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Generalized Hoeffding-Sobol Decomposition for Dependent Variables -Application to Sensitivity Analysis

Gaëlle Chastaing[†] Fabrice Gamboa[‡] Clémentine Prieur[†]

Abstract

In this paper, we consider a regression model built on dependent variables. This regression modelizes an input output relationship. Under boundedness assumptions on the joint distribution 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.

List of abbreviations

- SA = Sensitivity Analysis
- HOFD = Hierarchically Orthogonal Functional Decomposition
- IPDV = Independent Pairs of Dependent Variables
- DVP = Da Veiga Procedure

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 stochastic approach whose objective is to determine a global criterion based on density of the joint probability distribution function of the output and the inputs of a deterministic model. The most usual quantification is the variance-based method, widely studied in SA literature. Hoeffding decomposition [1] (see also Owen [2]) states that the variance of the output can be uniquely decomposed into summands of increasing dimensions under orthogonality constraints. Following this approach, Sobol [3] introduces variability measures, the so called *Sobol sensitivity indices*, to estimate the contribution of each input on a system.

Different methods have been exploited to estimate Sobol indices. The Monte Carlo algorithm was proposed by Sobol [4], and has been later improved by the Quasi Monte Carlo technique, performed by Owen [5]. FAST methods are also widely used to estimate Sobol indices. Introduced earlier by Cukier & al. [6] [7], they are well known to reduce the computational cost of multidimensional integrals thanks to Fourier transformations. Later, Tarantola & al. [8] adapted the Random Balance Designs (RBD) to FAST method for SA (see also recent advances on the subject by Tissot & al. [9]).

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However, these indices are constructed on the hypothesis that input variables are independent, which seems unrealistic for many real life phenomena. If correlations are not zero, the analytical Hoeffding decomposition is not true anymore. So that, the Sobol indices are irrelevant. If we use them, conclusions on variables sensitivity can be completely wrong even on very simple models (see, for example, Da Veiga's illustration [10]). In terms of estimation, useful methods also rely on the inputs independence. Hence, when they are used on dependent variables, they lead to an important source of errors. It is then necessary to take dependency into account in analytical indices and in estimation methods.

Recent researches have been led to deal with this issue : Jacques & al [11] proposed a model with groups of correlated incomes independent of one another, and expanded classical Sobol indices on these groups. Mara [12] studied the particular case of additive dependence. In order to use Polynomial Chaos as meta models, he orthogonalized inputs by the Gram-Schmidt process to come back to independent variables. Approximating the output by a linear model, Xu & Gertner [13] have proposed to decompose the partial variance due to an input into a correlated and uncorrelated parts. The estimation of these new quantities was made by linear regression. More generally, Li & Rabitz [14] exploited this approach with Generalized Additive Models (GAM). GAM components were approximated by suitable basis functions. Thus, global variance were decomposed and estimated accordingly. An extension of the FAST method has been proposed by Xu & Gertner [15]: The extension is based on the reordering of the independent sample in the traditional FAST. Sensitivity indices are then derived by FAST. The construction of a new generalized moment free sensitivity index was initiated by Borgonovo & al. [16] [17]. Based on geometrical consideration, these indices measure the shift area between the outcome density and this same density conditionally to a parameter.

Thus, none of these works gave 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, sensitivity measures based on functional ANOVA could neither be deduced in the dependent frame.

In a pionnering work, Hooker [18], inspired by Stone [19], shed new lights on hierarchically orthogonal function decomposition. Nevertheless, the right assumption to get this kind of decomposition is not completely clear in [18], as there is a gap to show the uniqueness of the decomposition. In the present paper, 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 decorrelated. 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. In the general case, the computation of the summands of the HOFD involves a minimization problem under constraints (see Proposition 1). This optimization procedure will be studied for statistical purposes in the future. Here, we will focus on the special case where the inputs are independent pairs of dependent variables (IPDV). As a matter of fact, in the simplest case of a single pair of dependent variables, the HOFD may be performed by solving a functional linear system of equations involving suitable projection operators (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 [11]. 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. We also compare these generalized indices to the classical Sobol ones (independent case). 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 assumption on density of the joint distribution function of the inputs. Further, we introduce the generalized indices.

In Section 3, we give examples of distribution functions that satisfy the boundedness assumption. A sufficient condition is proposed for any model, and more specific conditions are given in the IPDV case. In Section 4, the HOFD is performed by using adapted projection operators in the case of IPDV models. In the case of a single pair of dependent variables, the components of the HOFD are found by solving a functional linear system. Otherwise, a preliminary step of classical decomposition on independent pairs is necessary to come back to the resolution of linear systems. Section 5 is devoted to numerical applications. Through three toy functions, we estimate generalized indices and compare their performances with the analytical values. In Section 6, we give conclusions and discuss upcoming work. Technical proofs and further details are postponed to Section 7.

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

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

Let ν be a measure on $(\mathbb{R}^p, \mathcal{B}(\mathbb{R}^p))$. Assume that $P_X \ll \nu$ and let p_X be the density of P_X with respect to ν , that is $p_X = \frac{dP_X}{d\nu}$.

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

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

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 $\text{Cov}(\cdot, *) = \mathbb{E}[(\cdot - \mathbb{E}(\cdot))(* - \mathbb{E}(*))]$ 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.

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

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

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

At this stage, we do not make assumptions on the support of \mathbf{X} . For $u \in S \setminus \emptyset$, the support of X_u is denoted by \mathcal{X}_u .

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 $P_X = P_{X_1} \otimes \dots \otimes P_{X_p}$.

The usual presentation is done when $\mathbf{X} \sim \mathcal{U}([0, 1]^p)$ [3], but the Hoeffding decomposition remains true in general case [20].

Let $\mathbf{x} = (x_1, \dots, x_p) \in \mathbb{R}^p$ and assume that $\eta \in \mathbb{L}^2(\mathbb{R}^p, P_X)$. The decomposition consists in writing $\eta(\mathbf{x}) = \eta(x_1, \dots, x_p)$ as the sum of increasing dimension functions:

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

The expansion (1) exists and is unique under one of the hypothesis:

$$\left\{ \begin{array}{l} \text{i) } \int \eta_u(x_u) dP_{X_i} = 0 \quad \forall i \in u, \forall u \subseteq \{1 \dots p\} \\ \text{or} \\ \text{ii) } \int \eta_u(x_u) \eta_v(x_v) dP_X = 0 \quad \forall u, v \subseteq \{1 \dots p\}, \quad u \neq v \end{array} \right.$$

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 $V(Y) = \sum_{u \in S} V(\eta_u(X_u))$.

Moreover, by integration, each term η_u has an explicit expression, given by:

$$\eta_0 = \mathbb{E}(Y), \quad \eta_i = \mathbb{E}(Y/X_i) - \mathbb{E}(Y), \quad i = 1, \dots, p, \quad \eta_u = \mathbb{E}(Y/X_u) - \sum_{v \subset u} \eta_v, \quad |u| \geq 2 \quad (2)$$

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

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

Furthermore,

$$\sum_{u \in S} S_u = 1$$

However, the main assumption is that the input parameters are independent. This is unrealistic in many cases. The use of expressions previously set up is not excluded in case of inputs' dependence, but they could lead to an unobvious and sometimes a wrong interpretation. Also, technics exploited to estimate them may mislead final results because most of them are built on the hypothesis 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. 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_X is a product measure. Nevertheless, we assume:

$$\boxed{\begin{array}{l} \text{where} \\ P_X \ll \nu \\ \nu(dx) = \nu_1(dx_1) \otimes \cdots \otimes \nu_p(dx_p) \end{array}} \quad (\text{C.1})$$

Our main assumption is :

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

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

The section is organized as follows: a preliminary lemma gives the main result to show that H^0 is a complete space. Then, this ensures the existence and the uniqueness of the projection of η onto H^0 . The generalized decomposition of η is finally obtained by adding a residual term orthogonal to every summand, as suggested in [18]. The first part of the reasoning is mostly inspired by Stone's work [19], except that our assumptions are more general. Indeed, we have a relaxed condition on the inputs distribution function. Moreover, the support \mathcal{X} of \mathbf{X} is general.

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 $v \in T$.

The next Lemma is a generalization of the Lemma 3.1 of [19]. As already mentioned, it will be the key to show the hierarchical decomposition.

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:

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

The proof of Lemma 1 is postponed to the Appendix. Our main theorem follows:

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

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

Moreover, this decomposition is unique.

The proof is given in the Appendix.

Notice that, in case where the input variables X_1, \dots, X_p are independent, $\delta = 1$ and Inequality (4) of Lemma 1 is an equality. Indeed, in this case, this equality is directly obtained by orthogonality of the summands.

The variational counterpart of Theorem 1 is a minimization problem under conditional constraints.

Proposition 1. Suppose that (C.1) and (C.2) hold. Let (\mathcal{P}) be the minimization problem under constraints:

$$(\mathcal{P}) \begin{cases} \min_{(\tilde{\eta}_u)_{u \in S}} \mathbb{E}[(Y - \sum_{u \in S} \tilde{\eta}_u(X_u))^2] \\ \mathbb{E}(\tilde{\eta}_u(X_u)/X_{u \setminus i}) = 0, \forall i \in u, \forall u \in S \setminus \emptyset \end{cases}$$

Then (\mathcal{P}) admits a unique solution $\eta^* = (\eta_u)_{u \in S}$.

Proof of Proposition 1 is postponed to the Appendix. Notice that a similar result for the Lebesgue measure is given in [18]. Its purpose was to provide diagnostics for high-dimensional functions. Here, we will no more exploit this idea. This will be done in a forthcoming work. Instead, we are going to construct stochastic sensitivity indices based on the new decomposition (5) and focus on a specific estimation method for IPDV models.

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. So, we can define generalized sensitivity indices.

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

$$S_u = \frac{V(\eta_u(X_u)) + \sum_{\substack{v \neq \emptyset \\ u \cap v \neq u, v}} \text{Cov}(\eta_u(X_u), \eta_v(X_v))}{V(Y)} \quad (6)$$

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

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

An immediate consequence is given in Proposition 2 (see proof in the Appendix) :

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

$$\sum_{u \in \mathcal{S} \setminus \{\emptyset\}} S_u = 1 \quad (8)$$

Thus, sensitivity indices are summed to 1. Furthermore, the covariance terms included in these new indices allow to take into account the inputs dependence. Thus, we are now able 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. We can distinguish the full contribution of a variable and its contribution into another correlated income.

Note that for independent inputs, the summands η_u are mutually orthogonal, so $\text{Cov}(\eta_u, \eta_v) = 0$, $u \neq v$, and we recover the well known Sobol indices. Hence, these new sensitivity indices can be seen as a generalization of Sobol indices.

However, the HOFD and subsequent indices are only obtained under constraints (C.1) and (C.2). In the following, we give illustrations of distribution functions satisfying these main assumptions.

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 of measures, 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 3 (the proof is postponed to the Appendix):

Proposition 3. Assume that there exist $M_1, M_2 > 0$ with

$$\boxed{M_1 \leq p_X \leq M_2} \quad (C.3)$$

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_X is a 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 $p = 2$. 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 of inputs $\mathbf{X} = (X_1, X_2)$. 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 modeled by copulas. Copulas [21] give a relationship between a joint distribution and its marginals. Sklar's theorem [22] 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:*

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

Furthermore,

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

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

Proposition 4. *For a two-dimensional model, the three following conditions are equivalent:*

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

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

$$3. \quad \boxed{C(u, v) = Muv + (1 - M)\tilde{C}(u, v), \forall (u, v) \in [0, 1]^2 \text{ for some 2-D copula } \tilde{C}} \quad (C.6)$$

The proof of Proposition 4 is postponed to the Appendix.

Hence, the generalized Hoeffding decomposition holds for a wide class of examples. The first example is the Morgenstern copulas [23]:

Example 2: The expression of the Morgenstern copulas is given by:

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

For $\theta \in] - 1, 1[$, (C.6) holds, and

$$C_\theta(u, v) = (1 - |\theta|)uv + |\theta|uv[1 + \frac{\theta}{|\theta|}(1 - u)(1 - v)]$$

Let now consider the class of Archimedean copulas,

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

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 5:

Proposition 5. *If there exist $M_1, M_2 > 0$ such that:*

$$-\varphi'(u) \geq M_1 \quad \forall u \in [0, 1] \quad (12)$$

$$\frac{d}{du} \left(\frac{1}{2} \frac{1}{\varphi'(u)^2} \right) \geq M_2, \quad \forall u \in [0, 1] \quad (13)$$

Then, Condition (C.5) holds.

The proof is straightforward. Now, we will see three illustrative Archimedean copulas satisfying (C.5).

Example 3: The Frank copula is characterized by the generator:

$$\varphi_1(x) = \log \left(\frac{e^{-\theta x} - 1}{e^{-\theta} - 1} \right), \quad \theta \in \mathbb{R} \setminus \{0\}$$

Condition (C.5) holds, and $c(u, v) \geq -\theta(e^{-\theta} - 1)e^{-2\theta}$ if $\theta > 0$, $c(u, v) \geq -\theta(e^{-\theta} - 1)$ elsewhere.

The next two examples also satisfy (C.5) by the intermediate Proposition 5.

Example 4: Let $\alpha < 0$, $\theta > 0$ and β with $\beta < -\alpha e^{-\theta}$. Set

$$\varphi_2(x) = -\frac{\alpha}{\theta} e^{-\theta x} + \beta x + \left(\frac{\alpha}{\theta} e^{-\theta} - \beta \right), \quad x \in [0, 1] \quad (14)$$

Example 5: Let $C < 0$ and set

$$\varphi_3(x) = x \ln x + (C - 1)x + (1 - C), \quad x \in [0, 1] \quad (15)$$

Leaving the class of copulas, we now directly work with the joint density function. Proposition 6 gives a general form of distribution for our framework:

Proposition 6. *If p_X has the form*

$$p_X(x_1, x_2) = \alpha \cdot f_{X_1}(x_1)f_{X_2}(x_2) + (1 - \alpha) \cdot g_X(x_1, x_2), \quad \alpha \in]0, 1[\quad (16)$$

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_X satisfies (C.5).

The proof is straightforward.

Example 6: As an illustration of Proposition 6, take $\nu = \nu_L$, $f_X = f_{X_1}f_{X_2}$ a normal density with a diagonal covariance matrix Σ , and g_X a normal density of covariance matrix Ω , with $\Omega_{ii} = \Sigma_{ii}$, $i = 1, 2$. Notice that because a copula of Gaussian mixture distribution is a mixture of Gaussian copulas (see [24]), this example can be directly recovered by the copula approach.

Example 7: Let generalize Example 6. If P_X is a Gaussian mixture

$$\alpha \cdot N_2(m, \Sigma) + (1 - \alpha) \cdot N_2(\mu, \Omega), \quad \alpha \in]0, 1[$$

with

$$m = \begin{pmatrix} m_1 \\ m_2 \end{pmatrix}, \quad \mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \quad \Sigma = \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{pmatrix}, \quad \Omega = \begin{pmatrix} \omega_1^2 & \rho\omega_1\omega_2 \\ \rho\omega_1\omega_2 & \omega_2^2 \end{pmatrix}, \quad \rho \in]-1, 1[$$

then (C.4) holds iff $\omega_1^2 \leq \sigma_1^2$ and $\omega_2^2 \leq \sigma_2^2$.

Thus, for many distributions, the generalized decomposition holds, and generalized sensitivity indices may thus be defined.

For the remaining part of the paper, we will assume that the set of inputs is an IPDV. If p is odd, we will assume that an input variable is independent to all the others.

The next section is devoted to the estimation of HOFD components. The simplest case of a single pair of dependent variables is first discussed. Then, the more general IPDV case is studied. In this last part, 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

Using the property of hierarchical orthogonality ($H_u^0 \perp H_v^0, \forall v \subset u$), we will see that the summands of the decomposition are solution of a functional linear system. For $u \in S$, the projection operator onto H_u^0 is denoted by $P_{H_u^0}$.

In this section, we present the HOFD terms computation, based on the resolution of a functional linear system. The result relies on projection operators previously set up. Further, we expose the linear system estimation for practice.

4.1 Models of $p = 2$ input variables

This part is devoted to the simple case of bidimensional models. Let

$$Y = \eta(X_1, X_2)$$

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

Procedure 1

1. *HOFD of the output:*

$$Y = \eta_0 + \eta_1(X_1) + \eta_2(X_2) + \eta_{12}(X_1, X_2) \quad (17)$$

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:*

$$\begin{pmatrix} Id & 0 & 0 & 0 \\ 0 & Id & P_{H_1^0} & 0 \\ 0 & P_{H_2^0} & Id & 0 \\ 0 & 0 & 0 & Id \end{pmatrix} \begin{pmatrix} \eta_0 \\ \eta_1 \\ \eta_2 \\ \eta_{12} \end{pmatrix} = \begin{pmatrix} P_{H_\emptyset}(\eta) \\ P_{H_1^0}(\eta) \\ P_{H_2^0}(\eta) \\ P_{H_{12}^0}(\eta) \end{pmatrix} \quad (18)$$

3. *Computation of the right-hand side vector of (18):*

$$\begin{pmatrix} P_{H_\emptyset}(\eta) \\ P_{H_1^0}(\eta) \\ P_{H_2^0}(\eta) \\ P_{H_{12}^0}(\eta) \end{pmatrix} = \begin{pmatrix} \mathbb{E}(\eta) \\ \mathbb{E}(\eta/X_1) - \mathbb{E}(\eta) \\ \mathbb{E}(\eta/X_2) - \mathbb{E}(\eta) \\ \eta - \mathbb{E}(\eta/X_1) - \mathbb{E}(\eta/X_2) + \mathbb{E}(\eta) \end{pmatrix} \quad (19)$$

In this frame, we have:

Proposition 7. *Let η be any function of $L_{\mathbb{R}}^2(\mathbb{R}^p, \mathcal{B}(\mathbb{R}^p), P_X)$. Then, under (C.1) and (C.2), the linear system*

$$(\mathcal{S}) \begin{pmatrix} Id & 0 & 0 & 0 \\ 0 & Id & P_{H_1^0} & 0 \\ 0 & P_{H_2^0} & Id & 0 \\ 0 & 0 & 0 & Id \end{pmatrix} \begin{pmatrix} h_0 \\ h_1 \\ h_2 \\ h_{12} \end{pmatrix} = \begin{pmatrix} P_{H_\emptyset}(\eta) \\ P_{H_1^0}(\eta) \\ P_{H_2^0}(\eta) \\ P_{H_{12}^0}(\eta) \end{pmatrix} \quad (20)$$

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

4. *Reduction of the system (18). As the constant term corresponds to the expected value of η , and the residual one can be deduced from the others, the dimension of the system (20) can even be reduced to:*

$$\underbrace{\begin{pmatrix} Id & P_{H_1^0} \\ P_{H_2^0} & Id \end{pmatrix}}_{A_2} \underbrace{\begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix}}_{\Delta} = \underbrace{\begin{pmatrix} \mathbb{E}(\eta/X_1) - \mathbb{E}(\eta) \\ \mathbb{E}(\eta/X_2) - \mathbb{E}(\eta) \end{pmatrix}}_B \quad (21)$$

5. *Practical resolution:* The numerical resolution of (21) is achieved by an iterative Gauss Seidel algorithm [25] 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:

$$\Delta^{(k+1)} := \begin{pmatrix} \Delta_1^{(k+1)} \\ \Delta_2^{(k+1)} \end{pmatrix} = L_2^{-1}(B - U_2 \cdot \Delta^{(k)}) \quad (22)$$

Using expression of A_2 , we get:

$$\Delta^{(k+1)} = \begin{pmatrix} \mathbb{E}(Y - \Delta_2^{(k)}/X_1) - \mathbb{E}(Y - \Delta_2^{(k)}) \\ \mathbb{E}(Y - \Delta_1^{(k+1)}/X_2) - \mathbb{E}(Y - \Delta_1^{(k+1)}) \end{pmatrix} \quad (23)$$

6. *Convergence of the algorithm:* now, we hope that the Gauss Seidel algorithm converges to the true solution. Looking back at (18), 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 [26], Gauss Seidel algorithm converges to the true solution Δ if A_2 is strictly diagonally dominant, which is implied by :

$$\|P_{H_i^0}\| < \|Id\|, \quad i = 1, 2 \quad (24)$$

i.e.

$$\sup_{\substack{\mathbb{E}(U^2)=1 \\ U \in H_j^0}} \mathbb{E}[P_{H_i^0}(U)^2] < 1, \quad i = 1, 2, j \neq i \quad (25)$$

Equality (19) reveals that $P_{H_i^0}(U) = \mathbb{E}(U/X_i) - \mathbb{E}(U)$. Hence, by the Jensen inequality [27] for conditional expectations, $\|P_{H_i^0}\|, i = 1, 2$ admits an upper bound:

Take $U \in H_1^0$:

$$\begin{aligned} \|P_{H_2^0}\| &= \sup_{\substack{\mathbb{E}(U^2)=1 \\ U \in H_1^0}} \mathbb{E}[(\mathbb{E}(U/X_2) - \mathbb{E}(U))^2] = \sup_{\substack{\mathbb{E}(U^2)=1 \\ U \in H_1^0}} \mathbb{E}[\mathbb{E}(U/X_2)^2] \quad \text{as } U \in H_1^0 \\ &\leq \sup_{\substack{\mathbb{E}(U^2)=1 \\ U \in H_1^0}} \mathbb{E}[\mathbb{E}(U^2/X_2)] = 1 \quad \text{by Jensen} \end{aligned}$$

The same holds for $U \in H_2^0$, and we also have $\|P_{H_2^0}\| \leq 1$.

Moreover, the Jensen's inequality is strict if U is not X_i -measurable. As U is a function of X_j (that is $j = 2$ if $i = 1$ and conversely), the condition of convergence holds if X_1 is not a measurable function of X_2 . Hence, Gauss Seidel algorithm converges if X_1 is not a function of X_2 .

7. *Estimation procedure: Suppose that we get a sample of n observations $(Y_k, \mathbf{X}_k)_{k=1, \dots, n}$.*

- *Estimation of the components of the HOFD: the iterative scheme (23) requires to estimate conditional expectations. As extended in Da Veiga & al [28], we propose to estimate them by local polynomial regression at each point of observation. 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 & Gijbels [29]), the Sherman-Morrison formula [30] is applied to reduce the computational time.*

A more detailed procedure is given in the Appendix. The iterative algorithm is easy to implement. We stop when $\|\Delta^{(k+1)} - \Delta^{(k)}\| \leq \varepsilon$, for a small positive ε .

Once (η_1, η_2) have been estimated, we estimate η_0 by the empirical mean of the output. Then, an estimation of η_{12} is obtained by subtraction.

- *We use empirical variance and covariance estimation to estimate sensitivity indices S_1, S_2 and S_{12} .*

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 $X^{(i)} := (X_1^{(i)}, X_2^{(i)})$, $i = 1, \dots, k$. By rearrangement, we may assume that:

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

SA for IPDV models has already been treated in [11]. Indeed, they proposed to estimate usual sensitivity indices on groups of variables via Monte Carlo estimation. 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 effects of the independent pairs.

To begin with, as a slight generalization of [3] and used in [11], let apply the Sobol decomposition on groups of dependent variables,

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

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

Thus, we obtain independent components of IPDV. Under the assumptions discussed in the previous section, we can apply the HOFD of each of these components, that is,

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

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 $i = 1, \dots, k$, the first order sensitivity index measuring the contribution of $X_1^{(i)}$ (respectively $X_2^{(i)}$) on the output of the model is:*

$$S_{i,1} = \frac{V(\varphi_{i,1}) + \text{Cov}(\varphi_{i,1}, \varphi_{i,2})}{V(Y)}, \quad \left(\text{resp. } S_{i,2} = \frac{V(\varphi_{i,2}) + \text{Cov}(\varphi_{i,1}, \varphi_{i,2})}{V(Y)} \right) \quad (26)$$

The second order sensitivity index for the pair $X^{(i)}$, $i = 1, \dots, k$, is defined as:

$$S_{i,12} = \frac{V(\varphi_{i,12})}{V(Y)} \quad (27)$$

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

Procedure 2

1. Estimation of $(\eta_i)_{i=1,\dots,k}$: as reminded in Part 2.2 with Equations (2), $\eta_i = \mathbb{E}(Y/X^{(i)}) - \mathbb{E}(Y)$. Step 7 of Procedure 1 gives method to estimate the conditional expectations. So that, we will have estimations of η_i , $i = 1, \dots, k$.
2. For $i = 1, \dots, k$, we apply step 2 to step 7 of Procedure 1, considering η_i as the 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. We consider IPDV models and a Gaussian mixture distribution on the input variables. We choose covariance matrices of the mixture satisfying conditions of Example 1.

We give estimations of our new indices, and compare them to the analytical ones, computed from expressions (6). We also compute dispersions of the estimated new indices.

In [28], Da Veiga & al. proposed to estimate the classical Sobol indices $S_u = (V[\mathbb{E}(Y/X_u)] - \sum_{v \subset u} V[\mathbb{E}(Y/X_v)]) / V(Y)$, $u \subseteq \mathcal{P}_p$, by nonparametric tools. Indeed, the local polynomial regression were used to estimate conditional moments $\mathbb{E}(Y/X_u)$, $u \subseteq \mathcal{P}_p$. This method, used further, will be called Da Veiga procedure (DVP). Results given by DVP are compared with the ones given by our method. The goal is to show that the usual sensitivity indices are not appropriate in the dependence frame, even if a relevant estimation method is used.

5.1 Two-dimensional IPDV model

Let consider the model

$$Y = X_1 + X_2 + X_1 X_2$$

Here, ν and P_X are of the form given by Example 1, with $m = \mu = 0$.

Thus, the analytical decomposition of Y is

$$\eta_0 = \mathbb{E}(X_1 X_2), \quad \eta_1 = X_1, \quad \eta_2 = X_2 \quad \eta_{12} = X_1 X_2 - \mathbb{E}(X_1 X_2)$$

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.

The analytical classical Sobol indices are difficult to obtain, but we give estimators of the classical Sobol indices with DVP.

		S_1	S_2	S_{12}	$\sum_u S_u$
New indices	Estimation	0.42 ± 0.041	0.41 ± 0.043	0.17 ± 0.026	1 ± 9.10^{-16}
	Analytical	0.39	0.39	0.22	1
DVP indices	Estimation	0.64 ± 0.045	0.65 ± 0.044	0.41 ± 0.038	1.7 ± 0.09

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

We notice that estimations with our method give quite good results in comparison with their analytical values. The estimation error of the interaction term is due to the fact that the component $\hat{\eta}_{12}$ is obtained by difference between the output and the other estimated components. The DVP indices are difficult to interpret as the sum is higher than 1.

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

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

The new indices estimations given in Table 1 are decomposed in Table 2. As previously, the number at the right of \pm indicates the standard deviation on L simulations.

	S_i^v	S_i^c	S_i
X_1	0.28 ± 0.04	0.14 ± 0.01	0.42 ± 0.041
X_2	0.27 ± 0.043	0.14 ± 0.01	0.41 ± 0.043
Analytical	0.25	0.14	0.39

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

For each index, the covariate itself explains 28% (in estimation, 25% in reality) of the part of the total variability. However, the contribution embedded in the correlation is not negligible as it represents 14% of the total variance. Considering the shape of the model, and coefficients of parameters distribution, it is quite natural to get the same contribution of X_1 and X_2 into the global variance. 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).

From now, we take $\rho_{12} = 0$, i.e. we assume that the inputs are independent. Let compare our new estimated indices with their analytical values in Table 3. We again decompose new indices into a variance (S_i^v) and a covariance (S_i^c) contribution.

	New indices			Theoretical
	S_i^v	S_i^c	S_i	S_i
X_1	0.39 ± 0.039	-0.01 ± 0.01	0.38 ± 0.036	0.375
X_2	0.38 ± 0.045	-0.01 ± 0.024	0.37 ± 0.037	0.375
X_1X_2	0.26 ± 0.038	-0.01 ± 0.01	0.25 ± 0.027	0.25

Table 3: Comparison between analytical and estimated indices with $\rho_{12} = 0$

Thus, the new indices are well tailored if we have a small idea on inputs dependence in a system. Indeed, Table 3 shows that our new indices take dependence into account if it exists, and the covariance contribution is estimated by 0 if not. New indices recover the classical Sobol indices in case of independence.

5.2 Linear Four-dimensional model

The test model is

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

Actually, Condition (C.2) only needs to be satisfied on groups of correlated variables. Let consider the two blocks $X^{(1)} = (X_1, X_3)$ and $X^{(2)} = (X_2, X_4)$ of correlated variables. The previous form of density can be taken for $X^{(1)}$ and $X^{(2)}$. $P_{X^{(i)}}$ is then the Gaussian mixture $\alpha_i \cdot N_2(0, \mathbf{I}_2) + (1 - \alpha_i) \cdot N_2(0, \Omega_i)$, $i = 1, 2$. The analytical sensitivity indices are given by (26) & (27).

For $L = 50$ simulations and $n = 1000$ observations, we took $\varphi_1^{2(1)} = \varphi_2^{2(1)} = 0.5$, $\varphi_1^{2(2)} = 0.7$, $\varphi_2^{2(2)} = 0.3$, $\rho_{12}^{(1)} = 0.4$, $\rho_{12}^{(2)} = 0.37$ and $\alpha_1 = \alpha_2 = 0.2$.

Figure 1 displays the dispersion of indices of first order for all variables and second order for grouped variables. We compare them to their analytical values. In the same figure, we also represented the estimators of classical Sobol indices with DVP.

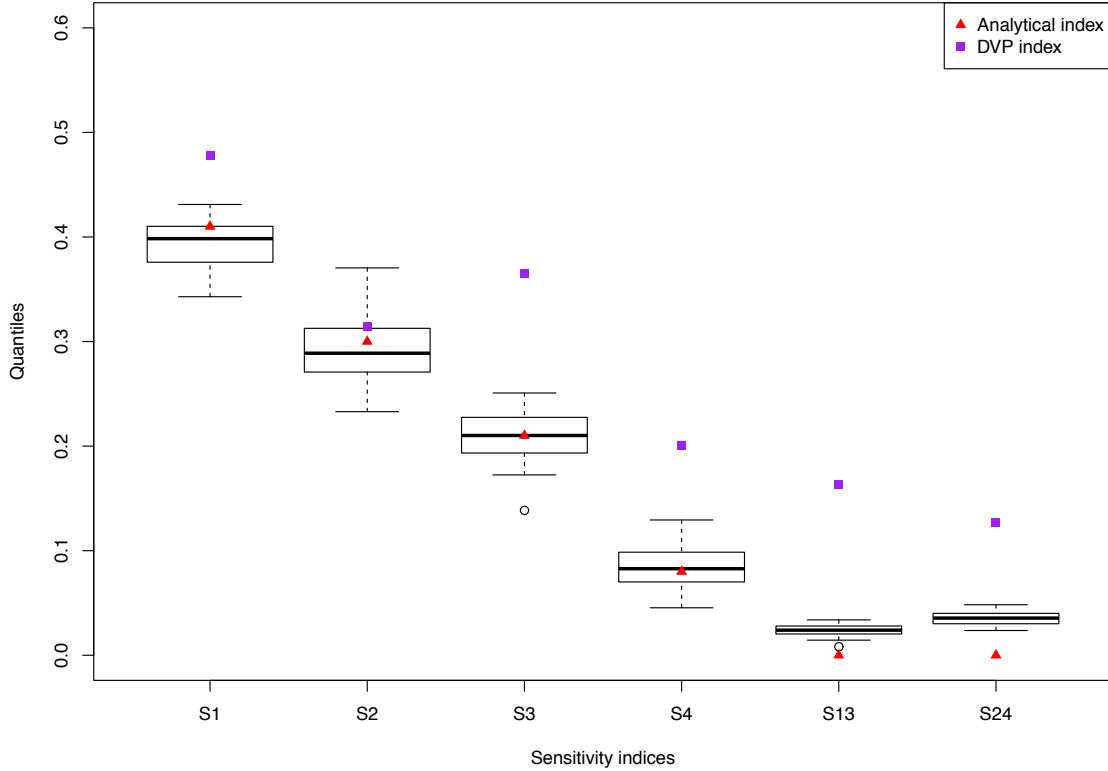


Figure 1: Boxplots representation of new indices-Comparison with analytical and DVP indices

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 , $i = 1, \dots, 4$. Also, interaction terms are well estimated, as they are closed to 0. For each case, the dispersion on 50 simulations is very low. As for the DVP estimation, it is once again very high compared with the true indices values.

5.3 The Ishigami function

This function is well known in SA ([31]). It is defined by:

$$Y = \sin(X_1) + a \sin^2(X_2) + bX_3^3 \sin(X_1)$$

We assume that X_3 is the independent variable, and that X_1 and X_2 are correlated. P_X is again the Gaussian mixture $\alpha \cdot N_3(0, I_3) + (1 - \alpha) \cdot N_3(0, \Omega)$.

With $L = 50$ simulations of $n = 1000$ observations, we fixed parameters of distribution at $\varphi_1^2 = 0.15$, $\varphi_2^2 = 0.85$, $\varphi_3^2 = 0.75$, $\rho_{12} = 0.3$ and $\alpha = 0.2$.

In Figure 2, the dispersion of the new measures is represented for fixed $b = 0.1$ and different values of a . In addition, the analytical new indices and estimated classical Sobol indices with DVP are displayed.

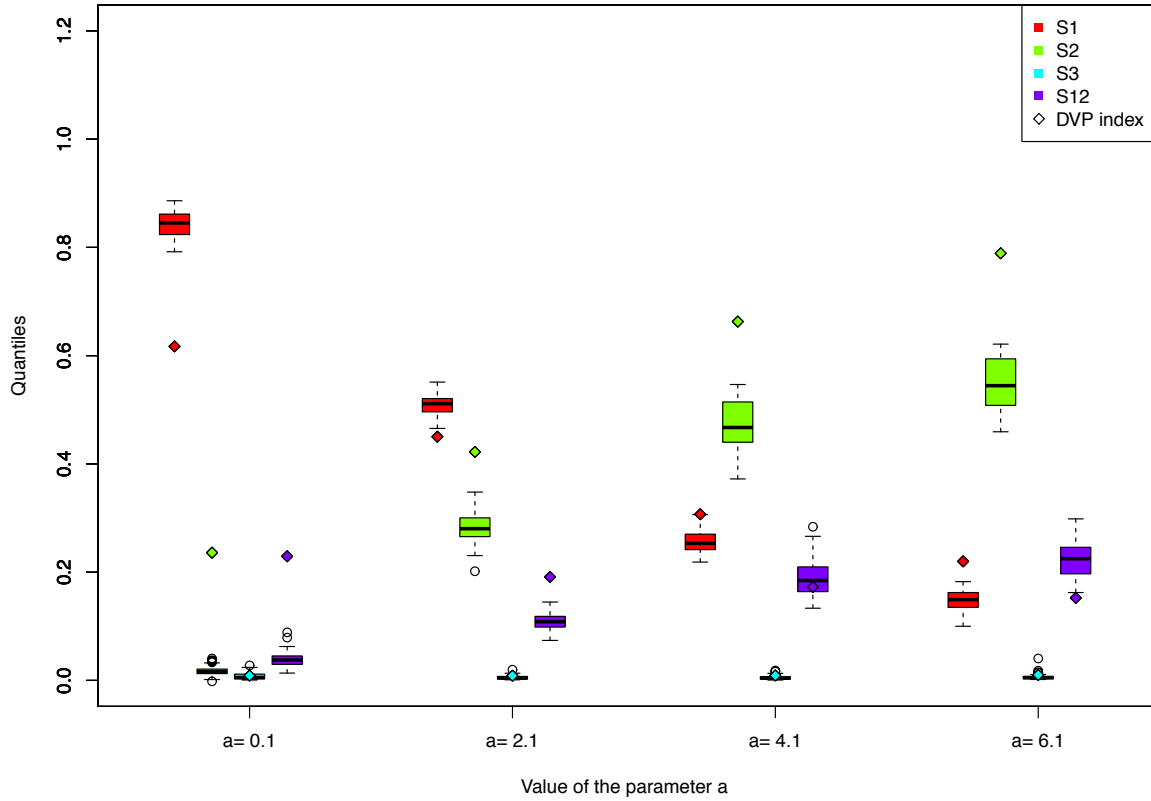


Figure 2: Boxplots of new indices for different values of a for Ishigami function

Every boxplot shows that there is a small dispersion. For all estimations, DVP indices are larger than the new ones. The figure clearly shows that, for all values of a , the sum of these four indices is greater than 1. It again shows their non adaptation to a situation of dependence.

If we have a look on the values taken by our new sensitivity indices, we see that, for small values of a , the variable X_1 contributes the most to the model's variability. This role decreases as a increases, and X_2 then gets the biggest contribution. For any value of a , the input X_3 plays a very negligible role, which seems realistic as b is a small fixed value. As for the interaction index S_{12} , it is getting bigger with the increasing importance of a , but the contribution remains low.

6 Conclusions and Perspectives

The Hoeffding decomposition and associated Sobol indices have been widely studied in SA over past years. Recently, a literature appears to treat the case of dependent input variables, in which authors propose different ways to deal with dependence. The goal of this paper is to conciliate the problem of inputs dependence with the Hoeffding decomposition. Indeed, we study a functional ANOVA decomposition in a generalized inputs distribution frame. Thus, we show that a model can be uniquely decomposed as a sum of hierarchically orthogonal functions of increasing dimension. Also, this approach generalizes the Hoeffding's one, as we recover it in case of independence.

Similarly to the classical Sobol decomposition, this leads to the construction of new sensitivity indices. They consist of a variance and a covariance contribution able to take into account the possible correlation among variables. In case of independence, these indices are the classical Sobol indices. However, the indices construction is only possible under specific assumptions on the joint distribution function of the inputs. We expose few cases that satisfy these assumptions for any p -dimensional models. More specifically, for two-dimensional models, the required assumption is equivalent to assumptions on copulas. In this context, we give examples satisfying one of these assumptions .

Focused on the IPDV models, summands of the decomposition are estimated thanks to projection operations. This leads to the numerical resolution of functional linear systems. The strength of this method is that it does not require to make assumptions on the form of the model or on the structure of dependence. We neither use meta-modelling and avoid in this way many sources of errors.

Through three applications on test models, we observe the importance of considering the inputs correlation, and show how our method could catch it. The comparison with estimators of classical indices with DVP shows that the Sobol indices are not appropriate in case of correlations, even when using nonparametric method. Also, when inputs independence holds, the new indices remain well suited to measure sensitivity into a model.

Nevertheless, only considering IPDV models for estimation is restrictive. The perspective is to explore other estimation methods suitable for more general models. Also, we intend to lead a systematic study on copulas satisfying or not our assumptions.

7 Appendix

A Generalized Hoeffding decomposition-Application to SA

A.1 Generalized decomposition for dependent inputs

The upcoming proof follows the guideline of the proof of Lemma 3.1 in Stone [19].

Proof of Lemma 1

By induction on the cardinal of T , let show that

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

- $\mathcal{H}(1)$ 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

$$\mathbb{E}[(\sum_{u \in T} h_u(\mathbf{X}))^2] \geq M \cdot \mathbb{E}(h_r^2(\mathbf{X})) \quad (28)$$

- 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

$$p_X \geq M \cdot p_{X_1} p_{X_2}$$

As a consequence,

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

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 $h_u \in H_{r \cap u}^0$, 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 (28) holds for any size of any maximal sets of T .

By using (28) with $\tilde{h}_r = h_r$ and $\tilde{h}_u = -\beta h_u, \forall u \neq r$, we get

$$\mathbb{E}[(h_r(\mathbf{X}) - \beta \sum_{u \neq r} h_u(\mathbf{X}))^2] \geq M\mathbb{E}(h_r^2(\mathbf{X})) \quad (29)$$

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

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

Hence,

$$[E(h_r(\mathbf{X}) \sum_{u \neq r} h_u(\mathbf{X}))]^2 \leq (1 - M) \cdot \mathbb{E}(h_r^2(\mathbf{X})) \cdot \mathbb{E}[(\sum_{u \neq r} h_u(\mathbf{X}))^2] \quad (30)$$

This implies

$$\mathbb{E}[(\sum_u h_u(\mathbf{X}))^2] \geq (1 - \sqrt{1 - M}) \left[\mathbb{E}(h_r^2(\mathbf{X})) + \mathbb{E}[(\sum_{u \neq r} h_u(\mathbf{X}))^2] \right] \quad (31)$$

Set $x = h_r(\mathbf{X})$ and $y = \sum_{u \neq r} h_u(\mathbf{X})$. (31) is rephrased as

$$\|x + y\|^2 \geq (1 - \sqrt{1 - M}) \{\|x\|^2 + \|y\|^2\} \quad (32)$$

Further, (30) is $\langle x, y \rangle \geq -\sqrt{1 - M} \|x\| \cdot \|y\|$. Thus,

$$\begin{aligned} \|x\|^2 + \|y\|^2 &\geq 2\langle x, y \rangle \\ &\geq -\frac{2}{\sqrt{1 - M}} \langle x, y \rangle \quad \text{by (32)} \end{aligned}$$

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

As $\mathcal{H}(n)$ is supposed to be true and (31) holds, it follows that:

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

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 $K^0 = \{\sum_{u \in S^-} h_u(X_u), h_u \in H_u^0, \forall u \in S^-\}$.

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 [32].

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 $h_{n,u} \rightarrow h_u$. As $(h_{n,u})_n \in H_u^0 \subset H_u$ complete, $h_u \in H_u$. Let $v \subset u$, and $h_v \in H_v^0$:

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

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 $h_n \rightarrow h \in K^0$.

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 :

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

As $(h_n)_n$ is a Cauchy sequence, by the above inequality, $(h_{n,u})_n$ is also Cauchy. As $h_{n,u} \rightarrow h_u \in H_u^0$, we deduce that $h_n \xrightarrow{n \rightarrow \infty} \sum_{u \in S^-} h_u = h \in K^0$.

Thus, K^0 is complete. By the projection theorem, we can deduce there exists a unique element into K^0 such that :

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

- Decomposition of η : following Hooker [18], we introduce the residual term as

$$\eta_{\mathcal{P}_p}(X_1, \dots, X_p) = \eta(X_1, \dots, X_p) - \sum_{u \in S^-} \eta_u(X_u)$$

By projection, $\langle \eta - \sum_{v \in S^-} \eta_v, h_u \rangle = 0 \quad \forall u \in S^-, \forall h_u \in H_u^0$. Hence, $\eta(\mathbf{X}) = \sum_{u \in S} \eta_u(X_u)$, $\eta_u \in H_u^0, \forall u \in S$, and this decomposition is well defined.

- Terms of the summand are unique: assume that $\eta = \sum_{u \in S} \eta_u = \sum_{u \in S} \tilde{\eta}_u$, $\tilde{\eta}_u \in H_u^0$. By Lemma 1, it follows that

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

■

Proof of Proposition 1

Let first prove the following equivalence :

$$\begin{aligned} \int \eta_u(x_u) \eta_v(x_v) p_X(x) d\nu(x) &= 0 \quad \forall v \subset u, \forall \eta_v \\ &\iff \\ \int \eta_u(x_u) p_X(x) d\nu_i(x_i) d\nu_{u^c}(x_{u^c}) &= 0 \quad \forall u \in S, \forall i \in u \end{aligned}$$

Let $v \subset u$ and $i \in u \setminus v$, then

$$\begin{aligned} \int \eta_v(x_v) \eta_u(x_u) p_X(x) d\nu(x) &= \int \eta_v(x_v) \eta_u(x_u) p_X(x) d\nu_i(x_i) d\nu_{u^c}(x_{u^c}) d\nu_{u \setminus i}(x_{u \setminus i}) \\ &= \int \eta_v(x_v) \left(\int \eta_u(x_u) p_X(x) d\nu_i(x_i) d\nu_{u^c}(x_{u^c}) \right) d\nu_{u \setminus i}(x_{u \setminus i}) \\ &= 0 \quad \text{by assumption} \end{aligned}$$

Conversely, assume that $\exists u, \exists i \in u$ such that $\int \eta_u(x_u) p_X(x) d\nu_i(x_i) d\nu_{u^c}(x_{u^c}) \neq 0$, then,

$$\eta_v = \int \eta_u(x_u) p_X(x) d\nu_i(x_i) d\nu_{u^c}(x_{u^c}) \quad \text{with } v = u \setminus i$$

and

$$\begin{aligned}
\int \eta_u(x_u)\eta_v(x_v)p_X(x)d\nu(x) &= \int \eta_u(x_u) \left(\int \eta_u(x_u)p_X(x)d\nu_i d\nu_{u^c} \right) p_X(x)d\nu_i d\nu_{u^c} d\nu_{u \setminus i} \\
&= \int \left(\int \eta_u(x_u)p_X(x)d\nu_i(x_i) d\nu_{u^c}(x_{u^c}) \right)^2 d\nu_{u \setminus i}(x_{u \setminus i}) \\
&> 0
\end{aligned}$$

There is a contradiction, so that $\int \eta_u(x_u)p_X(x)d\nu_i(x_i) d\nu_{u^c}(x_{u^c}) = 0 \quad \forall i \in u, \forall u$.
The second expression can be rewritten as :

$$\int \eta_u(x_u)p_X(x)d\nu_i(x_i) d\nu_{u^c}(x_{u^c}) = \mathbb{E}(\eta_u/X_{u \setminus i}) \quad \forall i \in u, \forall u \in S$$

Then, by Theorem 1, the minimization problem (\mathcal{P}) admits a unique solution. ■

A.2 Generalized sensitivity indices

Proof of Proposition 2

Under (C.1) and (C.2), Theorem 1 states the existence and the uniqueness decomposition of η :

$$\eta(\mathbf{X}) = \sum_{u \in S} \eta_u(X_u),$$

with $H_u^0 \perp H_v^0, \forall v \subset u$. Therefore,

$$\mathbb{E}(\eta(X)) = \mathbb{E}\left(\sum_{u \in S} \eta_u(X_u)\right) = \eta_0$$

and

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

Thus, (6) holds, and equalities (7) and (8) follow obviously. ■

B Examples of distribution function

B.1 Boundedness of the inputs density function

Proof of Proposition 3

Let $u \subset \mathcal{P}_p$, and $0 < M_1 \leq p_X \leq M_2$. As p_{X_u} and $p_{X_{u^c}}$ are marginals, they are upper bounded by M_2 .

As a consequence, $p_{X_u}p_{X_{u^c}} \leq \frac{M_2^2}{M_1}M_1 \leq \frac{M_2^2}{M_1}p_X$, so that $p_X \geq M_1M_2^{-2}p_{X_u}p_{X_{u^c}}$, with $0 < M_1M_2^{-2} < 1$. ■

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 $\nu_i \sim N(m_i, \sigma_i^2)$. So

$$\nu = \bigotimes_{i=1}^p \nu_i$$

- p_X is given by

$$\begin{aligned} p_X(\mathbf{x}) &= \frac{dP_X}{d\nu}(\mathbf{x}) = \frac{dP_X}{d\nu_L} \times \frac{d\nu_L}{d\nu}(\mathbf{x}) \\ &= \alpha + (1 - \alpha) \left| \frac{\Sigma}{\Omega} \right|^{1/2} \exp -\frac{1}{2} \mathbf{t}(\mathbf{x} - m)(\Omega^{-1} - \Sigma^{-1})(\mathbf{x} - m) \end{aligned} \quad (33)$$

First, we have $p_X(\mathbf{x}) \geq \alpha > 0$.

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

B.2 Examples of distribution of two inputs

Proof of Proposition 4

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, $\tilde{C}(0, u) = C(u, 0) = 0$ and $\tilde{C}(1, u) = \tilde{C}(u, 1) = u \quad \forall u \in [0, 1]$. 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). ■

C Estimation

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

Proof of Proposition 7

- 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

$$\begin{cases} \eta_0 \in H_0 \\ \eta_i \in H_i^0 \perp H_0, \quad i = 1, 2 \\ \eta_{12} \in H_{12}^0 \perp H_i^0, \quad i = 1, 2, H_{12}^0 \perp H_0 \end{cases}$$

Thus,

$$\begin{pmatrix} Id & 0 & 0 & 0 \\ 0 & Id & P_{H_1^0} & 0 \\ 0 & P_{H_2^0} & Id & 0 \\ 0 & 0 & 0 & Id \end{pmatrix} \begin{pmatrix} \eta_0 \\ \eta_1 \\ \eta_2 \\ \eta_{12} \end{pmatrix} = \begin{pmatrix} P_{H_0}(\eta) \\ P_{H_1^0}(\eta) \\ P_{H_2^0}(\eta) \\ P_{H_{12}^0}(\eta) \end{pmatrix} \quad (34)$$

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 $(\tilde{\eta}_0, \dots, \tilde{\eta}_{\mathcal{P}_p}) \in H_0 \times \dots \times H_{\mathcal{P}_p}^0$, then

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

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

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

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

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

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

As 0 can be uniquely decomposed into H^0 as a sum of zero, then,

$$\eta_1 - \tilde{\eta}_1 = \eta_2 - \tilde{\eta}_2 = 0$$

- Let now compute

$$\begin{pmatrix} P_{H_0}(\eta) \\ P_{H_1^0}(\eta) \\ P_{H_2^0}(\eta) \\ P_{H_{12}^0}(\eta) \end{pmatrix}$$

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 :

$$\varphi(X_i) = \varphi_0 + \varphi_i(X_i), \quad \varphi_0 \in H_0, \quad \varphi_i \in H_i^0$$

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

$$\begin{pmatrix} P_{H_0}(\eta) \\ P_{H_1^0}(\eta) \\ P_{H_2^0}(\eta) \\ P_{H_{12}^0}(\eta) \end{pmatrix} = \begin{pmatrix} \mathbb{E}(\eta) \\ \mathbb{E}(\eta/X_1) - \mathbb{E}(\eta) \\ \mathbb{E}(\eta/X_2) - \mathbb{E}(\eta) \\ \eta - \mathbb{E}(\eta/X_1) - \mathbb{E}(\eta/X_2) + \mathbb{E}(\eta) \end{pmatrix} \quad (35)$$

■

Numerical procedure

Gauss-Seidel algorithm requires the estimation of conditional expectation at each iteration. To do this, we use the local polynomial estimation with a leave-one-out technique. To considerably reduce time cost in application, the Sherman-Morrison formula is exploited.

We are going to review these methods for estimating $\mathbb{E}(Y/X = x)$, when Y and X are supposed to be real random variable.

The local polynomial estimation [29] consists in approximating $m(x) = \mathbb{E}(Y/X = x)$ by a q^{th} -order polynomial fitted by a weight least squared estimation.

An explicit solution of $\hat{m}(x)$ is given by :

$$\hat{m}(x) = {}^t(1 \ 0 \ \dots \ 0)[{}^t\mathbb{X}(x)D(x)\mathbb{X}(x)]^{-1} \cdot {}^t\mathbb{X}(x)D(x)\mathbb{Y} \quad (36)$$

with

$$\mathbb{X}(x) = \begin{pmatrix} 1 & X_1 - x & \dots & (X_1 - x)^q \\ \vdots & \vdots & & \vdots \\ 1 & X_n - x & \dots & (X_n - x)^q \end{pmatrix} \quad D(x) = \begin{pmatrix} K\left(\frac{X_1 - x}{h}\right) & \dots & 0 \\ & \ddots & \\ 0 & \dots & K\left(\frac{X_n - x}{h}\right) \end{pmatrix}$$

$$\mathbb{Y} = \begin{pmatrix} Y_1 \\ \vdots \\ Y_n \end{pmatrix}$$

The leave-one-out technique on local estimation consists in estimating m in every observation point X_1, \dots, X_n , i.e. computing Equation (36) when the k^{th} line of matrices has been removed for estimating $\hat{m}(X_k)$. It means that we would need to inverse ${}^t\mathbb{X}_{-k}(x)D_{-k}(x)\mathbb{X}_{-k}(x)$ n times, which is very expensive. To avoid these expensive computations, Sherman and Morrison [30] proposed a formula :

Lemma 2. *If A is a square invertible matrix, and u, v are vectors such that $1 + {}^t v A^{-1} u \neq 0$, then*

$$(A + u {}^t v)^{-1} = A^{-1} - \frac{A^{-1} u {}^t v A^{-1}}{1 + {}^t v A^{-1} u} \quad (37)$$

In our problem, set $S_n(x) = {}^t\mathbb{X}(x)D(x)\mathbb{X}(x)$. $S_n(x)$ can be rewritten as :

$$S_n(x) = \sum_{i=1}^n \Phi_i(x) {}^t \Phi_i(x) = \underbrace{\sum_{i \neq k} \Phi_i(x) {}^t \Phi_i(x)}_{S_{-k}(x)} + \Phi_k(x) {}^t \Phi_k(x) \quad (38)$$

where

$$\Phi_i(x) = {}^t(K(\frac{X_i - x}{h})\mathbb{X}_i(x)), \quad \mathbb{X}_i(x) = (1 \dots (X_i - x)^q), \quad \forall i = 1, \dots, n$$

Thus, $S_{-k}(x)$, corresponding to ${}^t\mathbb{X}(x)D(x)\mathbb{X}(x)$ when the k^{th} line has been removed, is of the form :

$$S_{-k}(x) = S_n(x) - \Phi_k(x) {}^t \Phi_k(x), \quad \forall k = 1, \dots, n$$

The Sherman-Morrison formula gives :

$$S_{-k}^{-1}(x) = S_n^{-1}(x) + \frac{S_n^{-1}(x)\Phi_k(x)^t\Phi_k(x)S_n^{-1}(x)}{1 - {}^t\Phi_k(x)S_n^{-1}(x)\Phi_k(x)}, \quad \forall k = 1, \dots, n \quad (39)$$

As $\hat{m}(X_k) = {}^t(1 \ 0 \ \dots \ 0)S_{-k}^{-1}(X_k) \cdot {}^t\mathbb{X}_{-k}(X_k)D_{-k}(X_k)\mathbb{Y}$, $\forall k$, it is faster to estimate $S_n^{-1}(x)$ and $\Phi_k(x)$ at each point of the design.

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