Generalized Hoeffding Decomposition

and the (surprising) linear nature of non-linearity

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UQSay Seminar #69
Online - Saclay, France.
February 8, 2024

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Some context

Does Hoeffding's functional decomposition hold when the inputs are not mutually independent?

Classical Hoeffding's decomposition: **Unique** decomposition $G(X) = \sum_{A \in \mathcal{P}_D} G_A(X_A)$ for any square-integrable $G(X)$, where the inputs X are **mutually independent**.

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However... Achieving this result requires **an unusual methodological journey**.

In this talk: Mix the fields of **probability theory** and **functional analysis**, with a sprinkle of **algebraic combinatorics**, to **generalize Hoeffding's decomposition to dependent inputs**.

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They showed that the generalized decomposition hold, **but under fairly restrictive assumptions on the inputs**.

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Our approach: Understand the relationships between these subspaces of $\mathbb{L}^2$ when the inputs are **not mutually independent**.

Random inputs, black-box model

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a **probability space**, and let $(E_1, \mathcal{E}_1), \ldots, (E_d, \mathcal{E}_d)$ be **standard Borel measurable spaces**.

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The **random inputs** are defined as a **measurable mapping** (i.e., **random element**):

$$X : \Omega \to E,$$

where $E = \bigtimes_{i=1}^{d} E_i$ is the **cartesian product of the d Polish spaces**.

(*This is just a way to say that $X = (X_1, \ldots, X_d)$ is not necessarily $\mathbb{R}^d$-valued*)

> **Remark .** We are mainly going to treat X as **a function**: although **its law is well-defined**, **we don't really need to control it directly**.
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Let $G : E \to \mathbb{R}$ be a **black-box model**, and denote by $G(X)$ the **random output** (it is a random variable).

Generated and $\mathbb{P}$-trivial σ-algebras

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For every $A \subset D$, denote by:

- $\sigma_A \subseteq \mathcal{F}$ the **σ-algebra generated by** X_A ;
- $\sigma_X \subseteq \mathcal{F}$ the **σ-algebra generated by** X.

And notice that **if** $B \subseteq A$**, then** $\sigma_B \subseteq \sigma_A$.

> **Lemma** *(Doob-Dynkin). If an $\mathbb{R}$-valued random variable Y is σ_X-measurable, then there exists some function $f : E \to \mathbb{R}$ such that $Y = f(X)$ a.s.*

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Finally, denote by $\sigma_\emptyset$ the $\mathbb{P}$**-trivial** σ**-algebra**, i.e., the σ-algebra that contains **every event of** $\mathcal{F}$ **of probability** 0.

> **Lemma** *(Kallenberg (2021, Lemma 4.9)). Every $\sigma_\emptyset$-measurable random variable is a.s. constant.*

Functional dependence

Assumption 1 *(Non-perfect functional dependence). Suppose that:*

- $\sigma_\emptyset \subset \sigma_i$, $i = 1, \ldots, d$ *(inputs are not constant).*
- *For* $B \subset A$, $\sigma_B \subset \sigma_A$ *(inputs add information).*
- *For every* $A, B \in \mathcal{P}_D$, $A \neq B$,
$$\sigma_A \cap \sigma_B = \sigma_{A \cap B}.$$

This assumption is purely functional: **we're just controlling the pre-image of the mappings** $(X_A)_{A \in \mathcal{P}_D}$.

Proposition . *Suppose that Assumption 1 hold. 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 ***such that***

$$X_B = T(X_A) \text{ a.e.}$$

In other words, if Assumption 1 hold, then **the inputs cannot be functions of each other**.

Output space

Recall that $(\Omega, \mathcal{F}, \mathbb{P})$ is our sample space, **and let** $\mathcal{G}$ be a **sub-σ-algebra** of $\mathcal{F}$.

Definition *(Lebesgue space). Denote by $\mathbb{L}^2(\mathcal{G})$ the **Lebesgue space** containing every **square-integrable, $\mathbb{R}$-valued random variables**. It is an (infinite-dimensional) Hilbert space with inner product, $\forall Z_1, Z_2 \in \mathbb{L}^2(\mathcal{G})$:*

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

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$\mathbb{L}^2(\sigma_X)$ is the space of **random outputs:** it **only contains random variable that can be expressed as functions of X.**

For every $A \subset D$, $\mathbb{L}^2(\sigma_A) \subset \mathbb{L}^2(\sigma_X)$ **only contains random variables that can be expressed as functions of X_A.**

$\mathbb{L}^2(\sigma_\emptyset)$ **only contains a.s constants.**

Generated Lebesgue subspaces

Theorem *(Sidák (1957, Theorem 2)). Let $\mathcal{B}_1 \subseteq \mathcal{B}_2 \subseteq \mathcal{F}$, then*

- $\mathbb{L}^2(\mathcal{B}_1) \subseteq \mathbb{L}^2(\mathcal{B}_2) \subseteq \mathbb{L}^2(\mathcal{F})$;
- $\mathbb{L}^2(\mathcal{B}_1) \cap \mathbb{L}^2(\mathcal{B}_2) = \mathbb{L}^2(\mathcal{B}_1 \cap \mathcal{B}_2)$.

Recall that, since for $B \subset A \in \mathcal{P}_D$ we have that $\sigma_B \subseteq \sigma_A$, then:

$$\mathbb{L}^2(\sigma_B) \textbf{ is a closed Hilbert subspace of } \mathbb{L}^2(\sigma_A)$$

and all of them are closed subspaces of $\mathbb{L}^2(\sigma_X)$: They are **nested in very a particular way** (more on that later in the talk).

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Controlling the Lebesgue spaces w.r.t. the σ-algebras allow to express **spaces of functions of subsets of inputs** (analogously to Chastaing, Gamboa, and Prieur (2012)).

The intuition

Recall the classical result:

Theorem *(Malliavin (1995, Chapter 3)). Let X and Y be two random elements. Then:*

$$X \perp\!\!\!\perp Y \iff \forall f(X) \in \mathbb{L}^2(\sigma_X),\ \forall g(Y) \in \mathbb{L}^2(\sigma_Y),\ \mathcal{C}orr(f(X), g(Y)) = 0,$$

or, in other words, $\mathbb{L}_0^2(\sigma_X) \perp \mathbb{L}_0^2(\sigma_Y)$, where $\mathbb{L}_0^2$ only contains centered random variables.

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Intuition:

Is it possible to control the **dependence structure** between the inputs by controlling the **angles between the subspaces** $\{\mathbb{L}^2(\sigma_A)\}_{A \in \mathcal{P}_D}$?

Dixmier's angle

Definition *(Dixmier's angle (Dixmier 1949)).* *Let M, N be **closed** subspaces of a Hilbert space H. The cosine of Dixmier's angle between M and N is defined as*

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Dixmier's angle is closely related to the notion of **maximal correlation** in probability theory (Koyak 1987), as a dependence measure between **random elements**.

Definition *(Maximal correlation (Gebelein 1941)). Let Z_1, Z_2 be two **random elements**. The maximal correlation between Z_1 and Z_2 is*

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Friedrich's angle is used in probability theory as a measure of **partial dependence** between two random elements (Bryc 1984, 1996; Dauxois, Nkiet, and Romain 2004).

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Remark .

$$\rho^*(Z_1,Z_2) = 0 \iff \mathbb{E}[\mathbb{E}[.\mid Z_1]\mid Z_2] = \mathbb{E}[\mathbb{E}[.\mid Z_2]\mid Z_1]$$

Closure and complements

These two angles are related to the **closedness of the sum of the two subspaces**:

- $c\,(M, N) < 1 \iff M + N$ is closed in H ;
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One **popular complement** of a closed subspace M is **its orthogonal complement** $M^\perp$.

Feshchenko matrix

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

These matrices resemble closely the ones used by **Feshchenko (2020)** to study the **closedness of an arbitrary sum of closed subspaces** of a Hilbert space.

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$\Longrightarrow$ **We're going to call them "Feshchenko matrices".**

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$$\Delta = I_{2^d} \iff X \text{ is mutually independent.}$$

Remark . Recall that we're working with **abstract-valued random elements** (and not necessarily a random vector).

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Our second assumption:

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

Note that this is a restriction of the inner product of $\mathbb{L}^2(\sigma_X)$, and thus **an indirect restriction on the law of** X.

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W is said to admit a ***direct-sum decomposition*** *if any $w \in W$ can be written* ***uniquely*** *as*

$$w = \sum_{i=1}^{n} w_i \text{ where } w_i \in W_i \text{ for } i = 1, \ldots, n.$$

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Intuition: Can we find a direct-sum decomposition for $\mathbb{L}^2(\sigma_A)$, for every $A \in \mathcal{P}_D$?

If so, we could uniquely decompose any **non-linear function** of X_A, $A \in \mathcal{P}_D$.

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<u>**Intuition:**</u> **Can we find a direct-sum decomposition for $\mathbb{L}^2(\sigma_A)$, for every $A \in \mathcal{P}_D$?**

If so, we could uniquely decompose any **non-linear function** of X_A, $A \in \mathcal{P}_D$.

But which subspaces should be involved in the direct-sum decomposition ?

Generalized Hoeffding decomposition

Theorem . *Under Assumptions 1 and 2, for every $A \in \mathcal{P}_D$, one has that*

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

where $V_\emptyset = \mathbb{L}^2(\sigma_\emptyset)$, and

$$V_B = \left[\sum_{C \in \mathcal{P}_B, C \neq B} V_C \right]^{\perp_B},$$

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Main intuition:

"Inductive generalized centering"

Intuition behind the result: One input

One input:

1. Let $i \in D$, and **fix** $\mathbb{L}^2(\sigma_i)$ **as the ambient space**.
2. We have that $V_\emptyset := \mathbb{L}^2(\sigma_\emptyset)$ **is a closed subspace of** $\mathbb{L}^2(\sigma_i)$ (thus it is **complemented**).
3. Denote $V_i = [V_\emptyset]^{\perp_i}$, **the orthogonal complement of** $V_\emptyset$ **in** $\mathbb{L}^2(\sigma_i)$.
4. One has that $\mathbb{L}^2(\sigma_i) = V_\emptyset \oplus V_i$.
5. Since $V_\emptyset$ only contains constants, $V_i = \mathbb{L}^2_0(\sigma_i)$.

In other words, we just showed that any $f(X_i) \in \mathbb{L}^2(\sigma_i)$ can be written as

$$f(X_i) = \underbrace{\mathbb{E}[f(X_i)]}_{\in V_\emptyset} + \underbrace{\mathbb{E}[f(X_i) - \mathbb{E}[f(X_i)]]}_{\in V_i}.$$

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And note that we can do this for any $i \in D$**.**

Intuition behind the result: Two inputs

Two inputs:

1. Let $i, j \in D$, and **fix** $\mathbb{L}^2(\sigma_{ij})$ **as the ambient space**.
2. We have that $\mathbb{L}^2(\sigma_i)$ and $\mathbb{L}^2(\sigma_j)$ are **closed subspaces of** $\mathbb{L}^2(\sigma_{ij})$.
3. **Assumptions 1 and 2 imply that** $\mathbb{L}^2(\sigma_i) + \mathbb{L}^2(\sigma_j)$ **is closed in** $\mathbb{L}^2(\sigma_{ij})$ (thus it is **complemented**).
4. Notice (previous step) that $\mathbb{L}^2(\sigma_i) + \mathbb{L}^2(\sigma_j) = V_\emptyset + V_i + V_j$.
5. Denote $V_{ij} = [V_\emptyset + V_i + V_j]^{\perp_{ij}}$, **the orthogonal complement in** $\mathbb{L}^2(\sigma_{ij})$.
6. We thus have that $\mathbb{L}^2(\sigma_{ij}) = V_\emptyset + V_i + V_j + V_{ij}$.

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In essence, we **"centered" a bivariate function from its "univariate and constant parts".**

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In essence, we **"centered" a bivariate function from its "univariate and constant parts".**

And we can continue the same induction up to d inputs.

Orthocanonical decomposition

As a direct consequence of the previous theorem:

Corollary *(Orthocanonical decomposition). Under Assumptions 1 and 2, any $G(X) \in \mathbb{L}^2(\sigma_X)$ can be* ***uniquely decomposed*** *as*

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

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

The term **"orthocanonical"** comes from the choice of the **orthogonal complement** in the "centering process".

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The subspaces V_A are comprised of **proper representants**, i.e., either 0 or **functions of exactly** X_A (they do not contain functions of fewer inputs).

Projectors

Recall that for any $G(X) \in \mathbb{L}^2(\sigma_X)$, we have

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Oblique projections

Denote the operator

$$Q_A : \mathbb{L}^2(\sigma_X) \to \mathbb{L}^2(\sigma_X), \text{ such that } \quad Q_A(G(X)) = G_A(X_A).$$

Q_A is the (canonical) **oblique projection** onto V_A, parallel to $\bigoplus_{B \in \mathcal{P}_D : B \neq A} V_A$.

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Denote the projector

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

the **orthogonal projection** onto V_A.

Hence, for any $G(X) \in \mathbb{L}^2(\sigma_X)$, one has that, $\forall A \in \mathcal{P}_D$

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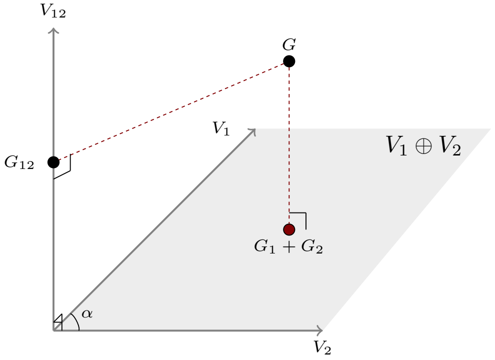

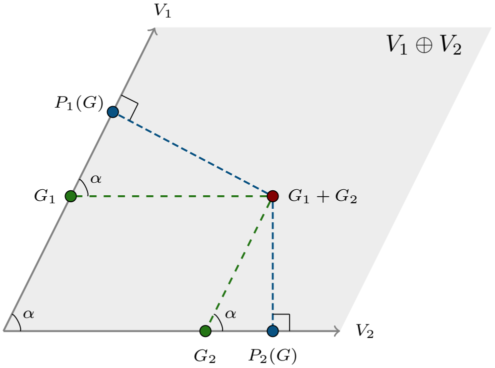

Illustration : $\mathbb{L}_0^2(\sigma_{12})$

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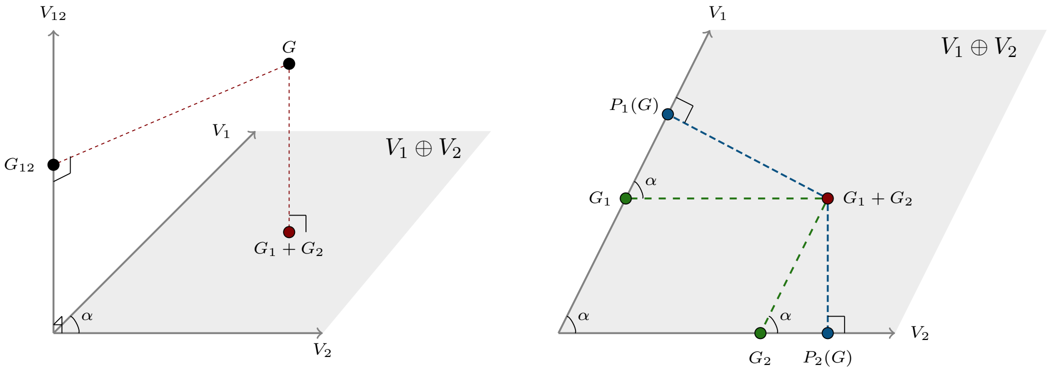

The oblique projection Q_A usually differ from the oblique projections P_A

Oblique and orthogonal projections

In fact,

Proposition . *Under Assumptions 1 and 2,*

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

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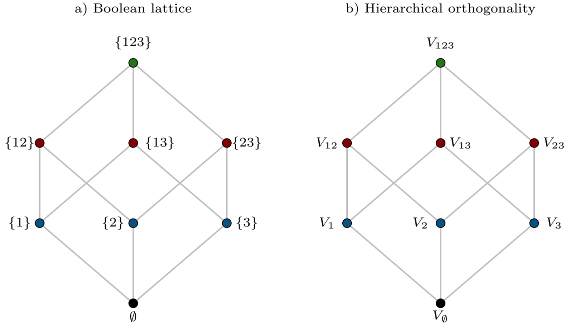
To illustrate this fact, we need some algebraic combinatorics.

Boolean lattice and hierarchical orthogonality

Our decomposition is **over the power-set** $\mathcal{P}_D$, which **which is not trivial**.

When endowed with the **binary relation** $\subseteq$ they form an algebraic structure called **a Boolean lattice**.



The subspaces $\{V_A\}_{A \in \mathcal{P}_D}$ are **hierarchically orthogonal** by design: they follow the same algebraic structure, but this time **w.r.t. to** $\perp$.

More projectors

Recall that:

- Q_A is the **oblique projection** onto V_A.
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But what about projections onto the subspaces $\left\{\mathbb{L}^2\left(\sigma_A\right)\right\}_{A\in\mathcal{P}_D}$**?**

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Is it possible to express the projections Q_A using $\mathbb{M}_A$?

Generalized Möbius inversion

Yes, because we're **working on the power-set** $\mathcal{P}_D$!

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Corollary *(Möbius inversion on power-sets (Rota 1964)). Let* $D = \{1, \dots, d\}$*. For any two set functions:*

$$f : \mathcal{P}_D \to \mathbb{A}, \quad g : \mathcal{P}_D \to \mathbb{A},$$

where $\mathbb{A}$ *is an* ***abelian group****, the following equivalence holds:*

$$f(A) = \sum_{B \in \mathcal{P}_A} g(B), \quad \forall A \in \mathcal{P}_D \quad \Longleftrightarrow \quad g(A) = \sum_{B \in \mathcal{P}_A} (-1)^{|A|-|B|} f(B), \quad \forall A \in \mathcal{P}_D.$$

In our case, we have, **by definition of the oblique projection onto** $\mathbb{L}^2(\sigma_A)$, that

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(This is what we call the **"model-centric"** approach)

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If the inputs are mutually independent, from Hoeffding (1948), we have that:

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Our approach actually generalizes Hoeffding's decomposition!

Variance decomposition

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Organic variance decomposition: separate **pure interaction effects** to **dependence effects**. The dependence structure of X is **unwanted**, and one wishes to study its effects.

Orthocanonical variance decomposition: the dependence structure of X is **inherent in the uncertainty modeling** of the studied phenomenon. It amounts to quantify **structural** and **correlative** effects.

Organic variance decomposition: Pure interaction

The notion of pure interaction is intrinsically linked with the notion of mutual independence.

Let $\widetilde{X} = (\widetilde{X}_1, \ldots, \widetilde{X}_d)^\top$ be the random vector such that

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Definition *(Pure interaction). For every $A \in \mathcal{P}_D$, define the **pure interaction of** X_A **on** $G(X)$ **as***

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

These indices are the **Sobol' indices** computed on the mutually independent version of X.

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This approach **strongly resembles the "independent Sobol' indices"** proposed by Mara, Tarantola, and Annoni (2015).

(see, also, Lebrun and Dutfoy (2009a, 2009b))

Organic variance decomposition: Dependence effects

Recall the following result:

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Definition *(Dependence effects).* *For every $A \in \mathcal{P}_D$, define the* ***dependence effects of X_A on $G(X)$ as***

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

Proposition . *Under Assumptions 1 and 2,*

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

Organic variance decomposition: Dependence effects

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What do they sum up to ?...

Probably some interesting global multivariate dependence measure!

Canonical variance decomposition

The structural effects represent the variance of each of the $G_A(X_A)$. It amounts to perform a **covariance decomposition** (Hart and Gremaud 2018; Da Veiga et al. 2021).

Definition *(Structural effects). For every $A \in \mathcal{P}_D$, define the* ***structural effects of X_A on $G(X)$ as***

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

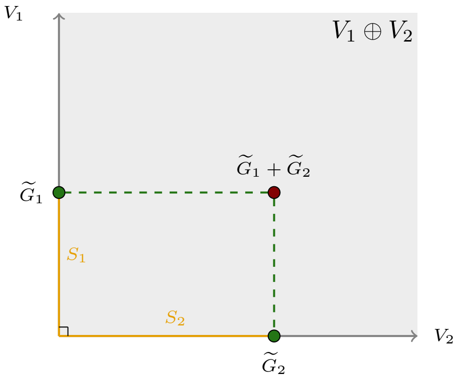
The **correlative effects** represent the part of variance that is due to the correlation between the $G_A(X_A)$.

Definition *(Correlative effects). For every $A \in \mathcal{P}_D$, define the* ***correlative effects of X_A on $G(X)$ as***

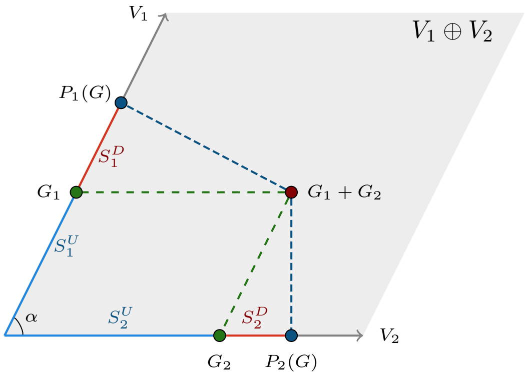
$$S_A^C = Cov\left(G_A(X_A), \sum_{B \in \mathcal{P}_D : B \neq A} G_B(X_B)\right).$$

Variance decomposition: Intuition

Pure interaction effects



Structural and dependence effects



Example: Two Bernoulli inputs

Let $E = \{0, 1\}^2$, and let $X = (X_1, X_2)$, where

$$X_1 \sim \mathcal{B}(q_1), \quad \text{and } X_2 \sim \mathcal{B}(q_2).$$

The joint law of X can be express using **three parameters**:

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

where $p_{ij} = \mathbb{P}(\{X_1 = i\} \cap \{X_2 = j\})$.

Any function $G : \{0, 1\}^2 \to \mathbb{R}$ can be expressed as the vector $G = (G_{00}, G_{01}, G_{10}, G_{11})^\top$.

Each value $G_{ij} = G(i, j)$, can be observed with probability p_{ij}.

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In this case, we can compute everything analytically.

It requires to solving 13 equations with 13 unknowns*.

*https://github.com/milidris/GeneralizedAnova

Feshchenko matrix and the Fréchet bounds

For the **Feshchenko matrix** Δ to be definite positive, one has that:

$$\max\left\{0, q_1q_2 - \sqrt{q_1q_2(1-q_1)(1-q_2)}\right\} < \rho < \min\left\{1, q_1q_2 - \sqrt{q_1q_2(1-q_1)(1-q_2)}\right\}.$$

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However, the **classical Fréchet bounds for ρ for bivariate Bernoulli random variables** (Joe 1997, p.210) are equal to

$$\max\{0, q_1 + q_2 - 1\} \leq \rho \leq \min\{q1, q2\},$$

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ρ strictly contained in the Fréchet bounds $\implies$ Assumptions 1 and 2 hold.

Our decomposition hold for virtually any dependence structure between two Bernoullis.

Conclusion

Main take-aways:

- Hoeffding-like decomposition of function with dependent inputs is **achievable under fairly reasonable assumptions.**
- Mixing **probability, functional analysis and combinatorics** lead to a **linear treatment of multivariate non-linear stochastic problems**.
- We can define **intuitive model-centric decompositions of quantities of interest**.
- We proposed candidates to separate **pure interaction** and **dependence effects**.

Perspectives

Main challenge: Estimation.

- We haven't found an **off-the-shelf method** to **estimate the oblique projections**...

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- We haven't found an **off-the-shelf method** to **estimate the oblique projections**...
- **But we have a lot of ideas on where to start :)**

A few perspectives:

- Causality and algebraic structures beyond the Boolean lattice.
- Link between Feshchenko matrices and copulas.
- Non $\mathbb{R}$-valued output.
- Beyond the MSE for surrogate modelling.
- Many methodological questions that seemed unreachable so far, but appear approachable using this framework.

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Thank you for your attention!

Any questions?

Annihilating property

Proposition *(Annihilating property).* *For any $A \in \mathcal{P}_D$ and any $B \subset A$*

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