Hoeffding decomposition of black-box models with dependent inputs

Marouane Il Idrissi, Nicolas Bousquet, Fabrice Gamboa, Bertrand Iooss, Jean-Michel Loubes

Hoeffding decomposition of black-box models with dependent inputs

Marouane Il Idrissi[a,b,c,e], Nicolas Bousquet[a,b,d], Fabrice Gamboa[c], Bertrand Iooss[a,b,c], Jean-Michel Loubes[c]

[a] *EDF Lab Chatou, 6 Quai Watier, 78401 Chatou, France*

[b] *SINCLAIR AI Laboratory, Saclay, France*

[c] *Institut de Mathématiques de Toulouse, 31062 Toulouse, France*

[d] *Sorbonne Université, LPSM, 4 place Jussieu, Paris, France*

[e] *Corresponding Author - Email: ilidrissi.m@gmail.com*

Abstract

One of the main challenges for interpreting black-box models is the ability to uniquely decompose square-integrable functions of non-independent random inputs into a sum of functions of every possible subset of variables. However, dealing with dependencies among inputs can be complicated. We propose a novel framework to study this problem, linking three domains of mathematics: probability theory, functional analysis, and combinatorics. We show that, under two reasonable assumptions on the inputs (non-perfect functional dependence and non-degenerate stochastic dependence), it is always possible to decompose such a function uniquely. This generalizes the well-known Hoeffding decomposition. The elements of this decomposition can be expressed using oblique projections and allow for novel interpretability indices for evaluation and variance decomposition purposes. The properties of these novel indices are studied and discussed. This generalization offers a path towards a more precise uncertainty quantification, which can benefit sensitivity analysis and interpretability studies whenever the inputs are dependent. This decomposition is illustrated analytically, and the challenges for adopting these results in practice are discussed.

Keywords: Hoeffding's decomposition ; oblique projection ; black-box model ; interpretability ; variance decomposition ; uncertainty quantification ; dependent inputs ; interaction effects

1. Introduction

When dealing with complex black-box models (e.g., predictive models, numerical simulation codes) with non-deterministic inputs, assessing the effects of the random nature of the inputs on the output is paramount in many studies. This general problem has broad application in many fields, such as sensitivity analysis (SA) [10] and explainability in artificial intelligence (XAI) [4]. In particular, in industrial practices (e.g., when dealing with critical systems), uncertainty quantification (UQ) enables the improvement of the studied phenomenon modeling process and can allow for scientific discoveries [14, 24].

One of the main challenges when it comes to UQ is to deal with dependent inputs [46]. The proposed methods usually assume mutual independence of the inputs [52, 38], either for the simplicity of the resulting estimation schemes or for the lack of a proper framework. However, the inputs are often endowed with a dependence structure intrinsic to the (observed or modeled) studied phenomena. Always assuming mutual independence can be seen as expedient and can lead to improper insights [25].

One classical way to assess the effects of input uncertainties is using functional decompositions, ob-

taining so-called *high-dimensional model representations* (HDMR) [44]. Formally, for random inputs $X = (X_1, \dots, X_d)^\top$, and an output $G(X)$, it amounts to finding the unique decomposition

$$G(X) = \sum_{A \in \mathcal{P}_D} G_A(X_A), \tag{1}$$

where $D = \{1, \dots, d\}$, $\mathcal{P}_D$ is the set of subsets of D, and $G_A(X_A)$ are functions of the subset of input $X_A = (X_i)_{i \in A}$. Whenever the X_i are assumed to be mutually independent, such a decomposition is known as *Hoeffding's decomposition*, due to his seminal work on the subject [26]. Whenever the inputs are not assumed to be mutually independent, many approaches have been proposed in the literature.

Notably, [25] proposed an approximation theoretic framework to address the problem and provides useful tools for importance quantification, but their approach lacks a proper and intuitive understanding of the quantities being estimated. On the one hand, in [7], the authors approached the problem differently and brought forward an intuitive view on the subject, but under very limiting assumptions on the probabilistic structure of the inputs. On the other hand, [27] and [33] proposed a projection-based approach under constraints derived from desirability criteria. [42] proposed a generalization under input exchangeability. However, these approaches do not offer completely satisfactory answers to uncertainty quantification with dependent inputs. Other approaches rely on transforming the dependent inputs to achieve mutual independence using, e.g., Nataf or Rosenblatt transforms [35, 36, 40]. While they offer seemingly meaningful indications, they do not quantify the effects due to the dependence.

To fill this gap, this article proposes a framework at the cornerstone of probability theory, functional analysis, and abstract algebra. By viewing random variables as measurable functions, we prove that a unique decomposition such as (1), for square-integrable black-box outputs $G(X)$, is indeed possible under two fairly reasonable assumptions on the inputs:

1. Non-perfect functional dependence;
2. Non-degenerate stochastic dependence.

To be more specific, denote σ_X the σ-algebra generated by X, and $\mathbb{L}^2(\sigma_X)$ the space of square-integrable σ_X-measurable real-valued functions (i.e., real-valued functions of X). From the proposed framework, defining a decomposition such as in (1) equates to defining a direct-sum decomposition of $\mathbb{L}^2(\sigma_X)$ of the form

$$\mathbb{L}^2(\sigma_X) = \bigoplus_{A \in \mathcal{P}_D} V_A,$$

where V_A are some linear vector subspaces of functions of X_A. We show that such a decomposition is achievable and we propose a complete characterization of the subspaces V_A. To the best of our knowledge, it offers a new way to approach multivariate dependence, relying on geometric considerations. We also show that Hoeffding's classical decomposition is a very special case of our framework.

Furthermore, we propose novel sensitivity indices based on this decomposition, along with theoretical arguments to justify their relevance. Notably, we show that the popular SHAP [38] method to decompose predictions is theoretically sound if and only if the inputs are mutually independent. Moreover, we propose four indices for quantifying the importance of inputs, based on the variance decomposition of $G(X)$. They allow the disentanglement of effects due to interactions and the effects due to the dependence structure.

This document is organized as follows. Section 2 is dedicated to introduce the overall framework, notations, and the required preliminaries. Section 3 is dedicated to the main result of this paper. Its proof is presented and discussed. In Section 4, some observations resulting from this novel decomposition are presented. Section 5 introduces novel decompositions for two quantities of interest: an evaluation of a model and its variance. The proposed indices are intuitive, disentangle interaction effects to effects due to the dependence, and allow for an original way of quantifying uncertainties. Section 6 is dedicated to the illustration of our result in the particular toy case of a model with two Bernoulli inputs. In

this illustration, the decomposition can be computed analytically, and the proposed indices also admit analytical formulas. Finally, Section 7 discusses the challenges for a broad acceptance of the proposed method in practice, as well as some motivating perspectives.

2. Framework and preliminaries

In the remainder of this document, the following notations are adopted. $\subset$ indicates a proper (strict) inclusion, while $\subseteq$ indicates a possible equality between sets. The positive integer d denotes the number of inputs (i.e., covariates), and $D := \{1, \ldots, d\}$. "Random element" is used if the domain of measurable functions is not necessarily $\mathbb{R}$ or $\mathbb{R}^d$. The term "random variables" is exclusive to *real-valued random elements*, and "random vector" is exclusive to a vector of random variables. Independence between random elements is denoted using $\perp\!\!\!\perp$. For a measurable space $(E, \mathcal{E})$ and $B \subset \mathcal{E}$, we denote by $\sigma[B]$ the smallest σ-algebra containing B. For a finite set, e.g., D, denote by $\mathcal{P}_D$ its power-set (i.e., the set of subsets of D, including D and $\emptyset$), and for any $A \in \mathcal{P}_D$, denote $\mathcal{P}_{-A} = \mathcal{P}_A \setminus \{A\}$ (i.e., the power-set of A without A). Depending on the context, when dealing with a set A, $|A|$ denotes its cardinality (i.e., the number of elements in A), while for a scalar $c \in \mathbb{R}$, $|c|$ denotes its absolute value.

2.1. General framework

2.1.1. Random inputs

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space, and let $(E_1, \mathcal{E}_1), \ldots, (E_d, \mathcal{E}_d)$ be a collection of standard Borel measurable spaces. For every $A \in \mathcal{P}_D, A \neq \emptyset$, denote:

$$E_A := \bigtimes_{i \in A} E_i, \quad \mathcal{E}_A := \bigotimes_{i \in A} \mathcal{E}_i,$$

where $\times$ denotes the Cartesian product between sets and $\otimes$ denotes the product of σ-algebras. Denote $E := E_D$ and $\mathcal{E} := \mathcal{E}_D$.

The *random inputs* are an E-valued, $(\mathcal{F})$-measurable mapping denoted $X = (X_1, \ldots, X_d)$. For every $A \subset D$, the E_A-valued random elements defined as $X_A := (X_i)_{i \in A}$ characterizes a *subset of the inputs*.

Denote by $\sigma_\emptyset$ the $\mathbb{P}$-trivial σ-algebra, i.e.,

$$\sigma_\emptyset := \sigma\left[\{A \in \mathcal{F} : \mathbb{P}(A) = 0\}\right]$$

i.e., the smallest σ-algebra containing every null sets of $\mathcal{F}$ w.r.t. $\mathbb{P}$. Denote by σ_X the σ-algebra generated by X. For every $A \in \mathcal{P}_D, A \notin \{\emptyset, D\}$, let σ_A be the σ-algebra generated by the subset of inputs X_A. For every $A \in \mathcal{P}_D, A \notin \{\emptyset, D\}$, denote by P_{X_A} the probability measure induced by X_A, and P_X the probability measure induced by X.

When it comes to random elements, especially when the very particular case of mutual independence is not assumed, one needs to restrict the inputs explicitly to avoid trivial situations (e.g., , constant a.s. inputs or redundancy). Throughout this paper, it is assumed that:

1. For every $i \in D$, $\sigma_\emptyset \subset \sigma_i$, i.e., the $\mathbb{P}$-trivial σ-algebra is strictly contained in the σ-algebras generated by individual inputs;
2. For every $A, B \in \mathcal{P}_D$ such that $B \subset A$, $\sigma_B \subset \sigma_A$, i.e., the σ-algebra generated by a subset of inputs is necessarily strictly contained in the σ-algebras generated by a bigger subset of inputs;

Remark 1. While (1.) is standard in many probabilistic theoretical frameworks (see, e.g., [51]), (2.) is less standard but remains reasonable. For instance, consider an example with three inputs. The fact that $\sigma_1 \subseteq \sigma_{12}$ comes naturally from the definition of generated σ-algebras. However, if one lets $\sigma_1 = \sigma_{12}$, that would entail that *every* σ_{12}-measurable random variable $f(X_1, X_2)$ can in fact be written as a function of only X_1, hence making the subset (X_1, X_2) "redundant" w.r.t. to X_1.

2.1.2. Space of square-integrable outputs and its subspaces

Denote $\mathbb{L}^2(\mathcal{F})$ the Lebesgue space of $\mathbb{R}$-valued square-integrable $\mathcal{F}$-measurable functions on $(\Omega, \mathcal{F}, \mathbb{P})$. For any sub σ-algebra $\mathcal{B} \subseteq \mathcal{F}$, denote $\mathbb{L}^2(\mathcal{B})$ the subspace of $\mathbb{L}^2(\mathcal{F})$ containing $\mathcal{B}$-measurable functions. $\mathbb{L}^2_0(\mathcal{B})$ denotes the subspace of centered elements of $\mathbb{L}^2(\mathcal{B})$.

These Lebesgue spaces show some intrinsic properties concerning the sub-σ-algebras they are defined on. First, recall the following well-known classical result [51, Theorem 2]:

Theorem 1. *For two sub σ-algebras $\mathcal{B}_1$ and $\mathcal{B}_2$ of $\mathcal{F}$, the following assertions hold.*

1. *If $\mathcal{B}_1 \subseteq \mathcal{B}_2$, then $\mathbb{L}^2(\mathcal{B}_1) \subseteq \mathbb{L}^2(\mathcal{B}_2)$.*
2. $\mathbb{L}^2(\mathcal{B}_1) \cap \mathbb{L}^2(\mathcal{B}_2) = \mathbb{L}^2(\mathcal{B}_1 \cap \mathcal{B}_2)$.

This article focuses on the Lebesgue space $\mathbb{L}^2(\sigma_X)$, i.e., the space of square-integrable, σ_X-measurable random variables. Recall that elements of $\mathbb{L}^2(\sigma_X)$ can *always be expressed as functions of* X, thanks to the Doob-Dynkin Lemma. Thus, in the following, $\mathbb{L}^2(\sigma_X)$ is referred to as the *output space*. Additionally, notice that $\mathbb{L}^2(\sigma_\emptyset)$ only contains constant a.s. functions [30, Lemma 4.9].

Notably, for every $A \in \mathcal{P}_{-D}$, the Hilbert space $\mathbb{L}^2(\sigma_A)$ is a *closed subspace of* $\mathbb{L}^2(\sigma_X)$ (due completeness). From Theorem 1, one can notice that the set of subspaces $\left\{\mathbb{L}^2(\sigma_A)\right\}_{A \in \mathcal{P}_D}$ are nested following the partial order of $\mathcal{P}_D$ (see Appendix Appendix A). In the following, for every $A \in \mathcal{P}_D$, the closed subspace $\mathbb{L}^2(\sigma_A)$ is referred to as *the Lebesgue space generated by* X_A.

The key point of the proposed approach is to study the relationships between these subspaces generated by the subsets of inputs. Studying different *angles between closed subspaces of a Hilbert space* offers relevant tools for this purpose.

2.2. Angles between subspaces

2.2.1. Dixmier's angle

Dixmier's angle [17] can be understood as the *minimal angle* between two closed subspaces of a Hilbert space. Its cosine is defined as follows.

Definition 1 (Dixmier's angle)**.** *Let H and K be closed subspaces of a Hilbert space $\mathcal{H}$ with inner product $\langle \cdot, \cdot \rangle$ and norm $\|\cdot\|$. The cosine of Dixmier's angle is defined as*

$$c_0(H, K) := \sup \left\{ |\langle x, y \rangle| : x \in H, \|x\| \leq 1, \quad y \in K, \|y\| \leq 1 \right\}.$$

Dixmier's angle can be understood as the smallest angle between two elements of the two closed subspaces (or limits of converging sequences of these elements). In probability theory, when applied to the Lebesgue spaces generated by two random elements, this angle is better known as the *maximal correlation*: a dependence measure between general random elements [23].Let Z_1 and Z_2 be two random elements, and denote σ_{Z_1} and σ_{Z_2} their generated σ-algebra. The *maximal correlation* between Z_1 and Z_2 is nothing more than the cosine of Dixmier's angle between $\mathbb{L}^2_0(\sigma_{Z_1})$ and $\mathbb{L}^2_0(\sigma_{Z_2})$, i.e., $c_0\left(\mathbb{L}^2_0(\sigma_{Z_1}), \mathbb{L}^2_0(\sigma_{Z_2})\right)$.

The maximal correlation has been extensively studied in the literature (see, e.g., [47, 31, 15, 11]). It also appears when studying the mixing properties of stochastic processes [18]. Obviously, we have:

$$c_0\left(\mathbb{L}^2_0(\sigma_{Z_1}), \mathbb{L}^2_0(\sigma_{Z_2})\right) = 0 \iff \mathbb{L}^2_0(\sigma_{Z_1}) \perp \mathbb{L}^2_0(\sigma_{Z_2}) \iff Z_1 \perp\!\!\!\perp Z_2,$$

where the independence is to be understood w.r.t. $\mathbb{P}$ (see [39, Chapter 3]).

2.2.2. Friedrichs' angle

Friedrichs' angle [21] differs from Dixmier's angle in one way: the intersection of the two subspaces is disregarded. It is defined as follows.

Definition 2 (Friedrichs' angle)**.** *Let H and K be closed subspaces of a Hilbert space $\mathcal{H}$ with inner product $\langle\cdot,\cdot\rangle$ and norm $\|\cdot\|$. The cosine of Friedrichs' angle is defined as*

$$c(H,K) := \sup\left\{ |\langle x,y\rangle| : \begin{cases} x \in H \cap (H\cap K)^{\perp}, \|x\| \leq 1 \\ y \in K \cap (H\cap K)^{\perp}, \|y\| \leq 1 \end{cases} \right\},$$

where the orthogonal complement is taken w.r.t. to $\mathcal{H}$.

In probability theory, this quantity is known as the maximal partial (or relative) correlation [5, 6, 12] between two random elements. It is suitable for deciphering conditional independence between σ-algebras. More precisely, it offers a sufficient and necessary condition for the commutativity of conditional expectations w.r.t. to those σ-algebras (see [30], Theorems 8.13 and 8.14).

Indeed, for a sub-sigma algebra $\mathcal{G} \subset \mathcal{F}$, denote $\mathbb{E}_{\mathcal{G}}$ the conditional expectation operator w.r.t. $\mathcal{G}$, then

$$c\left(\mathbb{L}_0^2(\sigma_{Z_1}), \mathbb{L}_0^2(\sigma_{Z_2})\right) = 0 \iff \mathbb{E}_{\sigma_{Z_1}} \circ \mathbb{E}_{\sigma_{Z_2}} = \mathbb{E}_{\sigma_{Z_2}} \circ \mathbb{E}_{\sigma_{Z_1}}. \tag{2}$$

Remark 2. In the remainder of this paper, for conciseness, any reference to Friedrichs' or Dixmier's angle refers to the *cosine of the angle* (taking values in $[0,1]$) instead of the angle itself (which takes its values in $[0,\pi/2]$).

2.2.3. Properties of Friedrichs' and Diximier's angles

Besides their links with probabilistic considerations, these angles are traditionally used in functional analysis as tools to assess the closedness of sums of closed subspaces of a Hilbert space. Some useful properties, relevant for proving our main result are displayed. The interested reader is referred to [16] for a more complete overview, as well as the proof of the results presented below.

Proposition 1 (Properties of Dixmier's angle)**.** *Let H, K be closed subspaces of a Hilbert space $\mathcal{H}$. Then, one has that $0 \leq c_0(H,K) = c_0(K,H) \leq 1$, and for any $x \in H$, and $y \in K$:*

$$|\langle x,y\rangle| \leq c_0(H,K)\,\|x\|\,\|y\|, \tag{3}$$

and for a proper closed subspace $\widetilde{H} \subset H$,

$$c_0\left(\widetilde{H},K\right) \leq c_0(H,K).$$

Moreover, the following statements are equivalent.

1. *$c_0(H,K) < 1$;*
2. *$H \cap K = \{0\}$ and $H + K$ is closed in $\mathcal{H}$.*

The previous result can be understood as follows. First, Dixmier's angle allows *to sharpen the Cauchy-Schwarz inequality* thanks to Eq. (3). For probabilistic considerations, this entails that the minimal angle between Lebesgue spaces (i.e., the maximal correlation) allows controlling the magnitude of the covariances between their elements. Moreover, whenever the angle is less than 1, the sum of the two subspaces is *closed*, and so their intersection reduces to $\{0\}$.

Proposition 2 (Properties of Friedrichs' angle)**.** *Let H, K be closed subspaces of a Hilbert space $\mathcal{H}$. Then, one has that*

$$0 \leq c(H,K) = c(K,H) \leq 1.$$

Notice that if $H \subseteq K$, then $c(H,K) = 0$. Moreover, the following statements are equivalent.

1. $c(H,K) < 1$;
2. $H + K$ *is closed in* $\mathcal{H}$.

For the purposes of this article, one property of Friedrichs' angle is of interest: whenever its value is less than 1, the sum of the two subspaces is *closed*. The closure of sums of subspaces plays a central part in the following developments.

These two angles are related, as highlighted by the following Lemma.

Lemma 1 (Relation between the two angles)**.** *Let* H, K *be closed subspaces of a Hilbert space* $\mathcal{H}$*. Then, one has that*

$$0 \leq c(H,K) \leq c_0(H,K) \leq 1.$$

Moreover, the following equality holds

$$c(H,K) = c_0\left(H \cap (H \cap K)^{\perp}, K\right) = c_0\left(H, K \cap (H \cap K)^{\perp}\right).$$

Furthermore, if $H \cap K = \{0\}$*, then* $c(H,K) = c_0(H,K)$*.*

2.2.4. Feshchenko matrix

As illustrated above, the maximal and partial correlation are good candidates to control the dependence structure of random elements. They can be understood as a generalization to random elements of the correlation and partial correlation of random variables. Hence, they offer a natural avenue for generalizing to the notion of *covariance and precision matrices*.

It is well-known that precision matrices (i.e., inverses of covariance matrices) can be written using partial correlations (see, e.g., [34, p.129]). Generalized precision matrices are not new. In the study of *graphical models*, generalized covariance and precision matrices have been used to study σ-algebras following a graph structure [37]. However, using Friedrichs' angle as a generalized partial correlation in such a setting does not seem to have been done yet in the probability theory literature.

We propose a novel generalization of precision matrices, called the *maximal coalitional precision matrix*. It is defined as follows.

Definition 3 (Maximal coalitional precision matrix)**.** *Let* $X = (X_1, \ldots, X_d)$ *be random inputs (i.e., a vector of random elements). The maximal coalitional precision matrix of* X *is the* $\left(2^d \times 2^d\right)$ *symmetric, set-indexed matrix* Δ*, defined entry-wise, for any* $A, B \in \mathcal{P}_D$*, by*

$$\Delta(A,B) = \begin{cases} 1 & \text{if } A = B; \\ -c\left(\mathbb{L}^2(\sigma_A), \mathbb{L}^2(\sigma_B)\right) & \text{otherwise.} \end{cases}$$

Moreover denote by $\Delta|_A$ *the principal* $\left(2^{|A|} - 1 \times 2^{|A|} - 1\right)$ *submatrix of* Δ *relative to the proper subsets of* $A \in \mathcal{P}_D$*.*

In the field of functional analysis, a similar type of matrix is used to derive a sufficient condition for sums of more than two closed subspaces of an abstract Hilbert space to be closed. The interested reader can refer to the pioneering works of Ivan Feshchenko [20, 19]. In the proof of our main theorem, this matrix is primarily used for that purpose. For conciseness, the matrix Δ defined in Definition 3 is referred to as the *Feshchenko matrix*.

One particular and interesting aspect of the Feshchenko matrix of a set of inputs is that *it is equal to the identity if and only if the inputs are mutually independent* (see Appendix Appendix C).

2.3. Closed subspaces, complements, and oblique projections

2.3.1. Closure and complement of a subspace

A closed proper subspace H of a Hilbert space $\mathcal{H}$ is always *complemented*, i.e., there exist some subspace K of $\mathcal{H}$ such that $\mathcal{H}$ admits the *direct-sum decomposition* (see Appendix Appendix B.1):

$$\mathcal{H} = H \oplus K.$$

For instance, the *orthogonal complement* $H^{\perp}$ (see, e.g., [49, Theorem 12.4]) of H in $\mathcal{H}$ is uniquely defined as

$$H^{\perp} := \{x \in \mathcal{H} : \langle x, y \rangle = 0, \quad \forall y \in H\}.$$

Additionally, orthogonal complements are always closed subspaces themselves. However, it is important to note that many other complements may exist for a single closed subspace.

For a subspace $H \subset \mathbb{L}^2(\sigma_B)$, denote by $H^{\perp_A}$ the *orthogonal complement of* H *in* $\mathbb{L}^2(\sigma_A)$. They have an interesting property:

Lemma 2. *Let $A, B \in \mathcal{P}_D$, such that $B \subseteq A$, and let H be a subspace of $\mathbb{L}^2(\sigma_B)$. Then*

$$H^{\perp_B} \subseteq H^{\perp_A}.$$

Proof of Lemma 2. From Theorem 1, one has that $\mathbb{L}^2(\sigma_B) \subseteq \mathbb{L}^2(\sigma_A)$. The result is a direct consequence of the definition of orthogonal complements. □

2.3.2. Oblique projections

For two Hilbert spaces $(\mathcal{M}_1, \|\cdot\|_1)$ and $(\mathcal{M}_2, \|\cdot\|_2)$, and a linear operator $T : \mathcal{M}_1 \to \mathcal{M}_2$ denote the range of T as

$$\mathrm{Ran}(T) := \{T(x) : x \in \mathcal{M}_1\} \subseteq \mathcal{M}_2,$$

and its nullspace as

$$\mathrm{Ker}(T) := \{x \in \mathcal{M}_1 : T(x) = 0\} \subseteq \mathcal{M}_1.$$

Let $\mathcal{H}$ be a Hilbert space and $P : \mathcal{H} \to \mathcal{H}$ be a bounded linear operator. If P is additionally idempotent (i.e., $P \circ P = P$), then $\mathcal{H}$ admits the direct sum decomposition $\mathcal{H} = \mathrm{Ran}(P) \oplus \mathrm{Ker}(P)$ (see [8, Proposition 3.2]). P is then called the oblique projector on $\mathrm{Ran}(P)$ parallel to $\mathrm{Ker}(P)$ and is defined as

$$\begin{aligned} P : \mathcal{H} = \mathrm{Ran}(P) \oplus \mathrm{Ker}(P) &\to \mathcal{H} \\ x = x_R + x_K &\mapsto x_R \end{aligned}$$

where $x_R \in \mathrm{Ran}(P)$ and $x_K \in \mathrm{Ker}(P)$. In this case, the operator $I - P$ is the oblique projection on $\mathrm{Ker}(P)$, parallel to $\mathrm{Ran}(P)$. On the other hand, if there are two closed subspaces M and N of a Hilbert space $\mathcal{H}$ such that $\mathcal{H} = M \oplus N$, then there exists a continuous idempotent operator (i.e., an oblique projector) P with range $\mathrm{Ran}(P) = M$ and $\mathrm{Ker}(P) = N$ (see [22, Theorem 7.90]). In this case, P is said to be the *canonical projector* (w.r.t. to the direct sum decomposition $\mathcal{H} = M \oplus N$).

If $\mathrm{Ker}(P) = \mathrm{Ran}(P)^{\perp}$, then the projection is said to be *orthogonal*, which is equivalent to P being self-adjoint (see [22, Theorem 7.71]). The direct-sum decomposition, in this case, is justified thanks to Hilbert's projection theorem.

It is well known that, for every $A \in \mathcal{P}_D$, one can consider the conditional expectation operators w.r.t. σ_A, denoted $\mathbb{E}_A[\cdot]$ as the *orthogonal projectors* of elements of $\mathbb{L}^2(\sigma_X)$ onto $\mathbb{L}^2(\sigma_A)$, parallel to $\mathbb{L}^2(\sigma_A)^{\perp}$.

3. Generalized Hoeffding decomposition

Being able to define a unique HDMR of a random output $G(X) \in \mathbb{L}^2(\sigma_X)$ can be seen as finding a direct-sum decomposition of $\mathbb{L}^2(\sigma_X)$. More precisely, it can be seen as expressing the direct-sum decomposition

$$\mathbb{L}^2(\sigma_X) = \bigoplus_{A \in \mathcal{P}_D} V_A,$$

where each V_A is a subspace of $\mathbb{L}^2(\sigma_A)$. By definition, such a decomposition entail that elements $G(X) \in \mathbb{L}^2(\sigma_X)$ can be uniquely decomposed as

$$G(X) = \sum_{A \in \mathcal{P}_D} G_A(X_A),$$

where $G_A(X_A) \in V_A$, which is reminiscent of Eq. (1).

This section shows that such a direct-sum decomposition is achievable under two reasonable assumptions on the inputs, which are less restrictive than mutual independence:

- Non-perfect functional dependence ;
- Non-degenerate stochastic dependence.

These two assumptions are introduced and discussed in the following, and then our main result is stated, proved, and discussed.

3.1. Assumptions

3.1.1. Non-perfect functional dependence

The first assumption can be formulated as a condition on the intersection of the σ-algebras generated by the subsets of inputs.

Assumption 1 (Non-perfect functional dependence). For any $A, B \in \mathcal{P}_D$,

$$\sigma_A \cap \sigma_B = \sigma_{A \cap B}$$

This restriction entails that "the subsets of inputs cannot be expressed as a function of other subsets", according to the following result.

Proposition 3. *Let $X = (X_1, \ldots, X_d)$ be inputs, and suppose that Assumption 1 holds. Then, for any $A, B \in \mathcal{P}_D$ such that $A \cap B \notin \{A, B\}$ (i.e., the sets cannot be subsets of each other), there is no mapping $T : E_A \to E_B$ such that $X_B = T(X_A)$ a.s.*

Proof of Proposition 3. Suppose that there exists a mapping $T : E_A \to E_B$ such that $X_B = T(X_A)$ a.s. Then, one has that $\sigma_B \subseteq \sigma_A$, which in turn implies that $\sigma_A \cap \sigma_B = \sigma_B$. Notice that necessarily $A \cap B \subset B$ and in the present framework $\sigma_{A \cap B} \subset \sigma_B$. Thus $\sigma_A \cap \sigma_B$ is necessarily different than $\sigma_{A \cap B}$, and thus Assumption 1 cannot hold. The result follows by taking the opposite implication. □

3.1.2. Non-degenerate stochastic dependence

The second assumption directly restricts the distribution of X through a condition on the *inner product of the Lebesgue space* $\mathbb{L}^2(\sigma_X)$. More precisely, it amounts to control the angles between the subspaces $\mathbb{L}^2(\sigma_A)$, $A \in \mathcal{P}_D$ using the Feshchenko matrix of the inputs X.

Assumption 2 (Non-degenerate stochastic dependence). The Feshchenko matrix Δ of X is positive definite.

Since Δ can be seen as a generalized precision matrix, this assumption is relatively reasonable since standard precision matrices are often assumed to be positive definite to ensure non-degeneracy of the probabilistic structure. One can notice that under this assumption, for any $A \in \mathcal{P}_D$, all the matrices $\Delta|_A$ are also positive definite. This assumption entails an interesting consequence regarding Friedrichs' angle between generated Lebesgue spaces.

Proposition 4. *Suppose that Assumption 2 hold. Then, for any $A, B \in \mathcal{P}_D$ such that $A \neq B$,*

$$c\left(\mathbb{L}^2\left(\sigma_A\right), \mathbb{L}^2\left(\sigma_B\right)\right) < 1.$$

Proof of Proposition 4. Suppose that Assumption 2 hold. Then, in particular, the principal submatrix of Δ

$$\begin{pmatrix} 1 & -c\left(\mathbb{L}^2\left(\sigma_A\right), \mathbb{L}^2\left(\sigma_B\right)\right) \\ -c\left(\mathbb{L}^2\left(\sigma_A\right), \mathbb{L}^2\left(\sigma_B\right)\right) & 1 \end{pmatrix}$$

is positive definite as well, and thus,

$$2 - 2c\left(\mathbb{L}^2\left(\sigma_A\right), \mathbb{L}^2\left(\sigma_B\right)\right) > 0 \quad \Longleftrightarrow \quad c\left(\mathbb{L}^2\left(\sigma_A\right), \mathbb{L}^2\left(\sigma_B\right)\right) < 1.$$

□

Thus, having a definite positive Feshchenko matrix entails that the maximal partial correlation between X_A and X_B is strictly less than 1 (i.e., the angle itself must be greater than zero).

3.2. Direct-sum decomposition of generated Lebesgue spaces

3.2.1. Statement

Our main result can be stated as follows.

Theorem 2 (Direct-sum decomposition of generated Lebesgue spaces)**.** *For every $A \in \mathcal{P}_D$, let $V_\emptyset = \mathbb{L}^2\left(\sigma_\emptyset\right)$ and for every $B \in \mathcal{P}_A$, let*

$$V_B = \left[\dotplus_{C \in \mathcal{P}_{-B}} V_C\right]^{\perp_B}.$$

If Assumptions 1 and 2 hold, then for every $A \in \mathcal{P}_D$, one has that

$$\mathbb{L}^2\left(\sigma_A\right) = \bigoplus_{B \in \mathcal{P}_A} V_B.$$

Then, the HDMR of a random output $G(X) \in \mathbb{L}^2\left(\sigma_X\right)$ follows directly as a corollary.

Corollary 1 (Orthocanonical decomposition)**.** *Let $X = (X_1, \ldots, X_d)$ be random inputs. Suppose that Assumptions 1 and 2 hold. Then, for any $G : E \to \mathbb{R}$ such that $G(X) \in \mathbb{L}^2\left(\sigma_X\right)$, $G(X)$ can be uniquely decomposed as*

$$G(X) = \sum_{A \in \mathcal{P}_D} G_A(X_A),$$

where each $G_A(X_A) \in V_A$.

Proof of Corollary 1. It is a direct consequence of Theorem 2. □

3.2.2. Proof of the main result

In order to prove Theorem 2, two preliminary results are required

Lemma 3. *Let $A \in \mathcal{P}_D$, and let $B, C \in \mathcal{P}_{-A}$ be non-empty proper subsets of A such that $B \neq C$. Let V_B, V_C be a closed subspace of $\mathbb{L}^2(\sigma_B)$ and $\mathbb{L}^2(\sigma_C)$ respectively. Suppose that Assumption 1 holds, and that*

$$V_B \subseteq \left[\mathbb{L}^2(\sigma_{B\cap C})\right]^{\perp}, \text{ and } V_C \subseteq \left[\mathbb{L}^2(\sigma_{B\cap C})\right]^{\perp}.$$

Then,

$$c_0(V_B, V_C) \leq c\left(\mathbb{L}^2(\sigma_B), \mathbb{L}^2(\sigma_C)\right).$$

Proof of Lemma 3. First, recall that, if Assumption 1 holds and thanks to Theorem 1

$$\mathbb{L}^2(\sigma_B) \cap \mathbb{L}^2(\sigma_C) = \mathbb{L}^2(\sigma_B \cap \sigma_C) = \mathbb{L}^2(\sigma_{B\cap C}).$$

Then, notice that since

$$V_B \subseteq \mathbb{L}^2(\sigma_B) \cap \left[\mathbb{L}^2(\sigma_{B\cap C})\right]^{\perp}, \quad \text{and } V_C \subseteq \mathbb{L}^2(\sigma_C) \cap \left[\mathbb{L}^2(\sigma_{B\cap C})\right]^{\perp},$$

one has that

$$\begin{aligned} c_0(V_B, V_C) &= c_0\left(\mathbb{L}^2(\sigma_B) \cap V_B, \mathbb{L}^2(\sigma_C) \cap V_C\right) \\ &\leq c_0\left(\mathbb{L}^2(\sigma_B) \cap \left[\mathbb{L}^2(\sigma_{B\cap C})\right]^{\perp}, \mathbb{L}^2(\sigma_C) \cap \left[\mathbb{L}^2(\sigma_{B\cap C})\right]^{\perp}\right). \end{aligned}$$

Hence, if Assumption 1 is assumed

$$\begin{aligned} c_0(V_B, V_C) &\leq c_0\left(\mathbb{L}^2(\sigma_B) \cap \left[\mathbb{L}^2(\sigma_B) \cap \mathbb{L}^2(\sigma_C)\right]^{\perp}, \mathbb{L}^2(\sigma_C) \cap \left[\mathbb{L}^2(\sigma_B) \cap \mathbb{L}^2(\sigma_C)\right]^{\perp}\right) \\ &= c\left(\mathbb{L}^2(\sigma_B), \mathbb{L}^2(\sigma_C)\right) \end{aligned}$$

where the last equality is achieved using Lemma 1. □

Lemma 4. *Let $A \in \mathcal{P}_D$, and let $(V_B)_{B\in\mathcal{P}_A, B\neq A}$ be a collection of closed subspaces of $\mathbb{L}^2(\sigma_A)$ such that, $\forall B, C \in \mathcal{P}_{-A}, B \neq C$,*

$$c_0(V_B, V_C) \leq c\left(\mathbb{L}^2(\sigma_B), \mathbb{L}^2(\sigma_C)\right).$$

Then, under Assumption 2, there exist a $\rho > 0$ such that, for any $\sum_{A\in\mathcal{P}_{-A}} Y_A \in +_{B\in\mathcal{P}_{-A}} V_B$

$$\sqrt{\mathbb{E}\left[\left(\sum_{B\in\mathcal{P}_{-A}} Y_A\right)^2\right]} \geq \rho \sum_{B\in\mathcal{P}_{-A}} \sqrt{\mathbb{E}\left[Y_A^2\right]},$$

and additionally, the sum of subspaces $+_{B\in\mathcal{P}_{-A}} V_B$ is closed in $\mathbb{L}^2(\sigma_A)$.

Proof of Lemma 4. Let $H_A = \bigoplus_{B\in\mathcal{P}_A: B\neq A} V_A$ be the Hilbert space external direct-sum (see Appendix Appendix B.2) of the collection of closed (and thus Hilbert) subspaces $(V_B)_{B\in\mathcal{P}_A, B\neq A}$. Let T_A be the operator defined as

$$\begin{aligned} T_A : H_A &\to \mathbb{L}^2(\sigma_A) \\ Y = (Y_B)_{B\in\mathcal{P}_{-A}} &\mapsto \sum_{B\in\mathcal{P}_{-A}} Y_B \end{aligned}$$

and notice that

$$\mathrm{Ran}\left(T_A\right) = \mathop{+}_{B\in\mathcal{P}_{-A}} V_B \subseteq \mathbb{L}^2\left(\sigma_A\right).$$

One then has that

$$\begin{aligned}
\mathbb{E}\left[\left(\sum_{B\in\mathcal{P}_{-A}} Y_B\right)^2\right] &= \sum_{B\in\mathcal{P}_{-A}} \mathbb{E}\left[Y_B^2\right] + \sum_{B,C\in\mathcal{P}_{-A}:B\neq C} \mathbb{E}\left[Y_A Y_B\right] \\
&\geq \sum_{B\in\mathcal{P}_{-A}} \mathbb{E}\left[Y_B^2\right] - \sum_{B,C\in\mathcal{P}_{-A}:B\neq C} c_0\left(V_A, V_B\right)\sqrt{\mathbb{E}\left[Y_A^2\right]}\sqrt{\mathbb{E}\left[Y_B^2\right]} \\
&\geq \sum_{B\in\mathcal{P}_{-A}} \mathbb{E}\left[Y_B^2\right] - \sum_{B,C\in\mathcal{P}_{-A}:B\neq C} c\left(\mathbb{L}^2\left(\sigma_A\right), \mathbb{L}^2\left(\sigma_B\right)\right)\sqrt{\mathbb{E}\left[Y_A^2\right]}\sqrt{\mathbb{E}\left[Y_B^2\right]}
\end{aligned}$$

where the first inequality is achieved thanks to Proposition 1. Denote $E_A = \left(\sqrt{\mathbb{E}\left[Y_B^2\right]}\right)_{B\in\mathcal{P}_{-A}}$ and notice that

$$\sum_{B\in\mathcal{P}_{-A}} \mathbb{E}\left[Y_B^2\right] - \sum_{B,C\in\mathcal{P}_{-A}:B\neq C} c\left(\mathbb{L}^2\left(\sigma_A\right), \mathbb{L}^2\left(\sigma_B\right)\right)\sqrt{\mathbb{E}\left[Y_A^2\right]}\sqrt{\mathbb{E}\left[Y_B^2\right]} = E_A^\top \Delta|_A E_A$$

Denote λ_A the smallest eigenvalue of $\Delta|_A$, and notice that if Assumption 2 holds, $\Delta|_A$ is definite positive and $\lambda_A > 0$. Thus, one has that

$$\begin{aligned}
E_A^\top \Delta|_A E_A &\geq \lambda_A E_A^\top E_A \\
&= \lambda_A \sum_{B\in\mathcal{P}_{-A}} \mathbb{E}\left[Y_A^2\right].
\end{aligned}$$

Hence, one has that

$$\begin{aligned}
\sqrt{\mathbb{E}\left[\left(\sum_{B\in\mathcal{P}_{-A}} Y_B\right)^2\right]} &\geq \sqrt{\lambda_A \sum_{B\in\mathcal{P}_{-A}} \mathbb{E}\left[Y_A^2\right]} \\
&\geq \sqrt{\frac{\lambda_A}{2^d-1}} \sum_{B\in\mathcal{P}_{-A}} \sqrt{\mathbb{E}\left[Y_A^2\right]}
\end{aligned}$$

where the last inequality is achieved using Jensen's inequality. Hence, one has that, for any $Y \in H_A$

$$\sqrt{\mathbb{E}\left[T_A(Y)^2\right]} \geq \sqrt{\frac{\lambda_A}{2^d-1}} \sum_{B\in\mathcal{P}_{-A}} \sqrt{\mathbb{E}\left[Y_A^2\right]}$$

where $\sqrt{\frac{\lambda_A}{2^d-1}} > 0$, and $\sum_{B\in\mathcal{P}_A} \sqrt{\mathbb{E}\left[Y_A^2\right]}$ is the norm of Y on H_A. Hence, by the closed ranged operator theorem (see [1, Theorem 2.5]),

$$\mathrm{Ran}\left(T_A\right) = \mathop{+}_{B\in\mathcal{P}_{-A}} V_B \text{ is closed in } \mathbb{L}^2\left(\sigma_A\right).$$

□

We can now proceed with the proof of Theorem 2.

Proof of Theorem 2. The proof is done in two steps. First, we prove by induction that, $\forall A \in \mathcal{P}_D$

$$\mathbb{L}^2(\sigma_A) = \bigdotplus_{C \in \mathcal{P}_A} V_C,$$

and then we show that this sum of subspaces is direct. The induction is done on the number of inputs up to d.

Statement. Let $n = 1, \dots, d-1$. We will show that if for every non-empty $B \in \mathcal{P}_D$, B such that $|B| = n$, one has that

$$\mathbb{L}^2(\sigma_C) = \bigdotplus_{Z \in \mathcal{P}_C} V_Z \quad \text{where} \quad V_C = \left[\bigdotplus_{Z \in \mathcal{P}_{-C}} V_Z \right]^{\perp_C}.$$

In this case, it follows that for every $A \in \mathcal{P}_D$ such that $|A| = n+1$,

$$\mathbb{L}^2(\sigma_A) = \bigdotplus_{C \in \mathcal{P}_A} V_C \quad \text{where} \quad V_A = \left[\bigdotplus_{Z \in \mathcal{P}_{-A}} V_Z \right]^{\perp_A}.$$

The induction is made on the passage from n to $n+1$.

Base case. We start for $n = 1$. For any $i \in D$, denote $V_i = [V_\emptyset]^{\perp_i}$, and notice that since $V_\emptyset$ is closed in $\mathbb{L}^2(\sigma_i)$

$$\mathbb{L}^2(\sigma_i) = V_\emptyset \oplus V_i.$$

and notice that $\forall i \in D$,

$$V_i = \left[\mathbb{L}^2(\sigma_\emptyset)\right]^{\perp_i} \subseteq \left[\mathbb{L}^2(\sigma_\emptyset)\right]^{\perp},$$

by Lemma 2.

Next, consider the case where $n = 2$. Notice from the previous step that for any $i, j \in D$ such that $i \neq j$, notice that $\mathbb{L}^2(\sigma_{i \cap j}) = \mathbb{L}^2(\sigma_\emptyset)$, and thus one has that

$$V_i \subset \left[\mathbb{L}^2(\sigma_\emptyset)\right]^{\perp} \text{ and } V_j \subset \left[\mathbb{L}^2(\sigma_\emptyset)\right]^{\perp}.$$

Hence, assuming that Assumption 1 hold, from Lemma 3, one can conclude that, for any $i, j \in D$ such that $i \neq j$,

$$c_0(V_i, V_j) \leq c\left(\mathbb{L}^2(\sigma_i), \mathbb{L}^2(\sigma_j)\right).$$

Now, let $A \in \mathcal{P}_D$ such that $|A| = 2$, and denote $A = \{i, j\}$, and notice that, under Assumption 2, by Lemma 4, one has that

$$V_\emptyset + V_i + V_j \text{ is closed in } \mathbb{L}^2(\sigma_A).$$

Hence, let

$$V_A = [V_\emptyset + V_i + V_j]^{\perp_A},$$

and notice that

$$\mathbb{L}^2(\sigma_A) = [V_\emptyset + V_i + V_j] \oplus V_A.$$

Since i and j have been chosen arbitrarily, this holds for any $A \in \mathcal{P}_D$ such that $|A| = 2$.

Induction. Suppose that, for every $B \in \mathcal{P}_D$ such that $|B| = n$, one has that

$$\mathbb{L}^2(\sigma_B) = \mathop{+}_{Z \in \mathcal{P}_B} V_Z, \text{ where } V_B = \left[\mathop{+}_{Z \in \mathcal{P}_{-B}} V_Z \right]^{\perp_B}.$$

Let $A \in \mathcal{P}_D$ such that $|A| = n+1$. Notice then that, for any non-empty $B, C \in \mathcal{P}_{-A}$, since $B \cap C \in \mathcal{P}_{-B} \cap \mathcal{P}_{-C}$, that

$$\mathbb{L}^2(\sigma_{B\cap C}) = \mathop{+}_{Z \in \mathcal{P}_{B\cap C}} V_Z,$$

is necessarily contained of $+_{Z\in\mathcal{P}_{-B}} V_Z$ and of $+_{Z\in\mathcal{P}_{-C}} V_Z$. Thus, one has that

$$V_B = \left[\mathop{+}_{Z \in \mathcal{P}_{-B}} V_Z \right]^{\perp_B} \subset \left[\mathop{+}_{Z \in \mathcal{P}_{-B}} V_Z \right]^{\perp} \subset \left[\mathbb{L}^2(\sigma_{B\cap C})\right]^{\perp}.$$

and analogously

$$V_C \subset \left[\mathbb{L}^2(\sigma_{B\cap C})\right]^{\perp}.$$

Hence, assuming that Assumption 1 hold, from Lemma 3, one can conclude that, for every non-empty $B, C \in \mathcal{P}_{-A}$ such that $B \neq C$,

$$c_0(V_B, V_C) \leq c\left(\mathbb{L}^2(\sigma_B), \mathbb{L}^2(\sigma_C)\right),$$

which, under Assumption 2 and thanks to Lemma 4, implies that $+_{Z\in\mathcal{P}_{-A}} V_Z$ is closed in $\mathbb{L}^2(\sigma_A)$. Denote $V_A = \left[+_{Z\in\mathcal{P}_{-A}} V_Z\right]^{\perp_A}$, and notice that

$$\mathbb{L}^2(\sigma_A) = \left[\mathop{+}_{Z \in \mathcal{P}_{-A}} V_Z \right] \oplus V_A = \mathop{+}_{Z \in \mathcal{P}_A} V_Z.$$

Since A has been taken arbitrarily, this holds for any $A \in \mathcal{P}_D$ such that $|A| = n$.

Now, we show that these decompositions are direct. Let $A \in \mathcal{P}_D$, and notice that for any non-empty $\forall B \in \mathcal{P}_A$, $V_B \perp \mathbb{L}^2(\sigma_\emptyset)$, meaning that any $f(X_B) \in V_B$ is centered. Next, notice that the principal $\left(2^{|A|} \times 2^{|A|}\right)$ submatrix of Δ, indexed by the elements of $\mathcal{P}_A$ and denoted Δ_A, is also definite-positive, and hence its smallest eigenvalue λ_A is positive. Notice further that for any $Y \in \mathbb{L}^2(\sigma_A)$, by definition, one has that:

$$Y = \sum_{B \in \mathcal{P}_A} Y_B, \quad \text{where } Y_B \in V_B.$$

Now, suppose that $Y = 0$ a.s., which is equivalent to $\mathbb{E}[Y] = 0$ and $\mathbb{E}\left[Y^2\right] = 0$. However, under Assumptions 1 and 2, notice that

$$\begin{aligned}
\mathbb{E}\left[Y^2\right] &= \mathbb{E}\left[\left(\sum_{B\in\mathcal{P}_A} Y_B\right)^2\right] \\
&= \sum_{B\in\mathcal{P}_A} \mathbb{E}\left[Y_B^2\right] + \sum_{B,C\in\mathcal{P}_A : B\neq C} \mathbb{E}\left[Y_B Y_C\right] \\
&\geq \sum_{B\in\mathcal{P}_A} \mathbb{E}\left[Y_B^2\right] - \sum_{B,C\in\mathcal{P}_A : B\neq C} c_0(V_B, V_C) \sqrt{\mathbb{E}\left[Y_B^2\right]}\sqrt{\mathbb{E}\left[Y_C^2\right]} \\
&\geq \sum_{B\in\mathcal{P}_A} \mathbb{E}\left[Y_B^2\right] - \sum_{B,C\in\mathcal{P}_A : B\neq C} c\left(\mathbb{L}^2(\sigma_B), \mathbb{L}^2(\sigma_C)\right) \sqrt{\mathbb{E}\left[Y_B^2\right]}\sqrt{\mathbb{E}\left[Y_C^2\right]}
\end{aligned}$$

Let $E_A = \left(\sqrt{\mathbb{E}\left[Y_B^2\right]}\right)_{B\in\mathcal{P}_A}^{\top}$ and notice that

$$\mathbb{E}\left[Y^2\right] \geq E_A^{\top}\Delta_A E_A \geq \lambda_A E_A^{\top} E_A = \lambda_A \sum_{B\in\mathcal{P}_A} \mathbb{E}\left[Y_B^2\right]$$

since Δ_A is definite positive, and $\lambda_A > 0$ is its smallest eigenvalue. Thus, one has that if $\mathbb{E}\left[Y^2\right] = 0$, then necessarily

$$\sum_{B\in\mathcal{P}_A} \mathbb{E}\left[Y_B^2\right] = 0,$$

and since this is a sum of positive elements, $\forall B \in \mathcal{P}_A$, $\mathbb{E}\left[Y_B^2\right] = 0$. In addition to the fact that each Y_B is centered, it is equivalent to every the summand Y_B being equal to 0 a.s. Hence,

$$Y = 0 \text{ a.s.} \implies \forall B \in \mathcal{P}_D, \quad Y_B = 0 \text{ a.s.}$$

which ultimately proves that

$$\mathbb{L}^2(\sigma_A) = \bigoplus_{B\in\mathcal{P}_A} V_B.$$

□

4. Some observations

Two main observations are discussed in this section. First, the "hierarchical orthogonality" structure that naturally arises from the orthocanonical decomposition developed above. Then, we leverage canonical projections due to the direct-sum decomposition of Theorem 2 to characterize the elements of the decomposition and we present some of their properties.

4.1. Hierarchical orthogonality

The set of subspaces $(V_A)_{A\in\mathcal{P}_D}$ benefit of a particular orthogonality structure, namely *hierarchical orthogonality*, reminiscent of the one described in [7].

Proposition 5 (Hierarchical orthogonality)**.** *We place ourselves in the framework of Theorem 2. For any $A \in \mathcal{P}_D$, and any $B \subset A$,*

$$V_A \perp V_B.$$

Proof of Proposition 5. It is a direct consequence of the definition of V_A. □

This particular structure can be illustrated using the Boolean lattice [13]. In order to formally differentiate between the structurally hierarchical subspaces and those that are not necessarily orthogonal, two different sets related to this structure are introduced. For any $A \in \mathcal{P}_D$, the first one is the set of *comparables* (i.e., the elements of $\mathcal{P}_D$ that are subsets of A or such that A is a subset of), denoted

$$\mathcal{C}_A = \mathcal{P}_A \cup \{B \in \mathcal{P}_D : A \subseteq D\},$$

and notice that, for any $B \in \mathcal{C}_A$, $V_B \perp V_A$. Then, we define the set of *uncomparables* of A as

$$\mathcal{U}_A = \mathcal{P}_D \setminus \mathcal{C}_A,$$

and notice that, in general, for every $B \in \mathcal{U}_A$, V_A is not necessarily orthogonal to V_B. And notice additionally that, for any $A \in \mathcal{P}_D$

$$\mathcal{P}_D = \mathcal{C}_A \cup \mathcal{U}_A.$$

Remark 3. It is important to note that the hierarchical orthogonality of the subspaces $(V_A)_{A\in\mathcal{P}_D}$ is a consequence of the *choice of inductively choosing orthogonal complements* in Theorem 2. Other complements, i.e., not necessarily orthogonal, could have been chosen, leading to a different structure. This is why the output decomposition in Corollary 1 is called "orthocanonical". A different choice of complements could lead to a different decomposition.

4.2. Canonical oblique projections and their properties

Two different projectors onto the subspaces V_A ($A \in \mathcal{P}_D$), can be defined. Let A be any element of $\mathcal{P}_D$. Denote by P_A the orthogonal projector onto V_A, i.e., ,

$$P_A : \mathbb{L}^2(\sigma_X) \to \mathbb{L}^2(\sigma_X), \quad \text{such that } \mathrm{Ran}(P_A) = V_A \text{ and } \mathrm{Ker}(P_A) = V_A^{\perp}.$$

Additionally, for every $A \in \mathcal{P}_D$, denote the following subspaces of $\mathbb{L}^2(\sigma_X)$

$$W_A = \bigoplus_{B\in\mathcal{P}_D : B\neq A} V_B,$$

and the operators

$$\begin{aligned} Q_A : \mathbb{L}^2(\sigma_X) &\to \mathbb{L}^2(\sigma_X) \\ G(X) = \sum_{B\in\mathcal{P}_D} G_B(X_B) &\mapsto G_A(X_A) \end{aligned}$$

and notice that Q_A is the projector onto V_A parallel to W_A, which is well-defined thanks to the direct-sum decomposition of Theorem 2 (see [45, Theorem 3.4]). For any $A \in \mathcal{P}_D$, the operators $P_A(\cdot)$ and $Q_A(\cdot)$ are both projectors onto V_A, but their nullspaces differ.

Now, we define the orthogonal projector onto $\mathbb{L}^2(\sigma_A)$, as

$$\mathbb{E}_A : \mathbb{L}^2(\sigma_X) \to \mathbb{L}^2(\sigma_X), \quad \text{such that } \mathrm{Ran}(\mathbb{E}_A) = \mathbb{L}^2(\sigma_A) \text{ and } \mathrm{Ker}(P_A) = \mathbb{L}^2(\sigma_A)^{\perp},$$

and notice, as mentioned before, that it is the conditional expectation operator of $H(X)$ given X_A (see [30, Chapter 8]). Additionally, denote the subspace

$$\widetilde{W}_A = \bigoplus_{B\in\mathcal{P}_D, B\notin\mathcal{P}_A} V_B$$

and the operator

$$\begin{aligned} \mathbb{M}_A : \mathbb{L}^2(\sigma_X) &\to \mathbb{L}^2(\sigma_X) \\ G(X) = \sum_{B\in\mathcal{P}_D} G_B(X_B) &\mapsto \sum_{B\in\mathcal{P}_A} G_B(X_B). \end{aligned}$$

Thanks to Theorem 2, notice that $\mathbb{M}_A$ is the projection onto $\mathrm{Ran}(\mathbb{M}_A) = \mathbb{L}^2(\sigma_A)$ parallel to $\mathrm{Ker}(\mathbb{M}_A) = \widetilde{W}_A$. For any $A \in \mathcal{P}_D$, the operators $\mathbb{E}_A[\cdot]$ and $\mathbb{M}_A[\cdot]$ are two projections onto $\mathbb{L}^2(\sigma_A)$, but with different nullspaces.

The first result is a particular consequence of the hierarchical orthogonality structure, known as the *annihilating property* (see, e.g., [27, Lemma 1] or [33]). This property admits a generalization in the framework of Theorem 2.

Proposition 6 (Annihilating property)**.** *We place ourselves in the framework of Theorem 2 and Corollary 1. For any $A \in \mathcal{P}_D$ and any $B \subset A$,*

$$P_B(Q_A(G(X))) = P_B(G_A(X_A)) = 0.$$

Proof of Proposition 6. From Proposition 5, for every $B \subset A$, one has that $V_B \perp V_A$, and thus $G_A(X_A) \in V_A \subset V_B^{\perp}$. □

Another interesting result is the fact that the oblique projections $(Q_A)_{A\in\mathcal{P}_D}$ onto the V_A can be expressed in terms of the oblique projections $(\mathbb{M}_A)_{A\in\mathcal{P}_D}$ onto the generated Lebesgue spaces.

Proposition 7 (Formula for oblique projections)**.** *We place ourselves in the framework of Theorem 2 and Corollary 1. One has that, for any $G(X) \in \mathbb{L}^2(\sigma_X)$, and for any $A \in \mathcal{P}_D$*

$$Q_A(G(X)) = \sum_{B\in\mathcal{P}_A} (-1)^{|A|-|B|}\mathbb{M}_A(G(X)).$$

Proof of Proposition 7. By definition of $\mathbb{M}_A$, one has that

$$\forall A \in \mathcal{P}_D, \quad \mathbb{M}_A(G(X)) = \sum_{B\in\mathcal{P}_A} Q_A(G(X)),$$

which, thanks to Rota's generalization of the Möbius inversion formula [48, 28], is equivalent to

$$\forall A \in \mathcal{P}_D, \quad Q_A(G(X)) = \sum_{B\in\mathcal{P}_A} (-1)^{|A|-|B|}\mathbb{M}_A(G(X)).$$

□

5. Sensitivity analyses with dependent inputs

This section is dedicated to introduce the notion of *orthocanonical decompositions of quantities of interest (QoIs)* by leveraging the decomposition offered in Theorem 2. In particular, two QoI decompositions are presented: the decomposition of an evaluation of the model and the decomposition of its variance.

5.1. Orthocanonical evaluation decomposition

For $\omega \in \Omega$, denote $x = X(\omega) \in E$ a realisation of X. Subsequently, denote $G(x) \in \mathbb{R}$ the evaluation on x of a random output $G(X) \in \mathbb{L}^2(\sigma_X)$. In the XAI literature, "explanation" methods aim at decomposing $G(x)$ into parts for which each input is responsible [4]. They often rely on cooperative game theory, particularly on the Shapley values [50], an allocation with seemingly reasonable properties [38]. However, allocations can be understood as aggregations of coalitional decompositions [28], which can be trivially chosen. However, Theorem 2, and in particular Corollary 1 offers an orthocanonical approach.

Definition 4 (Orthocanonical decomposition of an evaluation)**.** *Let $X = (X_1, \dots, X_d)$ be a vector of random elements, let $G(X)$ be in $\mathbb{L}^2(\sigma_X)$ and assume that Assumptions 1 and 2 hold. For any $\omega \in \Omega$, denote $x = X(\omega)$. The orthocanonical coalitional decomposition of the evaluation $G(x)$ is defined as*

$$G(x) = \sum_{A\in\mathcal{P}_D} G_A(x_A),$$

where $x_A = X_A(\omega)$, and

$$G_A(x_A) = Q_A(G(x)) = \sum_{B\in\mathcal{P}_A} (-1)^{|A|-|B|}\mathbb{M}_B(G(x)),$$

where Q_A is the projection onto V_A parallel to W_A and $\mathbb{M}_A$ is the projection onto $\mathbb{L}^2(\sigma_A)$ parallel to $\widetilde{W}_A$.

The usual coalitional decomposition of choice, even for dependent inputs, relies on choosing conditional expectations (also known as "conditional Shapley values") [38]. However, the following results show that this choice entails a canonical decomposition if and only if the inputs are mutually independent.

Proposition 8. *Let $X = (X_1, \dots, X_d)$ be a vector of random elements, let $G(X)$ be in $\mathbb{L}^2(\sigma_X)$, and assume that Assumptions 1 and 2 hold. Then,*

$$G_A(x_A) = \sum_{B \in \mathcal{P}_A} (-1)^{|A|-|B|} \mathbb{E}_B\left(G(x)\right), \quad \forall A \in \mathcal{P}_D$$

if and only if X is mutually independent.

Proof of Proposition 8. First, notice that $\mathbb{M}_A = \mathbb{E}_A$ if and only if $\widetilde{W}_A$ is the orthogonal complement of $\mathbb{L}^2(\sigma_A)$. One can notice that, $\widetilde{W}_A$ is a complement of $\mathbb{L}^2(\sigma_A)$ in $\mathbb{L}^2(\sigma_X)$, and from Proposition 14, one has that

$$\mathbb{L}^2(\sigma_A) = \bigoplus_{B \in \mathcal{P}_A} V_B \perp \widetilde{W}_A = \bigoplus_{B \in \mathcal{P}_D, B \notin \mathcal{P}_A} V_B,$$

holds for every $A \in \mathcal{P}_D$ if and only if X is mutually independent. In this case, $\widetilde{W}_A$ is an orthogonal complement of $\mathbb{L}^2(\sigma_A)$, and by uniqueness, $\widetilde{W}_A = \mathbb{L}^2(\sigma_A)^\perp$, and thus $\mathbb{M}_A = \mathbb{E}_A$. □

5.2. Variance decomposition

Performing a variance decomposition of a black-box model is paramount in quantifying a set of inputs' importance towards a multivariate model [10]. Let $G(X)$ be a random output and denote its variance

$$\mathbb{V}\left(G(X)\right) = \mathbb{E}\left[\left(G(X) - \mathbb{E}\left[G(X)\right]\right)^2\right] = \mathbb{E}\left[G(X)^2\right] - \mathbb{E}\left[G(X)\right]^2.$$

We propose two ways to approach the problem of decomposing $\mathbb{V}\left(G(X)\right)$. The *orthocanonical variance decomposition* relies on the decomposition of $G(X)$ offered by Corollary 1. In contrast, the *organic variance decomposition* aims at defining and disentangling *pure interaction effects* from *dependence effects*.

5.2.1. Orthocanonical variance decomposition

In light of Corollary 1, the orthocanonical variance decomposition of $G(X)$ is rather intuitive. It relies on the following rationale:

$$\begin{aligned}
\mathbb{V}\left(G(X)\right) &= \mathrm{Cov}\left(G(X), G(X)\right) \\
&= \sum_{A \in \mathcal{P}_D} \mathrm{Cov}\left(G_A(X_A), G(X)\right) \\
&= \sum_{A \in \mathcal{P}_D} \left[\mathbb{V}\left(G_A(X_A)\right) + \sum_{B \in \mathcal{U}_A} \mathrm{Cov}\left(G_A(X_A), G_B(X_B)\right)\right].
\end{aligned}$$

reminiscent of the "covariance decomposition" [53, 7, 25, 10]. Two indices arise from this decomposition.

Definition 5 (Orthocanonical variance decomposition)**.** *We place ourselves in the framework of Theorem 2. For any $A \in \mathcal{P}_D$, let*

$$S_A^U = \mathbb{V}\left(G_A(X_A)\right),$$

defines the structural contribution of X_A to $G(X)$*, while*

$$S_A^C = \sum_{B \in \mathcal{U}_A} Cov\left(G_A(X_A), G_B(X_B)\right),$$

represents the correlative contribution of X_A to $G(X)$.

The orthocanonical decomposition of $\mathbb{V}(G(X))$ is suitable in practice if the dependence structure of X is assumed to be inherent in the modeling of the studied phenomenon. These indices can be expressed using the oblique projections $\{\mathbb{M}_A\}_{A\in\mathcal{P}_D}$ onto the subspaces $\left\{\mathbb{L}^2(\sigma_A)\right\}_{A\in\mathcal{P}_D}$.

Proposition 9. *We place ourselves in the framework of Theorem 2. Then, for any $A \in \mathcal{P}_D$*

$$S_A^C = \sum_{B\in\mathcal{P}_A} (-1)^{|A|-|B|} Cov\left(\mathbb{M}_B(G(X)), [I-\mathbb{M}_A](G(X))\right).$$

Proof of Proposition 9. First, recall that, for any $A \in \mathcal{P}_D$,

$$G_A(X_A) = \sum_{B\in\mathcal{P}_A} (-1)^{|A|-|B|}\mathbb{M}_B(G(X)),$$

and hence,

$$\begin{aligned}\sum_{B\in\mathcal{P}_A} (-1)^{|A|-|B|}\mathrm{Cov}\left(\mathbb{M}_B(G(X)), [I-\mathbb{M}_A](G(X))\right) &= \mathrm{Cov}\left(G_A(X_A), [I-\mathbb{M}_A](G(X))\right)\\ &= \sum_{B\in\mathcal{P}_D:B\notin\mathcal{P}_A} \mathrm{Cov}\left(G_A(X_A), G_B(X_B)\right).\end{aligned}$$

However, notice that $\mathcal{U}_A \subset \mathcal{P}_D \setminus \mathcal{P}_A$, and that, for any $B \in \mathcal{P}_D \setminus \mathcal{P}_A$ with $B \notin \mathcal{U}_A$,

$$\mathrm{Cov}\left(G_A(X_A), G_B(X_B)\right) = 0,$$

and hence,

$$\begin{aligned}\sum_{B\in\mathcal{P}_A} (-1)^{|A|-|B|}\mathrm{Cov}\left(\mathbb{M}_B(G(X)), [I-\mathbb{M}_A](G(X))\right) &= \sum_{B\in\mathcal{P}_D:B\notin\mathcal{P}_A} \mathrm{Cov}\left(G_A(X_A), G_B(X_B)\right)\\ &= \sum_{B\in\mathcal{U}_A} \mathrm{Cov}\left(G_A(X_A), G_B(X_B)\right)\\ &= S_A^C.\end{aligned}$$

□

Proposition 10. *We place ourselves in the framework of Theorem 2. Then, for any $A \in \mathcal{P}_D$*

$$S_A^U = \sum_{B\in\mathcal{P}_A} (-1)^{|A|-|B|}\left[\mathbb{V}\left(\mathbb{M}_B(G(X))\right) - Cov\left(\mathbb{M}_B(G(X)), [I-\mathbb{M}_A](G(X))\right)\right].$$

Proof of Proposition 10. First, recall that

$$\mathbb{M}_A(G(X)) = \sum_{B\in\mathcal{P}_A} G_B(X_B).$$

Thus,

$$\begin{aligned}\mathbb{V}\left(\mathbb{M}_A(G(X))\right) = \mathbb{V}\left(\sum_{B\in\mathcal{P}_A} G_B(X_B)\right) &= \sum_{B\in\mathcal{P}_A} \mathbb{V}\left(G_B(X_B)\right) + \sum_{C\in\mathcal{U}_A} \mathrm{Cov}\left(G_B(X_B), G_C(X_C)\right)\\ &= \sum_{B\in\mathcal{P}_A} S_B^U + S_B^C\end{aligned}$$

which is equivalent to

$$\mathbb{V}\left(\mathbb{M}_A(G(X))\right) - \sum_{B\in\mathcal{P}_A} S_B^C = \sum_{B\in\mathcal{P}_A} S_B^U.$$

However, notice that, $\forall A \in \mathcal{P}_D$,

$$\sum_{B \in \mathcal{P}_A} S_B^C = \mathrm{Cov}\left(\mathbb{M}_A(G(X)), [I - \mathbb{M}_A]\left(G(X)\right)\right),$$

and thus, $\forall A \in \mathcal{P}_D$,

$$\mathbb{V}\left(\mathbb{M}_A(G(X))\right) - \mathrm{Cov}\left(\mathbb{M}_A(G(X)), [I - \mathbb{M}_A]\left(G(X)\right)\right) = \sum_{B \in \mathcal{P}_D} S_B^U.$$

Using Rota's generalization of the Möbius inversion formula applied to the power-set, it yields that, $\forall A \in \mathcal{P}_D$,

$$S_A^U = \sum_{B \in \mathcal{P}_A} (-1)^{|A|-|B|} \left[\mathbb{V}\left(\mathbb{M}_B(G(X))\right) - \mathrm{Cov}\left(\mathbb{M}_B(G(X)), [I - \mathbb{M}_A]\left(G(X)\right)\right)\right].$$

□

5.2.2. Organic variance decomposition

The goal of the *organic variance decomposition* is to separate "pure interaction effects" to "dependence effects". Pure interaction can be seen as the study of the functional relation between the inputs X and the random output $G(X)$ *under mutual independence of* X. Formally, let $X = (X_1, \ldots, X_d)$ be a vector of random elements. The induced probability measure P_X is not necessarily the product measure $\bigtimes_{i \in D} P_{X_i}$. Now, denote $\widetilde{X} = (\widetilde{X}_1, \ldots, \widetilde{X}_d)$ the vector of random elements such that

$$\forall i \in D, \quad \widetilde{X}_i \text{ and } X_i \text{ have the same distribution} \quad \text{and} \quad P_{\widetilde{X}} := \bigtimes_{i \in D} P_{X_i}.$$

In other words, X and $\widetilde{X}$ have the same univariate marginals, but $\widetilde{X}$ is the mutual independent version of X and, for any $A \in \mathcal{P}_D$, denote $\widetilde{X}_A$ its marginals. Suppose that $G(X) \in \mathbb{L}^2\left(\sigma_X\right)$ and $G\left(\widetilde{X}\right) \in \mathbb{L}^2\left(\sigma_{\widetilde{X}}\right)$.

Notice that, since $\widetilde{X}$ is mutually independent, it respects both Assumptions 1 and 2, and hence, one can perform the following orthocanonical decomposition in $\mathbb{L}^2\left(\sigma_{\widetilde{X}}\right)$

$$G\left(\widetilde{X}\right) = \sum_{A \in \mathcal{P}_D} \widetilde{G}_A\left(\widetilde{X}_A\right),$$

where the $\widetilde{G}_A(\widetilde{X}_A)$ are all pairwise orthogonal (see Appendix Appendix C), and hence

$$\mathbb{V}\left(G\left(\widetilde{X}\right)\right) = \sum_{A \in \mathcal{P}_D} \mathbb{V}\left(\widetilde{G}_A\left(\widetilde{X}_A\right)\right).$$

We propose the following indices.

Definition 6 (Pure interaction effect)**.** *We place ourselves in the framework of Theorem 2. For any* $A \in \mathcal{P}_D$*, let*

$$S_A = \frac{\mathbb{V}\left(\widetilde{G}_A\left(\widetilde{X}_A\right)\right)}{\mathbb{V}\left(G\left(\widetilde{X}\right)\right)} \mathbb{V}\left(G(X)\right)$$

define the pure interaction indices.

These indices are, in fact, the Sobol' indices of $G\left(\widetilde{X}\right)$ [52], which are known in the literature as quantifying pure interaction [10]. These indices can also be expressed as functions of the orthogonal projections onto the subspaces $\mathbb{L}^2\left(\sigma_{\widetilde{X}_A}\right)$ as follows

$$S_A = \sum_{B \in \mathcal{P}_A} (-1)^{|A|-|B|} \mathbb{E}_B\left(G(\widetilde{X})\right).$$

For further considerations about these indices, we refer the interested reader to [40, 10].

Remark 4. In certain situations, when X is from a certain family of random vectors, it is possible to find a simple mapping $T : E \to E$ such that

$$\widetilde{X} = T(X).$$

In particular, if P_X is in the family of elliptical distribution, it amounts to performing a Nataf transform of the inputs [35, 36].

To define dependence effects, one desirability criterion can be brought forward: the set of indices must all be equal to zero if and only if X is mutually independent. Many quantities can be defined that respect this property. However, we focus on one particular quantity, which can be easily interpreted thanks to the following observation.

Lemma 5. *We place ourselves in the framework of Theorem 2. Let $G(X) \in \mathbb{L}^2(\sigma_X)$. Then,*

$$Q_A(G(X)) = P_A(G(X)) \ \text{ a.s.}, \quad \forall A \in \mathcal{P}_D \quad \Longleftrightarrow \quad X \text{ is mutually independent.}$$

Proof of Lemma 5. First, suppose that X is mutually independent. By Proposition 14, one has that

$$\forall A, B \in \mathcal{P}_D, B \neq A \quad V_A \perp V_B,$$

which entails that

$$V_A \perp W_A = \bigoplus_{B \in \mathcal{P}_D : B \neq A} V_B.$$

However, notice that W_A still complements V_A in $\mathbb{L}^2(\sigma_X)$. Furthermore, by unicity of the orthogonal complement, one has that $W_A = V_A^{\perp}$. Thus,

$$\mathrm{Ran}(Q_A) = V_A, \quad \mathrm{Ker}(Q_A) = V_A^{\perp},$$

and thus $Q_A = P_A$, leading to

$$Q_A(G(X)) = P_A(G(X)) \ \text{ a.s.}$$

Now, suppose that for any $A \in \mathcal{P}_D$, $Q_A(G(X)) = P_A(G(X))$ a.s. Hence, it implies that

$$\forall A \in \mathcal{P}_D, G_A(X_A) = P_A(G(X)).$$

which implies that $P_A = Q_A$, since the above equation defines the operator Q_A. Thus, P_A and Q_A must share the same ranges and nullspaces. In particular,

$$\mathrm{Ker}(Q_A) = \mathrm{Ker}(P_A) = V_A^{\perp},$$

implying that $W_A = V_A^{\perp}$, which leads to

$$V_A \perp W_A, \forall A \in \mathcal{P}_D \quad \Longleftrightarrow \quad V_A \perp V_B, \forall A, B \in \mathcal{P}_D, B \neq A.$$

Finally, thanks to Proposition 14, notice that this is equivalent to X being mutually independent. □

Hence, a rather intuitive index is the distance between these two projections.

Definition 7 (Dependence effects)**.** *We place ourselves in the framework of Theorem 2. For any* $A \in \mathcal{P}_D$*, let*

$$S_A^D = \mathbb{V}\left(Q_A(G(X)) - P_A(G(X))\right) = \mathbb{E}\left[\left(Q_A(G(X)) - P_A(G(X))\right)^2\right]$$

define the dependence effect of X_A*.*

Furthermore, these indices are naturally all zero if and only if X is mutually independent.

Proposition 11.

$$\forall A \in \mathcal{P}_D,\ S_A^D = 0 \quad \Longleftrightarrow \quad X \text{ is mutually independent.}$$

Proof of Proposition 11. This is a direct consequence of Lemma 5. □

6. Analytical formulas for two Bernoulli inputs

In order to illustrate Theorem 2, one can take an interest in a very particular case: X is comprised of two Bernoulli random variables. In this example, the orthocanonical decomposition can be achieved analytically.

6.1. Decomposition as a system of linear equations

Let $X = (X_1, X_2)$ where both inputs follow a Bernoulli distribution (here, $E = \{0,1\}^2$) with success probability q_1 and q_2 respectively. The joint law of X can be fully expressed using three free parameters: q_1, q_2, and $\rho = \mathbb{E}[X_1 X_2]$. More precisely, one has that:

$$p_{00} = 1 - q_1 - q_2 + \rho,\ p_{01} = q_2 - \rho,\ p_{10} = q_1 - \rho,\ p_{11} = \rho$$

where, for $i, j \in \{0,1\}$, one denotes $p_{ij} = \mathbb{P}(\{X_1 = i\} \cap \{X_2 = j\})$. Denote the (4×4) diagonal matrix $P = \mathrm{diag}(p_{00}, p_{01}, p_{10}, p_{11})$. Any function $G : \{0,1\}^2 \to \mathbb{R}$ can be represented as a vector in $\mathbb{R}^4$, where each element represents a value that G can take w.r.t. the values taken by X. For $i, j \in \{0,1\}$, denote $G_{ij} = G(i,j)$, and thus

$$G = (G_{00}, G_{01}, G_{10}, G_{11})^\top$$

where each G_{ij} can be observed with probability p_{ij}.

In this particular case, one can analytically compute the decomposition of G related to Theorem 2. It can be performed by finding suitable unit-norm vectors in $\mathbb{R}^4$

$$v_\emptyset = \begin{pmatrix} c \\ c \\ c \\ c \end{pmatrix}, v_1 = \begin{pmatrix} g_0 \\ g_0 \\ g_1 \\ g_1 \end{pmatrix}, v_2 = \begin{pmatrix} h_0 \\ h_1 \\ h_0 \\ h_1 \end{pmatrix}, v_{12} = \begin{pmatrix} k_{00} \\ k_{01} \\ k_{10} \\ k_{11} \end{pmatrix}$$

such that

$$\begin{cases} v_\emptyset^\top P v_1 = 0 \\ v_\emptyset^\top P v_2 = 0 \\ v_\emptyset^\top P v_{12} = 0 \\ v_{12}^\top P v_1 = 0 \\ v_{12}^\top P v_2 = 0 \end{cases}, \quad \text{and} \quad \begin{cases} v_\emptyset^\top P v_\emptyset = 1 \\ v_1^\top P v_1 = 1 \\ v_2^\top P v_2 = 1 \\ v_{12}^\top P v_{12} = 1 \end{cases} \tag{4}$$

which results in a system of nine equations with nine real unknown parameters (i.e., c for $v_\emptyset$, h_0, h_1 for v_1, g_0, g_1 for v_2, and $k_{00}, k_{01}, k_{10}, k_{11}$ for v_{12}). Given these vectors, one has that any function G can be written as

$$G = ev_\emptyset + \alpha v_1 + \beta v_2 + \delta v_{12},$$

resulting in four additional equations with four unknown parameters. These 13 equations and 13 parameters can be solved analytically.

We used the symbolic programming package `sympy` to perform these calculations [41]. We refer the interested reader to the accompanying GitHub repository[1] for the analytical formulas obtained for this decomposition, as well as the analytical formulas of the indices introduced in Section 5. The remainder of this section is dedicated to discussing one interesting finding.

6.2. Feshchenko matrix and the Fréchet bounds on copulas

Friedrichs' angle between V_1 and V_2 can be analytically computed. It is equal to:

$$c\left(\mathbb{L}^2\left(\sigma_1\right), \mathbb{L}^2\left(\sigma_2\right)\right) = \left|v_1^\top P v_2\right| = \left|\frac{-q_1 q_2 + \rho}{\sqrt{q_1}\sqrt{q_2}\sqrt{1-q_1}\sqrt{1-q_2}}\right|.$$

Hence, for the Feshchenko matrix Δ to be definite positive (and thus for Assumption 2 to hold), it entails that

$$\left|\frac{-q_1 q_2 + \rho}{\sqrt{q_1}\sqrt{q_2}\sqrt{1-q_1}\sqrt{1-q_2}}\right| < 1.$$

Let

$$B_0 := \max\left\{0, q_1 q_2\left(1 - \sqrt{\frac{(q_1-1)(q_2-1)}{q_1 q_2}}\right)\right\}$$

and

$$B_1 := \min\left(1, q_1 q_2\left(1 + \sqrt{\frac{\{q_1-1\}(q_2-1)}{q_1 q_2}}\right)\right),$$

and notice that ρ must necessarily be bounded by

$$B_0 < \rho < B_1.$$

However, the classical Fréchet bounds for ρ for bivariate Bernoulli random variables (see [29, p.210]) are equal to

$$H_0 := \max\left(0, q_1 + q_2 - 1\right) \leq \rho \leq \min\left(q1, q2\right) := H_1,$$

and notice that these bounds are attained if and only if X is counter-comonotonic or comonotonic. However, attaining these bounds violates Assumption 1 (and in particular Proposition 3). One can notice that the Fréchet bounds are always more restrictive than the bounds due to the positive definiteness of the Feshchenko matrix. Thus, Assumptions 1 and 2 hold for any copula between two distinct Bernoulli random variables.

7. Discussion and future work

In this article, we propose a framework to study the problem of decomposing functions of random inputs, which are not necessarily assumed to be mutually independent. This framework merges tools from probability theory, functional analysis, and some notions of combinatorics. This framework leads

[1] https://github.com/milidris/GeneralizedAnova

to a generalization of the Hoeffding decomposition [26]. It can be expressed using oblique projections of the random output on some particular subspaces. Based on this result, we propose methods to decompose two quantities of interest: an evaluation (i.e., observation) of the random output and its variance. For the latter, two approaches are proposed, which correspond to different situations one may encounter in practice. The properties of the resulting indices are studied, and an emphasis is put on their intuitive interpretation. Finally, a particular case is studied, where the inputs are composed of two Bernoulli random variables, for which the proposed decomposition can be computed analytically.

The first main challenge towards adopting the indices presented in Section 5 is estimation. While many methods exist to estimate conditional expectations. Many of these schemes rely on the variational problem offered by Hilbert's projection theorem, i.e., characterizing orthogonal projections as a distance-minimizing problem. A first idea would be to express oblique projections as a distance-minimizing optimization problem under constraints. A second idea would be to take advantage of the particular expression of oblique projections (see, e.g., [2, 9]). A final idea would be to find suitable bases for each $(V_A)_{A\in\mathcal{P}_D}$ to project $G(X)$ onto, analogously to [7]. Non-orthogonal polynomial bases would be a great start to study this problem whenever X is endowed with a multivariate Gaussian probabilistic structure.

The second main challenge is understanding the extent of such an approach. Aside from the uncertainty quantification that this framework offers, we believe it is a step towards a more global treatment of dependencies in (non-linear) multivariate statistics. As one can notice, our framework offers a (somewhat surprisingly) linear approach to possibly highly non-linear problems (due to the function G, and/or to the stochastic dependence on X). We believe that Assumptions 1 and 2 will play a pivotal role going forward.

Finally, we emphasize the importance of the Boolean lattice algebraic structure, which is intrinsically part of our framework. It is essential in our analysis and offers a path toward studying different algebraic structures. One can notice that several references to Rota's generalization of the Möbius inversion formula [48, 32] are made in our reasoning. This result is paramount to the well-foundedness of our approach. However, Rota's result is much more general and does not only apply to Boolean lattices (i.e., powersets). It holds for any (finite) partially ordered set. Our approach clearly identifies the role of the underlying algebraic structure in the resulting analyses. It paves the way for more complex analysis, where the relationship between the inputs may differ. For example, one can think of hierarchical structures (e.g., to represent physical causality) or the presence of trigger variables [43], which would result in a different algebraic structure, but still be partially ordered.

Acknowledgements

Support from the ANR-3IA Artificial and Natural Intelligence Toulouse Institute is gratefully acknowledged.

References

[1] Y. A. Abramovich and C. D. Aliprantis. *An invitation to operator theory*. Number v. 50 in Graduate studies in mathematics. American Mathematical Society, Providence, R.I, 2002.

[2] S. N. Afriat. Orthogonal and oblique projectors and the characteristics of pairs of vector spaces. *Mathematical Proceedings of the Cambridge Philosophical Society*, 53(4):800–816, 1957.

[3] S. Axler. *Linear Algebra Done Right*. Undergraduate Texts in Mathematics. Springer International Publishing, Cham, 2015.

[4] A. Barredo Arrieta, N. Díaz-Rodríguez, J. Del Ser, A. Bennetot, S. Tabik, A. Barbado, S. Garcia, S. Gil-Lopez, D. Molina, R. Benjamins, R. Chatila, and F. Herrera. Explainable Artificial

Intelligence (XAI): Concepts, taxonomies, opportunities and challenges toward responsible AI. *Information Fusion*, 58:82–115, 2020.

[5] W. Bryc. Conditional expectation with respect to dependent sigma-fields. In *Proceedings of VII conference on Probability Theory*, pages 409–411, 1984.

[6] W. Bryc. Conditional Moment Representations for Dependent Random Variables. *Electronic Journal of Probability*, 1:1–14, 1996. Publisher: Institute of Mathematical Statistics and Bernoulli Society.

[7] G. Chastaing, F. Gamboa, and C. Prieur. Generalized Hoeffding-Sobol decomposition for dependent variables - application to sensitivity analysis. *Electronic Journal of Statistics*, 6:2420–2448, 2012.

[8] J.B. Conway. *A Course in Functional Analysis*, volume 96 of *Graduate Texts in Mathematics*. Springer, New York, NY, 2007.

[9] G. Corach, A. Maestripieri, and D. Stojanoff. A classification of projectors. In *Topological Algebras, their Applications, and Related Topics*, pages 145–160, Bedlewo, Poland, 2005. Institute of Mathematics Polish Academy of Sciences.

[10] S. Da Veiga, F. Gamboa, B. Iooss, and C. Prieur. *Basics and Trends in Sensitivity Analysis: Theory and Practice in R*. Society for Industrial and Applied Mathematics, Philadelphia, PA, 2021.

[11] J. Dauxois and G. M. Nkiet. Canonical analysis of two euclidean subspaces and its applications. *Linear Algebra and its Applications*, 264:355–388, 1997.

[12] J Dauxois, G. M Nkiet, and Y Romain. Canonical analysis relative to a closed subspace. *Linear Algebra and its Applications*, 388:119–145, 2004.

[13] B. A. Davey and H. A. Priestley. *Introduction to Lattices and Order*. Cambridge University Press, Cambridge, 2 edition, 2002.

[14] E. de Rocquigny, N. Devictor, and S. Tarantola, editors. *Uncertainty in Industrial Practice*. John Wiley & Sons, Ltd, Chichester, UK, 2008.

[15] A. Dembo, A. Kagan, and L. A. Shepp. Remarks on the Maximum Correlation Coefficient. *Bernoulli*, 7(2):343–350, 2001.

[16] F. Deutsch. The Angle Between Subspaces of a Hilbert Space. In S. P. Singh, editor, *Approximation Theory, Wavelets and Applications*, NATO Science Series, pages 107–130. Springer Netherlands, Dordrecht, 1995.

[17] J. Dixmier. étude sur les variétés et les opérateurs de julia, avec quelques applications. *Bulletin de la Société Mathématique de France*, 77:11–101, 1949.

[18] P. Doukhan. *Mixing*, volume 85 of *Lecture Notes in Statistics*. Springer, New York, NY, 1994.

[19] I. Feshchenko. When is the sum of closed subspaces of a Hilbert space closed?, 2020. https://arxiv.org/abs/2012.08688.

[20] I. S. Feshchenko. On closeness of the sum of n subspaces of a Hilbert space. *Ukrainian Mathematical Journal*, 63(10):1566–1622, 2012.

[21] K. Friedrichs. On Certain Inequalities and Characteristic Value Problems for Analytic Functions and For Functions of Two Variables. *Transactions of the American Mathematical Society*, 41(3):321–364, 1937. Publisher: American Mathematical Society.

[22] A. Galántai. *Projectors and Projection Methods*. Springer US, Boston, MA, 2004.

[23] H. Gebelein. Das statistische Problem der Korrelation als Variations- und Eigenwertproblem und sein Zusammenhang mit der Ausgleichsrechnung. *ZAMM - Zeitschrift für Angewandte Mathematik und Mechanik*, 21(6):364–379, 1941.

[24] R. Ghanem, D. Higdon, and H. Owhadi, editors. *Handbook of uncertainty quantification*. Springer Reference. Springer Nature, Cham, Switzerland, 2017.

[25] J. Hart and P. A. Gremaud. An approximation theoretic perspective of Sobol' indices with dependent variables. *International Journal for Uncertainty Quantification*, 8(6), 2018.

[26] W. Hoeffding. A Class of Statistics with Asymptotically Normal Distribution. *The Annals of Mathematical Statistics*, 19(3):293–325, 1948.

[27] G. Hooker. Generalized Functional ANOVA Diagnostics for High-Dimensional Functions of Dependent Variables. *Journal of Computational and Graphical Statistics*, 16(3):709–732, 2007.

[28] M. Il Idrissi, N. Bousquet, F. Gamboa, B. Iooss, and J-M. Loubes. On the coalitional decomposition of parameters of interest. *Comptes Rendus. Mathématique*, 361:1653–1662, 2023.

[29] H. Joe. *Multivariate Models and Multivariate Dependence Concepts*. Chapman and Hall/CRC, New York, 1997.

[30] O. Kallenberg. *Foundations of Modern Probability*, volume 99 of *Probability Theory and Stochastic Modelling*. Springer International Publishing, Cham, 2021.

[31] R. A. Koyak. On Measuring Internal Dependence in a Set of Random Variables. *The Annals of Statistics*, 15(3):1215–1228, 1987.

[32] J. P. S. Kung, G-C. Rota, and C. Hung Yan. *Combinatorics: the Rota way*. Cambridge University Press, New York, 2012. OCLC: 1226672593.

[33] F. Y. Kuo, I. H. Sloan, G. W. Wasilkowski, and H. Woźniakowski. On decompositions of multivariate functions. *Mathematics of Computation*, 79(270):953–966, 2009.

[34] S.L. Lauritzen. *Graphical Models*. Oxford Statistical Science Series. Oxford University Press, Oxford, New York, 1996.

[35] R. Lebrun and A. Dutfoy. Do Rosenblatt and Nataf isoprobabilistic transformations really differ? *Probabilistic Engineering Mechanics*, 24(4):577–584, 2009.

[36] R. Lebrun and A. Dutfoy. A generalization of the Nataf transformation to distributions with elliptical copula. *Probabilistic Engineering Mechanics*, 24(2):172–178, 2009.

[37] P-L Loh and M. J. Wainwright. Structure estimation for discrete graphical models: Generalized covariance matrices and their inverses. *The Annals of Statistics*, 41(6), 2013.

[38] S. M. Lundberg and S-I. Lee. A Unified Approach to Interpreting Model Predictions. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 30. Curran Associates, Inc., 2017.

[39] P. Malliavin. *Integration and Probability*, volume 157 of *Graduate Texts in Mathematics*. Springer, New York, NY, 1995.

[40] T. A. Mara, S. Tarantola, and P. Annoni. Non-parametric methods for global sensitivity analysis of model output with dependent inputs. *Environmental Modelling & Software*, 72:173–183, 2015.

[41] A. Meurer, C.P. Smith, M. Paprocki, O. Čertík, S.B. Kirpichev, M. Rocklin, A. Kumar, S. Ivanov, J.K. Moore, S. Singh, T. Rathnayake, S. Vig, B.E. Granger, R.P. Muller, F. Bonazzi, H. Gupta, S. Vats, F. Johansson, F. Pedregosa, M.J. Curry, A.R. Terrel, Š. Roučka, A. Saboo, I. Fernando, S. Kulal, R. Cimrman, and A. Scopatz. Sympy: symbolic computing in python. *PeerJ Computer Science*, 3:e103, 2017.

[42] Giovanni Peccati. Hoeffding-ANOVA decompositions for symmetric statistics of exchangeable observations. *The Annals of Probability*, 32(3):1796–1829, 2004. Publisher: Institute of Mathematical Statistics.

[43] J. Pelamatti and V. Chabridon. Sensitivity Analysis in the Presence of Hierarchical Variables. In *Programme and abstracts of the 23th Annual Conference of the European Network for Business and Industrial Statistics (ENBIS)*, volume 1, page 84, Valencia, 2023. Department of Applied Statistics and Operational Research, and Quality, Universitat Politecnica de Valencia.

[44] H. Rabitz and O. Aliş. General foundations of high-dimensional model representations. *Journal of Mathematical Chemistry*, 25(2):197–233, 1999.

[45] D. S Rakic and D. S Djordjevic. A note on topological direct sum of subspaces. *Funct. Anal. Approx. Comput*, 10(1):9–20, 2018.

[46] S. Razavi, A. Jakeman, A. Saltelli, C. Prieur, B. Iooss, E. Borgonovo, E. Plischke, S. Lo Piano, T. Iwanaga, W. Becker, S Tarantola, J.H.A. Guillaume, J. Jakeman, H. Gupta, N. Melillo, G. Rabitti, V. Chabridon, Q. Duan, X. Sun, S. Smith, R. Sheikholeslami, N. Hosseini, M. Asadzadeh, A. Puy, S. Kucherenko, and H. R. Maier. The Future of Sensitivity Analysis: An essential discipline for systems modeling and policy support. *Environmental Modelling & Software*, 137:104954, 2021.

[47] A. Rényi. On measures of dependence. *Acta Mathematica Academiae Scientiarum Hungarica*, 10(3):441–451, 1959.

[48] G-C. Rota. On the foundations of combinatorial theory I. Theory of Möbius Functions. *Zeitschrift für Wahrscheinlichkeitstheorie und Verwandte Gebiete*, 2(4):340–368, 1964.

[49] W. Rudin. *Functional analysis*. International series in pure and applied mathematics. McGraw-Hill, Boston, Mass., 2. ed., [nachdr.] edition, 1996.

[50] L. S. Shapley. Notes on the n-Person Game – II: The Value of an n-Person Game. Researach Memorandum ATI 210720, RAND Corporation, Santa Monica, California, 1951.

[51] Z. Sidák. On Relations Between Strict-Sense and Wide-Sense Conditional Expectations. *Theory of Probability & Its Applications*, 2(2):267–272, 1957.

[52] I.M Sobol'. Global sensitivity indices for nonlinear mathematical models and their monte carlo estimates. *Mathematics and Computers in Simulation*, 55(1):271–280, 2001.

[53] C. J. Stone. The Use of Polynomial Splines and Their Tensor Products in Multivariate Function Estimation. *The Annals of Statistics*, 22(1):118–171, 1994. Publisher: Institute of Mathematical Statistics.

Appendix A. Generated Lebesgue spaces

When it comes to $\mathbb{L}^2(\sigma_X)$, Theorem 1 implies that the set of subspaces $\left\{\mathbb{L}^2(\sigma_A)\right\}_{A\in\mathcal{P}_D}$ display some ordering structure w.r.t. the inclusion binary relation.

Lemma 6. *Let $A, B \in \mathcal{P}_D$, such that $B \subseteq A$. Then*

$$\mathbb{L}^2(\sigma_B) \subseteq \mathbb{L}^2(\sigma_A).$$

Proof of Lemma 6. Notice that, by definition, σ_A is a σ-algebra that contains $\cup_{i\in B}\sigma_i$ since $B \subseteq A$. Since σ_B is the smallest σ-algebra containing $\cup_{i\in B}\sigma_i$, then necessarily $\sigma_B \subseteq \sigma_A$. Applying Theorem 1 (1.) leads to the result. □

Lemma 6 can be understood as the fact that the Lebesgue space of *random outputs* w.r.t. a subset of inputs X_B *is included* in the Lebesgue space of *random outputs* w.r.t. a bigger subset of inputs X_A (i.e., provided $B \subseteq A$). For instance, for two inputs $X = (X_1, X_2)$, Lemma 6 entails that the set of random outputs which are only functions of X_1 is included in the set of random outputs which are functions of both X_1 *and* X_2. This behavior is rather intuitive due to the intrinsic definition of measurability, i.e., a random variable measurable w.r.t. σ_B is necessarily measurable w.r.t. σ_A provided $\sigma_B \subseteq \sigma_A$.

The Lebesgue spaces $\mathbb{L}^2$ of square-integrable random variables, display a remarkable property. It is well known that, whenever equipped with a particular inner product, they are Hilbert spaces, i.e., inner product spaces that are also complete metric spaces (see, e.g., [39, Theorem 9.4.1]).

Theorem 3. *Let $\mathcal{B} \subseteq \mathcal{F}$ be a sub-σ-algebra. The Lebesgue space $\mathbb{L}^2(\mathcal{B})$ is then a Hilbert space when equipped with the inner product defined, for any $Z_1, Z_2 \in \mathbb{L}^2(\mathcal{B})$, as:*

$$\mathbb{E}[XY] = \int_\Omega Z_1(\omega) Z_2(\omega) d\mathbb{P}(\omega).$$

Appendix B. Some notions from functional analysis

Appendix B.1. (Internal) direct-sum decompositions

An internal direct-sum decomposition of a vector space entails expressing this vector space as a particular sum of subspaces, having exclusively the zero vector as a common element. The adjective internal is omitted in the following for conciseness, except to avoid any confusion. Direct-sum decompositions of vector spaces can be characterized thanks to the following theorem (see, e.g., [3, Definition 1.40 and Proposition 1.44]).

Theorem 4 (Direct-sum decomposition)**.** *Let W be a vector space, and for a positive integer n, let $W_1, \ldots, W_n$ be proper subspaces of W (i.e., $W_i \subset W$ for every $i = 1, \ldots, n$). Then, the following statements are equivalent:*

1. *Any $w \in W$ can be written uniquely as $w = \sum_{i=1}^n w_i$ where $w_i \in W_i$ for $i = 1, \ldots, n$;*
2. *For $i = 1, \ldots, n$, one has that $W_i \cap (W_1 + W_2 + \cdots + W_{i-1} + W_{i+1} + \cdots + W_n) = \{0\}$;*
3. *$W = +_{i=1}^n W_i$ and additionally, for any $w = \sum_{i=1}^n w_i \in W$, where $w_i \in W_i$ one has that*

$$w = 0 \implies w_i = 0, \quad i = 1, \ldots, n.$$

If any of these three conditions are met, then W is said to admit a direct sum decomposition*, which is denoted*

$$W = \bigoplus_{i=1}^n W_i.$$

One can notice the resemblance between the sought-after decomposition in Eq. (1) and the one defined in Theorem 4 (1.). Since the random output $G(X)$ belongs to the (vector) Hilbert space $\mathbb{L}^2(\sigma_X)$, the problem of HDMR of random outputs can be seen as finding suitable subspaces of $\mathbb{L}^2(\sigma_X)$, where each subspace would be related to every Lebesgue space $\left\{\mathbb{L}^2(\sigma_A)\right\}_{A\in\mathcal{P}_D}$, and such that they form a direct-sum decomposition of $\mathbb{L}^2(\sigma_X)$. In order to properly characterize the subspaces involved in the decomposition, the notion of *complement of a subspace of a Hilbert space* is central and introduced in the following section.

Appendix B.2. Hilbert space external direct sums

Let $H_1, \ldots, H_n$ be a collection of Hilbert spaces with respective inner products $\langle .,. \rangle_1, \ldots, \langle .,. \rangle_n$ and induced norms $\|.\|_1, \ldots, \|.\|_n$. The Hilbert space (external) direct-sum is the space denoted and defined as (see [8, Definition 6.4])

$$\bigoplus_{i=1}^{n} H_i = \left\{ x = (x_1, \ldots, x_n) \in \bigtimes_{i=1}^{n} H_i : \sum_{i=1}^{n} \|x_i\|_i^2 < \infty \right\}.$$

A Hilbert space direct-sum is itself a Hilbert space w.r.t. the inner product $\langle .,. \rangle$ (see [8, Proposition 6.2])

$$\forall x, y \in \bigoplus_{i=1}^{n} H_i, \quad \langle x, y \rangle = \sum_{i=1}^{n} \langle x_i, y_i \rangle_i .$$

Appendix B.3. Closed range operator theorem

The following result can be found in [1, Theorem 2.5].

Theorem 5 (Closed range operator)**.** *Let $(\mathcal{M}_1, \|.\|_1)$ and $(\mathcal{M}_2, \|.\|_2)$ be two Banach spaces, and let $T : \mathcal{M}_1 \to \mathcal{M}_2$ be a continuous operator between the two spaces. T is bounded from below, i.e., there exists some $\gamma > 0$ such that, $\forall x \in \mathcal{M}_1$*

$$\|T(x)\|_2 \geq \gamma \|x\|_1 ,$$

if and only if T is one-to-one and $Ran(T)$ is closed in $\mathcal{M}_2$.

Appendix B.4. Intuition and interpretation behind of the proof of Theorem 2

Despite the somewhat formal nature of Theorem 2, its interpretation is rather intuitive. Given a univariate function $G_1(X_1) \in \mathbb{L}^2(\sigma_1)$, it is well known that it can always be decomposed as

$$G_1(X_1) = \mathbb{E}[G_1(X_1)] + [G_1(X_1) - \mathbb{E}[G_1(X_1)]] . \tag{B.1}$$

In other words, a random variable can always be decomposed as its expectation plus its centered version. The first step of the result formalizes this idea. $V_\emptyset = \mathbb{L}^2(\sigma_\emptyset)$ is comprised of constant a.e. random variables and is a closed subspace of $\mathbb{L}^2(\sigma_1)$. Thus $V_\emptyset$ is complemented in $\mathbb{L}^2(\sigma_1)$, and, in particular, it is complemented by V_1, its orthogonal complement. V_1 is thus comprised of every function of $\mathbb{L}^2(\sigma_1)$ which are orthogonal to the constants (i.e., they are centered). Thus, since $\mathbb{L}^2(\sigma_1) = V_\emptyset \oplus V_1$, one recovers the relation in (B.1).

For two inputs X_1 and X_2, Assumption 1 ensures that the subspaces $\mathbb{L}^2(\sigma_1)$ and $\mathbb{L}^2(\sigma_2)$ of $\mathbb{L}^2(\sigma_{12})$ are not comprised of the same random variables, due to a *functional relation between X_1 and X_2*. On the other hand, Assumption 2 ensures that these subspaces are not the same due to a *degenerate stochastic relation*. Under those two assumptions, the sum $\mathbb{L}^2(\sigma_1) + \mathbb{L}^2(\sigma_2) = V_\emptyset + V_1 + V_2$ is a closed subspace of $\mathbb{L}^2(\sigma_{12})$, and thus, is complemented by V_{12} which is none other than its orthogonal complement. Notice that V_1 and V_2 are *not necessarily orthogonal*, but both are orthogonal to $V_\emptyset$ and V_{12}.

The same reasoning can be applied with three inputs. The two assumptions ensure that $\mathbb{L}^2(\sigma_{12})$, $\mathbb{L}^2(\sigma_{23})$, and $\mathbb{L}^2(\sigma_{13})$ are not pairwise equal due to either a functional or a stochastic relation. In this case, their sum is a closed subspace in $\mathbb{L}^2(\sigma_{123})$, and thus, it is complemented by V_{123} (i.e., the orthogonal complement of $\mathbb{L}^2(\sigma_{12}) + \mathbb{L}^2(\sigma_{23}) + \mathbb{L}^2(\sigma_{13})$). However, notice that neither V_{12}, V_{13} and V_{23} are pairwise orthogonal, nor V_1, V_2 and V_3. The same mechanism can be continued for any number of inputs.

Hence, the subspaces $(V_A)_{A\in\mathcal{P}_D}$ in Theorem 2 can be interpreted as the subspaces of functions of X which, for any $A \in \mathcal{P}_D$, are σ_A-measurable (i.e., are functions of X_A), but are orthogonal to the linear combinations of functions in $(V_B)_{B\in\mathcal{P}_{-A}}$. In other words, the elements of V_A can only contain multivariate non-linear functions of *exactly* X_A and the zero vector. For instance, for two inputs X_1 and X_2, V_{12} can be seen as the space of functions of X_1 and X_2, that "are not" (in the sense of being the complement of) linear combinations of functions of X_1 and X_2. Given this construction, a natural interpretation of V_A would be the space of "functional interactions" between the inputs X_A.

Appendix C. The particular case of mutual independence

It is well-known that the independence of two random elements (w.r.t. to $\mathbb{P}$) is linked to the independence of the σ-algebras they generate, which can be characterized by the orthogonality of the centered generated Lebesgue spaces. More precisely, two sub σ-algebras $\mathcal{A}_1$ and $\mathcal{A}_2$ of a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ are said to be independent if $\mathbb{L}^2(\mathcal{A}_1)$ and $\mathbb{L}^2(\mathcal{A}_2)$ are orthogonal on the constant functions (see [39, Definition 3.0.1]). More precisely,

$$\mathcal{A}_1 \perp\!\!\!\perp \mathcal{A}_2 \iff c_0\left(\mathbb{L}^2_0(\mathcal{A}_1), \mathbb{L}^2_0(\mathcal{A}_2)\right) = 0,$$

where $\perp$ is defined relative to the inner product on $\mathbb{L}^2(\mathcal{F})$. Additionally, two random elements Z_1, Z_2 defined on $(\Omega, \mathcal{F}, \mathbb{P})$ are considered independent if their generated σ-algebras are independent.

When dealing with a vector of random elements $X = (X_1, \ldots, X_d)$, mutual independence can be defined w.r.t. the independence of their generated σ-algebras. More precisely, X is said to be mutually independent if

$$\forall A \in \mathcal{P}_D, \quad \sigma_A \perp\!\!\!\perp \sigma_{D\setminus A} \iff c_0\left(\mathbb{L}^2_0(\sigma_A), \mathbb{L}^2_0\left(\sigma_{D\setminus A}\right)\right) = 0.$$

Proposition 12. *Let X be a vector of random elements. If X is mutually independent, then Assumption 1 hold.*

Proof of Proposition 12. From [39], note that for two σ-algebras $\mathcal{B}_1$ and $\mathcal{B}_2$,

$$\mathcal{B}_1 \perp\!\!\!\perp \mathcal{B}_2 \quad \implies \quad \mathcal{B}_1 \cap \mathcal{B}_2 = \sigma_\emptyset.$$

Suppose that Assumption 1 does not hold. Hence, in particular, for any $A \in \mathcal{P}_D$,

$$\sigma_A \cap \sigma_{D\setminus A} \neq \sigma_\emptyset.$$

It implies that σ_A and $\sigma_{D\setminus A}$ cannot be independent. Hence, since this holds for any $A \in \mathcal{P}_D$, X cannot be mutually independent. The result is proven by taking the opposite implication. □

Proposition 13. *Let X be a vector of random elements and suppose that Assumption 1 holds. X is mutually independent if and only if $\forall A, B \in \mathcal{P}_D$, $A \neq B$,*

$$c\left(\mathbb{L}^2(\sigma_A), \mathbb{L}^2(\sigma_B)\right) = 0.$$

Proof of Proposition 13. Notice that, in general, if $B \subset A$, then $c\left(\mathbb{L}^2\left(\sigma_A\right), \mathbb{L}^2\left(\sigma_B\right)\right)$ is necessarily equal to zero. Thus, we focus on the case where $A \cap B = C \notin \{A, B\}$. Now, suppose that for any $A, B \in \mathcal{P}_D$, $c\left(\mathbb{L}^2\left(\sigma_A\right), \mathbb{L}^2\left(\sigma_B\right)\right) = 0$. Hence, in particular, under Assumption 1, notice that for every $A \in \mathcal{P}_D$

$$\begin{aligned} c\left(\mathbb{L}^2\left(\sigma_A\right), \mathbb{L}^2\left(\sigma_{D\setminus A}\right)\right) &= c_0\left(\mathbb{L}^2\left(\sigma_A\right) \cap \mathbb{L}^2\left(\sigma_\emptyset\right)^\perp, \mathbb{L}^2\left(\sigma_{D\setminus A}\right) \cap \mathbb{L}^2\left(\sigma_\emptyset\right)^\perp\right) \\ &= c_0\left(\mathbb{L}_0^2\left(\sigma_A\right), \mathbb{L}_0^2\left(\sigma_{D\setminus A}\right)\right). \end{aligned}$$

Thus, for every $A \in \mathcal{P}_D$,

$$c_0\left(\mathbb{L}_0^2\left(\sigma_A\right), \mathbb{L}_0^2\left(\sigma_{D\setminus A}\right)\right) = 0 \iff \sigma_A \perp\!\!\!\perp \sigma_{D\setminus A},$$

which is equivalent to X being mutually independent.

Now, suppose that X is mutually independent, and thus, $P_X = \bigtimes_{i\in D} P_{X_i}$, which implies that, for any $A, B \in \mathcal{P}_D$, with $A \cap B = C \notin \{A, B\}$,

$$\mathbb{E}_A \circ \mathbb{E}_B = \mathbb{E}_B \circ \mathbb{E}_A = \mathbb{E}_C,$$

Thus, the orthogonal projections onto $\mathbb{L}^2\left(\sigma_A\right)$ and $\mathbb{L}^2\left(\sigma_B\right)$ commute, which is equivalent to (see (2))

$$c\left(\mathbb{L}^2\left(\sigma_A\right), \mathbb{L}^2\left(\sigma_B\right)\right) = 0.$$

□

Corollary 2. *Let X be a vector of random elements and suppose that Assumption 1 holds. X is mutually independent if and only if its Feshchenko matrix Δ is the identity.*

Proof of Corollary 2. It is a direct consequence of Proposition 13, by definition of Δ. □

Hence, if the inputs are mutually independent, both Assumption 1 and Assumption 2 hold and lead to the very particular case of Δ being the identity matrix. One has the following result when it comes to the resulting decomposition of $\mathbb{L}^2\left(\sigma_X\right)$.

Proposition 14. *Let X be random inputs and suppose that Assumption 1 holds. X is mutually independent if and only if*

$$\forall A, B \in \mathcal{P}_D, B \neq A \quad V_A \perp V_B.$$

Proof of Proposition 14. Notice that, in general, if Assumption 1 hold, one has that for any $A, B \in \mathcal{P}_D$, $B \neq A$

$$c_0\left(V_A, V_B\right) \leq c\left(\mathbb{L}^2\left(\sigma_A\right), \mathbb{L}^2\left(\sigma_B\right)\right).$$

Note that, from Proposition 12, Assumption 1 holds for a mutually independent X. Moreover, notice from Proposition 13 that X is mutually independent if and only if, $\forall A, B \in \mathcal{P}_D$, $A \neq B$, $c\left(\mathbb{L}^2\left(\sigma_A\right), \mathbb{L}^2\left(\sigma_B\right)\right) = 0$, thus necessarily $c_0\left(V_A, V_B\right) = 0$, which is equivalent to $V_A \perp V_B$. □

Proposition 14 is, in fact, equivalent to the Hoeffding functional decomposition for mutually independent inputs, which can be seen as a very particular case of Theorem 2 where X admits a Feshchenko matrix equal to the identity, and provided Assumption 1 holds. In this very particular case, the subspaces V_A are all pairwise orthogonal, and the *canonical projectors are orthogonal.*

In a nutshell, Theorem 2 generalizes Hoeffding's decomposition to inputs with Feshchenko matrices *that are different from the identity*, or in other words, for not-necessarily mutually independent inputs.