 - \sqrt{1 - M}) \left[\mathbb{E}(h_r^2(\mathbf{X})) + \mathbb{E}[(\sum_{u \neq r} h_u(\mathbf{X}))^2] \right] \tag{25}$$

Set $x = h_r(\mathbf{X})$ and $y = \sum_{u \neq r} h_s(\mathbf{X})$.(25) is rephrased as

$$\|x + y\|^2 \geq (1 - \sqrt{1 - M})\{\|x\|^2 + \|y\|^2\} \tag{26}$$

Further, (24) is $\langle x, y\rangle \geq -\sqrt{1 - M}\|x\| \cdot \|y\|$. Thus,

$$\begin{aligned} \|x\|^2 + \|y\|^2 &\geq 2\langle x, y\rangle \\ &\geq -\frac{2}{\sqrt{1 - M}}\langle x, y\rangle \end{aligned}$$

So $\|x + y\|^2 \geq (1 - \sqrt{1 - M})\{\|x\|^2 + \|y\|^2\}$.

As $\mathcal{H}(n)$ is supposed to be true and (25) holds, it follows that:

$$\begin{aligned}\mathbb{E}[(\sum_u h_u(\mathbf{X}))^2] &\geq \delta\left[\mathbb{E}(h_r^2(\mathbf{X})) + \delta^{n-1}\sum_{u\neq r}\mathbb{E}(h_u^2(\mathbf{X}))\right] \\ &\geq \delta^n \sum_u \mathbb{E}(h_u^2(\mathbf{X})) \qquad \text{as} \quad \delta \in \;]0,1] \\ &= \delta^{\#(T)-1}\sum_u \mathbb{E}(h_u^2(\mathbf{X}))\end{aligned}$$

Hence, $\mathcal{H}(n+1)$ holds.

We can deduce that $\mathcal{H}(n)$ is true for any collection T of $\mathcal{P}_p$. □

Proof of Theorem 1.
Let define the vector space $K^0 = \{\sum_{u\in S^-} h_u(\mathbf{X_u}), h_u \in H_u^0, \forall\; u \in S^-\}$.

In the first step, we will prove that K^0 is a complete space to prove the existence and uniqueness of the projection of η in K^0, thanks to the projection theorem [26].

Secondly, we will show that η is exactly equal to the decomposition into H^0, and finally, we will see that each term of the summand is unique.

- We show that H_u^0 is closed into H_u (as H_u is a Hilbert space).

  Let $(h_{n,u})_n$ be a convergent sequence of H_u^0 with $h_{n,u} \to h_u$. As $(h_{n,u})_n \in H_u^0 \subset H_u$ complete, $h_u \in H_u$. Let $v \subset u$, and $h_v \in H_v^0$:

  $$\begin{array}{cccc} \langle h_u - h_{n,u}, h_v\rangle & = \langle h_u, h_v\rangle & -\langle h_{n,u}, h_v\rangle & \\ \downarrow & & \shortparallel & \\ 0 & & 0 & \text{as } H_u^0 \perp H_v^0 \end{array}$$

  Thus, $\langle h_u, h_v\rangle = 0$, so that $h_u \in H_u^0$. H_u^0 is then a complete space.

  Let $(h_n)_n$ be a Cauchy sequence in K^0 and we show that each component is of Cauchy and that $h_n \to h \in K^0$.
  As $h_n \in K^0$, $h_n = \sum_{u\in S^-} h_{n,u}$, $h_{n,u} \in H_u^0$. It follows that:

  $$\begin{aligned}\|h_n - h_m\|^2 &= \|\sum_u (h_{n,u} - h_{m,u})\|^2 \\ &\geq \delta^{\#(S^-)-1}\sum_{u\in S^-}\|h_{n,u} - h_{m,u}\|^2 \quad \text{by Inequality (4)}\end{aligned}$$

  As $(h_n)_n$ is a Cauchy sequence, by the above inequality, $(h_{n,u})_n$ is also Cauchy. As $h_{n,u} \to h_u \in H_u^0$, we deduce that $h_n \underset{n\to\infty}{\longrightarrow} \sum_{u\in S^-} h_u = h \in K^0$.
  Thus, K^0 is complete. By the projection theorem, we can deduce there exists a unique element into K^0 such that:

  $$\|\eta - \sum_{u\in S^-}\eta_u\|^2 \leq \|\eta - h\|^2 \quad \forall\; h \in K^0$$

- Decomposition of η: following Hooker [14], we introduce the residual term as
$$\eta_{\mathcal{P}_p}(X_1,\dots,X_p)=\eta(X_1,\dots,X_p)-\sum_{u\in S^-}\eta_u(\mathbf{X_u})$$
By projection, $\langle \eta-\sum_{v\in S^-}\eta_v, h_u\rangle = 0\ \forall\ u\in S^-,\ \forall\ h_u\in H_u^0$. Hence, $\eta(\mathbf{X})=\sum_{u\in S}\eta_u(\mathbf{X_u})$, $\eta_u\in H_u^0$, $\forall\ u\in S$, and this decomposition is well defined.
- Terms of the summand are unique: assume that $\eta=\sum_{u\in S}\eta_u=\sum_{u\in S}\widetilde{\eta}_u$, $\widetilde{\eta}_u\in H_u^0$.
By Lemma 1, it follows that

$$\left.\begin{array}{l}\sum_{u\in S}(\eta_u-\widetilde{\eta}_u)=0\\ \|\sum_{u\in S}(\eta_u-\widetilde{\eta}_u)\|^2\geq\delta^{\#(S)-1}\sum_{u\in S}\|\eta_u-\widetilde{\eta}_u\|^2\end{array}\right\}\ \Rightarrow\ \|\eta_u-\widetilde{\eta}_u\|^2=0\quad\forall\ u\in S$$

□

A.2. Generalized sensitivity indices

Proof of Proposition 1.

Under (C.1) and (C.2), Theorem 1 states the existence and the uniqueness decomposition of $\eta(\mathbf{X})=\sum_{u\in S}\eta_u(\mathbf{X_u})$,, with $H_u^0\perp H_v^0$, $\forall\ v\subset u$.

Therefore, $\mathbb{E}(\eta(X))=\mathbb{E}(\sum_{u\in S}\eta_u(\mathbf{X_u}))=\eta_0$, and

$$\begin{aligned}V(Y)=V(\eta(X)) &= \mathbb{E}(\eta^2(X))-\eta_0^2\\ &= \sum_{u\neq\emptyset}\mathbb{E}(\eta_u^2(\mathbf{X_u}))+\sum_{u\neq v}\mathbb{E}(\eta_u(\mathbf{X_u})\eta_v(\mathbf{X_v}))\\ &= \sum_{u\neq\emptyset}V(\eta_u(\mathbf{X_u}))+\sum_{\substack{u\neq\emptyset\\ u\neq\mathcal{P}_p}}\ \sum_{\substack{v\neq\emptyset\\ u\not\subseteq v, v\not\subseteq u}}\mathbb{E}(\eta_u(\mathbf{X_u}),\eta_v(\mathbf{X_v}))\\ &= \sum_{u\neq\emptyset}\left[V(\eta_u(\mathbf{X_u}))+\sum_{\substack{v\\ u\cap v\neq u,v}}\mathrm{Cov}(\eta_u(\mathbf{X_u}),\eta_v(\mathbf{X_v}))\right]\end{aligned}$$

Thus, (6) holds, and equalities (7) and (8) follow naturally. □

Appendix B: Examples of distribution function

B.1. Boundedness of the inputs density function

Proof of Example 1.

- ν is a product of measure as $\frac{d\nu}{d\nu_L}=\prod_{i=1}^p\nu_i(x_i)$, with $\nu_i\sim N(m_i,\sigma_i^2)$.

- $p_{\mathbf{X}}$ is given by

$$\begin{aligned} p_{\mathbf{X}}(\mathbf{x}) &= \frac{dP_{\mathbf{X}}}{d\nu}(\mathbf{x}) = \frac{dP_{\mathbf{X}}}{d\nu_L} \times \frac{d\nu_L}{d\nu}(\mathbf{x}) \\ &= \alpha + (1-\alpha)\left|\frac{\Sigma}{\Omega}\right|^{1|2} \exp -\frac{1}{2}{}^t(\mathbf{x}-m)(\Omega^{-1}-\Sigma^{-1})(\mathbf{x}-m) \end{aligned} \tag{27}$$

  First, we have $p_{\mathbf{X}}(\mathbf{x}) \geq \alpha > 0$. Further, the sufficient and necessary condition to have $p_{\mathbf{X}} \leq M_2 < \infty$ is to get $(\Omega^{-1} - \Sigma^{-1})$ positive definite. Indeed, if $(\Omega^{-1} - \Sigma^{-1})$ admits a negative eigenvalue, $p_{\mathbf{X}}$ can not be bounded. Thus, $0 < \alpha \leq p_{\mathbf{X}} \leq M_2$ iff $(\Omega^{-1} - \Sigma^{-1})$ is positive definite.

□

B.2. Examples of distribution of two inputs

Proof of Proposition 3.
Condition (C.5) is immediate with Equation 9. Let prove that (C.5) is equivalent to (C.6).

If (C.6) holds, then $c(u, v) \geq M$. Conversely, we assume that $0 < M < 1$, and

$$\tilde{C}(u, v) = \frac{C(u, v) - Muv}{1 - M}$$

It is enough to show it is a copula: Obviously, $\tilde{C}(0, u) = C(u, 0) = 0$, $\tilde{C}(1, u) = \tilde{C}(u, 1) = u \quad \forall\, u \in [0, 1]$. By second order derivation, it comes that $\tilde{c}(u, v) = \frac{c(u,v)-M}{1-M}$, so $\tilde{c}(u, v) \geq 0$ by hypothesis (C.5). □

Let consider the class of Archimedian copulas,

$$C(u, v) = \varphi^{-1}[\varphi(u) + \varphi(v)], \quad u, v \in [0, 1] \tag{28}$$

where the generator φ is a non negative two times differentiable function defined on $[0, 1]$ with $\varphi(1) = 0$, $\varphi'(u) < 0$ and $\varphi''(u) > 0$, $\forall\, u \in [0, 1]$.

A sufficient condition for (C.5) is given in Proposition 6:

Proposition 6. *If there exist M_1, $M_2 > 0$ such that:*

$$-\varphi'(u) \geq M_1 \ \forall\, u \in [0, 1] \tag{29}$$

$$\frac{d}{du}\left(\frac{1}{2}\frac{1}{\varphi'(u)^2}\right) \geq M_2,\ \forall\, u \in [0, 1] \tag{30}$$

Then, Condition (C.5) holds.

The proof is straightforward. Now, we will see two illustrative Archimedian copulas satisfying Proposition 6.

Example 3. Let $\alpha < 0$, $\theta > 0$ and β with $\beta < -\alpha e^{-\theta}$. Set

$$\varphi_2(x) = -\frac{\alpha}{\theta}e^{-\theta x} + \beta x + (\frac{\alpha}{\theta}e^{-\theta} - \beta), \quad x \in [0,1] \tag{31}$$

Example 4. Let $C < 0$ and set

$$\varphi_3(x) = x \ln x + (C-1)x + (1-C), \quad x \in [0,1] \tag{32}$$

Appendix C: Estimation

C.1. Model of $p = 2$ input variables

Proof of Proposition 5.

- We first show first that $(\mathcal{S})$ admits an unique solution. Under (C.1) and (C.2), by Theorem 1, the decomposition of $\eta(\mathbf{X})$ is unique and

$$\eta(X_1, X_2) = \eta_0 + \eta_1(X_1) + \eta_2(X_2) + \eta_{12}(X_1, X_2)$$

with $\begin{cases} \eta_0 \in H_\emptyset \\ \eta_i \in H_i^0 \perp H_\emptyset, \quad i = 1,2 \\ \eta_{12} \in H_{12}^0 \perp H_i^0, \quad i = 1,2, H_{12}^0 \perp H_\emptyset \end{cases}$

Thus,

$$\begin{pmatrix} \mathrm{Id} & 0 & 0 & 0 \\ 0 & \mathrm{Id} & P_{H_1^0} & 0 \\ 0 & P_{H_2^0} & \mathrm{Id} & 0 \\ 0 & 0 & 0 & \mathrm{Id} \end{pmatrix} \begin{pmatrix} \eta_0 \\ \eta_1 \\ \eta_2 \\ \eta_{12} \end{pmatrix} = \begin{pmatrix} P_{H_\emptyset}(\eta) \\ P_{H_1^0}(\eta) \\ P_{H_2^0}(\eta) \\ P_{H_{12}^0}(\eta) \end{pmatrix} \tag{33}$$

So $(\eta_0, \eta_1, \eta_2, \eta_{12})$ is solution of $(\mathcal{S})$. Now, assume there exists an another solution of the system, say $(\widetilde{\eta}_0, \ldots, \widetilde{\eta}_{\mathcal{P}_p}) \in H_\emptyset \times \cdots \times H_{\mathcal{P}_p}^0$, then

$$\begin{cases} \eta_0 - \widetilde{\eta}_0 = 0 \\ \eta_1 - \widetilde{\eta}_1 + P_{H_1^0}(\eta_2 - \widetilde{\eta}_2) = 0 \\ P_{H_2^0}(\eta_1 - \widetilde{\eta}_1) + \eta_2 - \widetilde{\eta}_2 = 0 \\ \eta_{12} - \widetilde{\eta}_{12} = 0 \end{cases} \quad \Rightarrow \quad \begin{cases} \eta_0 = \widetilde{\eta}_0 \\ P_{H_1^0}(\eta_1 - \widetilde{\eta}_1 + \eta_2 - \widetilde{\eta}_2) = 0 \\ P_{H_2^0}(\eta_1 - \widetilde{\eta}_1 + \eta_2 - \widetilde{\eta}_2) = 0 \\ \eta_{12} = \widetilde{\eta}_{12} \end{cases}$$

$$\Rightarrow \quad \begin{cases} \eta_0 = \widetilde{\eta}_0 \\ \eta_1 - \widetilde{\eta}_1 + \eta_2 - \widetilde{\eta}_2 \in H_1^{0\perp} \cap H_2^{0\perp} \\ \eta_{12} = \widetilde{\eta}_{12} \end{cases}$$

As $\eta_1 - \widetilde{\eta}_1 \in H_1^0$ and $\eta_2 - \widetilde{\eta}_2 \in H_2^0$, it follows that

$$\begin{cases} \langle \eta_1 - \widetilde{\eta}_1, \eta_1 - \widetilde{\eta}_1 + \eta_2 - \widetilde{\eta}_2 \rangle = 0 \\ \langle \eta_2 - \widetilde{\eta}_2, \eta_1 - \widetilde{\eta}_1 + \eta_2 - \widetilde{\eta}_2 \rangle = 0 \end{cases}$$

$$\Rightarrow \quad \begin{cases} \|\eta_1 - \widetilde{\eta}_1\|^2 + \langle \eta_1 - \widetilde{\eta}_1, \eta_2 - \widetilde{\eta}_2 \rangle = 0 \\ \|\eta_2 - \widetilde{\eta}_2\|^2 + \langle \eta_1 - \widetilde{\eta}_1, \eta_2 - \widetilde{\eta}_2 \rangle = 0 \end{cases}$$

$$\Rightarrow \quad \|\eta_1 - \widetilde{\eta}_1 + \eta_2 - \widetilde{\eta}_2\|^2 = 0$$

$$\Rightarrow \quad \eta_1 - \widetilde{\eta}_1 + \eta_2 - \widetilde{\eta}_2 = 0$$

As 0 can be uniquely decomposed into H^0 as a sum of zero, then, $\eta_1 - \widetilde{\eta}_1 = \eta_2 - \widetilde{\eta}_2 = 0$.

- Let now compute $\begin{pmatrix} P_{H_\emptyset}(\eta) \\ P_{H_1^0}(\eta) \\ P_{H_2^0}(\eta) \\ P_{H_{12}^0}(\eta) \end{pmatrix}$.

  First of all, it is obvious that the constant term $\eta_0 = \mathbb{E}(\eta)$ and that η_{12} is obtained by subtracting η with all other terms of the right of the decomposition.
  Now, let us use the projector's property of embedded spaces. Indeed, as $H_i^0 \subset H_i$, $\forall\ i = 1, 2$, it comes

$$P_{H_i^0}(\eta) = P_{H_i^0}(P_{H_i}(\eta)) = P_{H_i^0}[\underbrace{\mathbb{E}(\eta|X_i)}_{\varphi(X_i)}]$$

  φ is a function of X_i, so it can be decomposed into the following expression:

$$\varphi(X_i) = \varphi_0 + \varphi_i(X_i), \quad \varphi_0 \in H_\emptyset,\ \varphi_i \in H_i^0$$

  with $\varphi_0 = \mathbb{E}(\varphi) = \mathbb{E}(\eta)$. Hence, one can easily deduce $P_{H_i^0}(\eta)$, $i = 1, 2$, as the term $\varphi_i = \mathbb{E}(\eta|X_i) - \mathbb{E}(\eta)$
  We obtain

$$\begin{pmatrix} P_{H_\emptyset}(\eta) \\ P_{H_1^0}(\eta) \\ P_{H_2^0}(\eta) \\ P_{H_{12}^0}(\eta) \end{pmatrix} = \begin{pmatrix} \mathbb{E}(\eta) \\ \mathbb{E}(\eta|X_1) - \mathbb{E}(\eta) \\ \mathbb{E}(\eta|X_2) - \mathbb{E}(\eta) \\ \eta - \mathbb{E}(\eta|X_1) - \mathbb{E}(\eta|X_2) + \mathbb{E}(\eta) \end{pmatrix} \tag{34}$$

□

Acknowledgement

The authors would like to warmly thank the anonymous referees and the associate editor for their insightful comments that have allowed to merely improve the article. The authors would also like to thank Bertrand Iooss for his help in providing the river flood model.

This work has been supported by French National Research Agency (ANR) through COSINUS program (project COSTA-BRAVA number ANR-09-COSI-015).

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