# Generalized Hoeffding Decomposition

## and the (surprising) linear nature of non-linearities


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***CRM-ISM Montreal Probability seminar***
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# Hi!

## Marouane IL IDRISSI

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☞ **Before:** Ph.D. Candidate (2021-2024)

**EDF R&D - Institut de Mathématiques de Toulouse**

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*Interpretability methods for certifying machine learning models applied to critical systems*

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☞ **Now:** Postdoctoral Researcher (2024-2026+)

**UQÀM - IID** (ULaval)

Arthur Charpentier (UQÀM), Marie-Pier Côté (ULaval)

*Interpretability, fairness and causal inference of black-box models*

**(Some) Topics of interest:**

*XAI* ● *Uncertainty quantification* ● *Sensitivity analysis* ● *Industrial risks* ● *Probabilistic modelling* ● *Statistics* ● *Statistical Learning* ● *Applied cooperative game theory* ● *Functional analysis*

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**This is the case for Hoeffding's functional decomposition**

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- **Non-perfect functional dependence**
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What we mean by "non-mutually independent inputs":

- **Non-perfect functional dependence**
- **Non-degenerate stochastic dependence**

☞ Somewhat *unusual* way to **deal with dependence**

But it involves a lot of interesting mathematics!

At least in my opinion :)

# Random inputs, black-box model

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☞ The **black-box model** is a mapping $G : E \to \mathbb{R}$
☞ The **random output** is the ($\mathbb{R}$-valued) random variable $G(X)$

# Generated $\sigma$-algebras

☞ Denote by $\sigma_X$ the **$\sigma$-algebra generated by** $X$:

$$\sigma_X = \left\{ X^{-1}[B] \,:\, \forall B \in \bigotimes_{i \in D} \mathcal{E}_i \right\} \subset \mathcal{F}$$

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☞ Denote by $\sigma_\emptyset$ the $\mathbb{P}$**-trivial** $\sigma$**-algebra**:

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

**Lemma** *(Doob-Dynkin)*.

Let $Y$ be an $\mathbb{R}$-value random variable, and let $X$ be random inputs.
If $Y$ is $\sigma_X$-measurable, then there exists a function $f : E \to \mathbb{R}$ such that

$$Y = f(X) \text{ a.s.}$$

# Measurability and Lebesgue spaces

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**Lemma** *(Kallenberg (2021, Lemma 4.9))*.

Let $Y$ be an $\mathbb{R}$-value random variable.
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**Definition** *(Lebesgue spaces $\mathbb{L}^2$)*.

For a sub-$\sigma$-algebra $\mathcal{G} \subset \mathcal{F}$, denote by $\mathbb{L}^2(\mathcal{G})$ the **Lebesgue space of square-integrable, $\mathbb{R}$-valued, $\mathcal{G}$-measurable** random variables.

It is a **Hilbert space** with the inner product, $\forall Z_1, Z_2 \in \mathbb{L}^2(\mathcal{G})$:

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

# Non-perfect functional dependence

- ☞ $\mathbb{L}^2(\sigma_X)$ **contains random variables that are functions of** $X$.
- ☞ For every $A \subset D$, $\mathbb{L}^2(\sigma_A)$ **contains random variables that are functions of** $X_A$.
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**Theorem** *Sidák (1957, Theorem 2)*. Let $\mathcal{G}_1, \mathcal{G}_2 \subseteq \mathcal{F}$, then

- If $\mathcal{G}_1 \subset \mathcal{G}_2$, then $\mathbb{L}^2(\mathcal{G}_1) \subset \mathbb{L}^2(\mathcal{G}_2) \subseteq \mathbb{L}^2(\mathcal{F})$ ;
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**Assumption 1** *(Non-perfect functional dependence)*.

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

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

# Output space

Consequences of Assumption 1:

☞ $\mathbb{L}^2(\sigma_\emptyset) \subset \mathbb{L}^2(\sigma_A)$, for every $A \in \mathcal{P}_D$

**There are non-constant random variables in the Lebesgue spaces**

☞ For $B \subset A$, $\mathbb{L}^2(\sigma_B) \subset \mathbb{L}^2(\sigma_A)$

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**Proposition** . Suppose that Assumption 1 hold. Then, for any $A, B \in \mathcal{P}_D$ such that $A \cap B \notin \{A, B\}$, **there is no mapping $T$ such that**

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

☞ Hence the name **"non-perfect functional dependence"**

# Dependence and maximal angles between Lebesgue spaces

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

$$X \perp\!\!\!\perp Y \iff \forall f(X) \in \mathbb{L}^2_0(\sigma_X), \forall g(Y) \in \mathbb{L}^2_0(\sigma_Y), \quad \mathbb{E}[f(X)g(Y)] = 0,$$

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## Our intuition:

**Control the dependence structure of** $X$ by **controlling the magnitude of the inner product between the functions of** $X_A$ for every $A \in \mathcal{P}_D$.

# Minimal angle, maximal correlation

Dixmier's angle: the **maximal value** the inner product can take **between the elements of two closed subspaces** of a Hilbert space

**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

$$c_0(M, N) := \sup \{ |\langle x, y\rangle| : x \in M, \|x\| \leq 1, \quad y \in N, \|y\| \leq 1 \}.$$

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

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**Remark** . The independence relation from the previous slide can be written as:

$$X \perp\!\!\!\perp Y \iff c_0\left(\mathbb{L}_0^2\left(\sigma_X\right), \mathbb{L}_0^2\left(\sigma_Y\right)\right) = 0.$$

# Maximal partial correlation

Friedrichs' angle: Restriction to the **elements orthogonal to the intersection of the subspaces**

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**Remark** . It is closely related **to the commutativity of conditional expectations**.

$$c\left(\mathbb{L}^2(\sigma_X), \mathbb{L}^2(\sigma_Y)\right) = 0 \iff \mathbb{E}\left[\mathbb{E}\left[. \mid X\right] \mid Y\right] = \mathbb{E}\left[\mathbb{E}\left[. \mid Y\right] \mid X\right]$$

## Closure and complements

☞ They assess the **closedness of the sum of subspaces** (for an infinite-dimensional $H$):

- $c\,(M,N) < 1 \iff M + N$ is closed in $H$ ;
- $c_0\,(M,N) < 1 \iff M \cap N = \{0\}$ and $M + N$ is closed in $H$.

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☞ In Hilbert spaces, **a closed subspace is always complemented**:
If $M$ is closed, then there exists **another subspace** $K$ such that

$$H = M + K \text{ and } M \cap K = \{0\}.$$

## Closure and complements

☞ They assess the **closedness of <u>the sum</u> of subspaces** (for an infinite-dimensional $H$):

- $c(M, N) < 1 \iff M + N$ is closed in $H$ ;
- $c_0(M, N) < 1 \iff M \cap N = \{0\}$ and $M + N$ is closed in $H$.

☞ In Hilbert spaces, **a closed subspace is always complemented**:
If $M$ is closed, then there exists **another subspace** $K$ such that

$$H = M + K \text{ and } M \cap K = \{0\}.$$

☞ ***K* is what's missing from *M* to span the ambient space *H*.**
**One** popular complement of closed subspaces are their **orthogonal complement (**$M^{\perp}$**)**.

# Feshchenko matrix

- ☞ For every $A \in \mathcal{P}_D$, $\mathbb{L}^2(\sigma_A)$ contains **the functions of** $X_A$
- ☞ Dixmier's and Friedrichs' angles to **pairwise** control the inner products in these spaces

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Intuition: A **generalized precision matrix** to control the *global magnitude of all the angles*

**Definition** *(Maximal coalitional precision matrix)*.

Let $\Delta$ be the $(2^d \times 2^d)$, symmetric **set-indexed** matrix, defined element-wise, $\forall A, B \in \mathcal{P}_D$ as

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

We use **Friedrichs' angles** (partial correlation), hence the **precision** part

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## We're calling them "Feshchenko matrices".

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**Proposition** . Suppose that Assumption 1 hold. Then,

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**Assumption 2** *(Non-degenerate stochastic dependence)*.

The Feshchenko matrix $\Delta$ of the inputs $X$ is definite-positive.

It's a **restriction on the inner product of** $\mathbb{L}^2(\sigma_X) \implies$ **A restriction on the law of** $X$

☞ Hence the *stochastic dependence* (in opposition to *functional dependence*).

# Direct-sum decomposition

**Definition** *Direct-sum decomposition (Axler 2015)*.

Let $H$ be a vector space and let $H_1, \dots, H_n$ be proper subspaces of $H$.

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

$$h = \sum_{i=1}^{n} h_i \text{ where } h_i \in H_i \text{ for } i = 1, \dots, n.$$

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**Goal: Find a direct-sum decomposition of** $\mathbb{L}^2(\sigma_X)$ **w.r.t. the subspaces** $\{\mathbb{L}^2(\sigma_A)\}_{A \in \mathcal{P}_D}$

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☞ **Consider Hoeffding's decomposition as a direct-sum decomposition of $\mathbb{L}^2(\sigma_X)$**

# 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

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**Intuition of the proof:**

**Inductive functional centering**

# Intuition of the proof: 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** $\mathbb{L}^2(\sigma_i)$ (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 $\mathbb{L}^2(\sigma_i) = V_\emptyset \oplus V_i$

We just showed that any $f(X_i) \in \mathbb{L}^2(\sigma_i)$ can be written as

$$f(X_i) = \underbrace{\mathbb{E}[f(X_i)]}_{\in V_\emptyset} + \underbrace{\mathbb{E}[f(X_i) - \mathbb{E}[f(X_i)]]}_{\in V_i = \mathbb{L}^2_0(\sigma_i)}$$

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**And note that** $\mathbb{L}^2(\sigma_i) = V_\emptyset \oplus V_i$ **hold for any** $i \in D$ **(induction)**

# Intuition of the proof: Two inputs

**Two inputs:**

1. Let $i, j \in D$, and **fix** $\mathbb{L}^2(\sigma_{ij})$ **as the ambient space**
2. **Assumptions 1 and 2 imply that** $\mathbb{L}^2(\sigma_i) + \mathbb{L}^2(\sigma_j)$ **is closed in** $\mathbb{L}^2(\sigma_{ij})$ (it is **complemented**)
3. Notice **(previous step)** that $\mathbb{L}^2(\sigma_i) + \mathbb{L}^2(\sigma_j) = V_\emptyset + V_i + V_j$
4. Denote $V_{ij} = [V_\emptyset + V_i + V_j]^{\perp_{ij}}$, **the orthogonal complement in** $\mathbb{L}^2(\sigma_{ij})$
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We **"centered" a bivariate function from its "univariate and constant parts"**

**We continue the induction up to $d$ inputs.**

# Orthocanonical decomposition

**Corollary** *(Orthocanonical decomposition)*.

Suppose that Assumptions 1 and 2 hold.

Then, any random variable $G(X) \in \mathbb{L}^2\left(\sigma_X\right)$ can be **uniquely decomposed** as

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

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

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**Is it possible to characterize the *representants* $G_A(X_A)$?**

## Projectors

- ☞ Let $H$ be a Hilbert space, and let $P : H \to H$ be an operator
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If $P$ is an idempotent ($P \circ P = P$), linear, and bounded operator, it is then called the **oblique projector onto $\mathbf{Ran}\,(P)$ parallel to $\mathbf{Ker}\,(P)$** and

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Conversely, suppose that

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then there exists a projector $P$ such that $\mathrm{Ran}\,(P) = M$ and $\mathrm{Ker}\,(P) = N$ (Galántai 2004)

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If in addition $N = M^{\perp}$ ($P$ is self-adjoint), then $P$ is called the **orthogonal projector** onto $M$
☞ The orthogonal projector onto $\mathbb{L}^2\,(\sigma_A)$ is the conditional expectation $\mathbb{E}\,[. \mid \sigma_A]$

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**Oblique projection onto $V_A$**

The operator

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

$Q_A$ is the (canonical) **oblique projection** with

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## Orthogonal projections onto $V_A$

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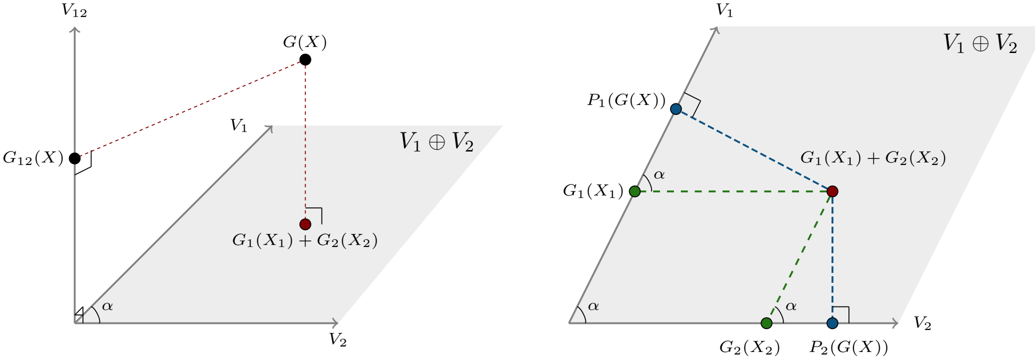
is the **orthogonal projection** onto $V_A$.

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

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

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



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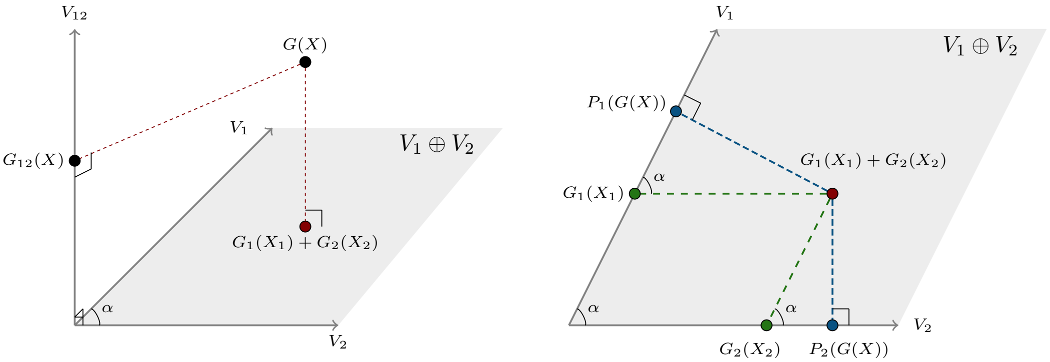


**The oblique projection $Q_A$ usually differ from the orthogonal projections $P_A$**

# Oblique and orthogonal projections

In fact,

**Proposition .**

Under Assumptions 1 and 2,

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

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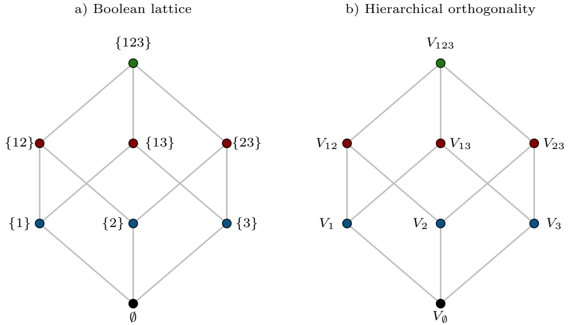
But, under Assumptions 1 and 2, they **may not be all orthogonal**

**There is a more visual way to illustrate that**

# Boolean lattice and hierarchical orthogonality

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

☞ Endowed with the **binary relation** $\subseteq$, $(\mathcal{P}_D, \subseteq)$ forms **a Boolean lattice**




The subspaces $\{V_A\}_{A \in \mathcal{P}_D}$ are **hierarchically orthogonal** **by design**

☞ They form the same algebraic structure **w.r.t. to** $\perp$

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**(Canonical) oblique projection onto $\mathbb{L}^2(\sigma_A)$:**

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**Can we characterize $Q_A$ w.r.t. $\mathbb{M}_A$?**

# Generalized Möbius inversion

Because $(\mathcal{P}_D, \subseteq)$ forms a **Boolean lattice**, yes!

**Corollary** *(Möbius inversion on power-sets (Rota 1964)).*

For any two set functions:

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

valued in an abelian group $\mathbb{A}$, the following equivalence holds:

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

☞ Analogous to the *inclusion-exclusion principle*

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

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

which is equivalent to

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

# Generalized Hoeffding decomposition

Hoeffding (1948) found that **for mutually independent inputs**:

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

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**Proposition .**

Under Assumptions 1 and 2,

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**Our approach generalizes Hoeffding's original decomposition!**

# Illustrative example: Two Bernoulli inputs

Let $X = (X_1, X_2)$, where

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

The joint law of $X$ can be characterized 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 $p_{ij} = \mathbb{P}\left(\{X_1 = i\} \cap \{X_2 = j\}\right)$

The functions of $X$ $G : \{0,1\}^2 \to \mathbb{R}$ can be expressed as a vector

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**In this case, we can compute everything analytically**

It requires solving 13 equations with 13 unknowns*

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

# Feshchenko matrix and the Fréchet bounds

For the **Feshchenko matrix** $\Delta$ to be definite positive, one has that:

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

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

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and are **more restrictive than the previous bounds**

**$\rho$ strictly contained in the Fréchet bounds $\implies$ Assumptions 1 and 2 hold**

**The generalized decomposition holds for any (non-comonotone) copula between two Bernoulli random variables**

# Main take-aways

☞ Under **mild assumptions** on the random inputs $X$, for any $G(X) \in \mathbb{L}^2(\sigma_X)$,

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

(Virtually) any model can be **decomposed** as a **sum of (pure) interactions of increasing dimensionality**

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Which **control the maximal angles** between **Lebesgue spaces generated by the subsets of inputs**

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Thanks to the **algebraic structure of the power-set**

**Non-linear problem in $d$ dimensions becomes linear in $2^d$ dimensions**

# Some perspectives

☞ **Main challenge: Estimating the orthocanonical projections from observations**

They sure look a lot like conditional expectations...

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☞ **Beyond the power-set**

Other algebraic structures to model different data generating processes

Links with causality and probabilistic graphical models

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Thank you for your attention!

Any questions?

**Let's talk about variance decomposition.**

We propose **two complementary approaches** for decomposing $\mathbb{V}(G(X))$ based on this generalized decomposition.

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

$$\widetilde{X}_i \stackrel{d}{=} X_i, \qquad \text{and } \widetilde{X} \text{ is mutually independent.}$$

**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 $X$.

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:

**Proposition** . Under Assumptions 1 and 2,

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

Which motivates the definition of dependence effects.

**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,

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

**What do they sum up to ?...**

Probably some interesting global multivariate dependence effect 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**

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

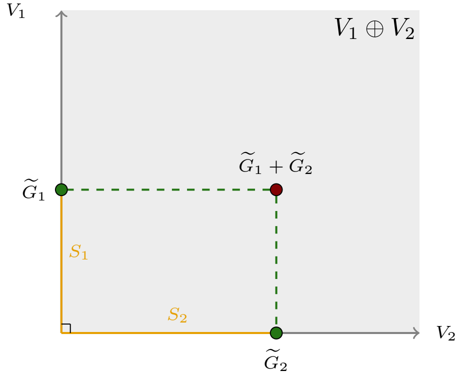
The **correlative effects** represent the part of variance that is due to the correlation between the $G_A(X_A)$

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

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

# Variance decomposition: Intuition

Pure interaction effects




Structural and dependence effects