Black-Box Model Decomposition with Dependent Random Inputs

The (surprising) linear nature of non-linearity

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Context

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$\Longrightarrow$ **No definitive answer to the problem.**

However, a generalization holds under **two reasonable assumptions**, which leads to **intuitive importance measures**.

Framework and notations

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space and let $X = (X_1, \dots, X_d)$ be random inputs, i.e.,

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

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

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For every $A \subset D$, denote $X_A = (X_i)_{i \in A}$ a **the subset of inputs in** A.

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Denote by $\sigma_\emptyset \subset \mathcal{F}$ the $\mathbb{P}$**-trivial** σ**-algebra** (smallest σ-algebra containing the elements of Ω of probability 0).

Proposition *(Resnick 2014). If an $\mathbb{R}$-valued random variable is $\sigma_\emptyset$-measurable, it is **constant a.e.***

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$\forall A \subset D$, denote by $\sigma_A \subset \mathcal{F}$ the σ**-algebra generated by** X_A, and σ_X the one generated by X.

Some probability theory

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

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Definition *(Lebesgue space). Let $\mathcal{G} \subset \mathcal{F}$ be a sub-σ-algebra. Denote by $\mathbb{L}^2(\mathcal{G})$ the* ***Lebesgue space*** *containing every* ***real-valued random variables****, which are $\mathcal{G}$-measurable, and, if $Y \in \mathbb{L}^2(\sigma_{\mathcal{G}})$*

$$\mathbb{E}\left[Y^2\right] = \int_\Omega Y(\omega)^2 d\mathbb{P}(\omega) < \infty.$$

Remark . $\mathbb{L}^2(\sigma_X)$ is the space of **random outputs** of the form $G(X)$.

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Proposition . *$\mathbb{L}^2(\sigma_X)$ is an (infinite-dimensional) Hilbert space, with inner product*

$$\langle f(X), g(X)\rangle = \mathbb{E}\left[f(X)g(X)\right] = \int_E f(x)g(x)dP_X(x) = \int_\Omega f(X(\omega))g(X(\omega))d\mathbb{P}(\omega).$$

Angles between subspaces of Hilbert spaces

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 *(Friedrich's angle (Friedrichs 1937)).* *The cosine of Friedrichs' angle is defined as*

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

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

Friedrich's angle is used in probability theory as a measure of **partial dependence** (Bryc 1984, 1996).

Direct-sum decompositions

Definition *(Direct-sum decomposition). Let $W_1, \dots, W_d$ be vector subspaces of a vector space W. W is said to admit a* ***direct-sum decomposition****, denoted:*

$$W = \bigoplus_{i=1}^{d} W_i,$$

if any element $w \in W$ can be written ***uniquely*** *as a sum of elements of the W_i.*

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Hence, a Hoeffding-like (coalitional) decomposition of a **black-box model** entails **finding a direct-sum decomposition for** $\mathbb{L}^2(\sigma_X)$, i.e., writting

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

where the V_A needs to be defined.

Assumptions

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

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

Remark . This assumption has nothing to do with the law of X. It is purely functional.

Lemma . *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*** $X_B = T(X_A)$ ***a.e***.

Remark . In other words, under Assumption 1, **the inputs cannot be functions of each other**.

Assumptions

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

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

Δ can be seen as a generalization of **precision matrices**.

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

We are now ready to state the second assumption.

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Assumption 2 *(Non-degenerate stochastic dependence).* Δ *is definite-positive.*

Main result

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

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

where $\perp_B$ denotes the orthogonal complement in $\mathbb{L}^2(\sigma_B)$.

Corollary (Canonical 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 $G_A(X_A) \in V_A$.

Intuition behind the result

<u>**One input:**</u>

Let $i \in D$. Then, any $f(X_i) \in \mathbb{L}^2(\sigma_i)$ can be written as

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

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Two inputs:

Let $i, j \in D$. We have that $\mathbb{L}^2(\sigma_i)$ and $\mathbb{L}^2(\sigma_j)$ are **closed subspaces of** $\mathbb{L}^2(\sigma_{ij})$.

Assumptions 1 and 2 implies that $\mathbb{L}^2(\sigma_i) + \mathbb{L}^2(\sigma_j)$ is closed, and thus **is complemented in $\mathbb{L}^2(\sigma_{ij})$ by**

$$V_{ij} := \left[\mathbb{L}^2(\sigma_i) + \mathbb{L}^2(\sigma_j)\right]^{\perp_{ij}} = [V_\emptyset + V_i + V_j]^{\perp_{ij}}.$$

And then,

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And we can continue up to d inputs by induction.

Projectors

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 **oblique projection** onto V_A, parallel to $\bigoplus_{B \in \mathcal{P}_D : B \neq A} V_A$.

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Orthogonal projections

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

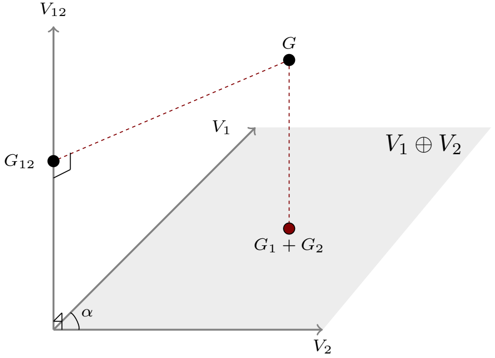
the **orthogonal projection** onto V_A.

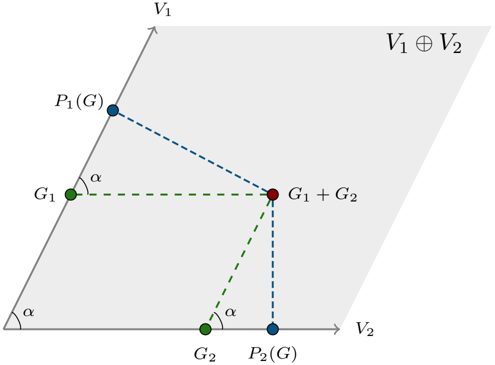
Illustration : $\mathbb{L}_0^2(\sigma_{12})$

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

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

which **usually differ from the orthogonal projection** $P_A(G(X))$.





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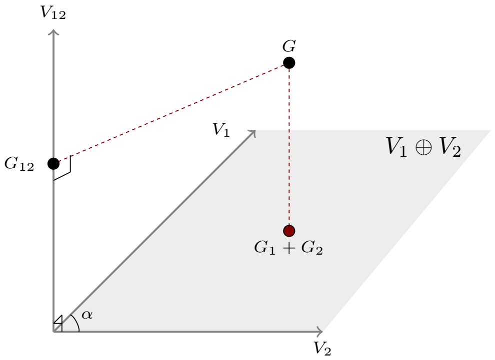

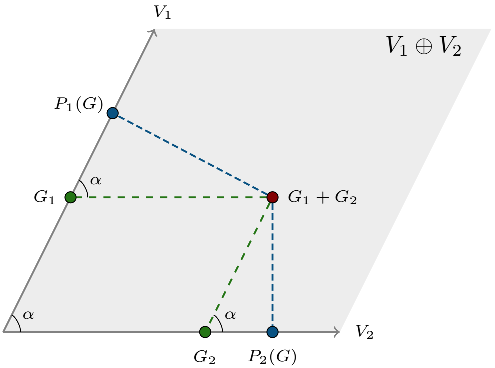

Assumptions 1 + 2 $\implies$ **V_1 and V_2 are distinct.**

Variance decomposition

We propose two complementary approaches for decomposing $\mathbb{V}\left(G(X)\right)$.

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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.

Canonical 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

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

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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.

Organic variance decomposition: Dependence effects

Recall that **usually,** $P_A(G(X))$ **and** $Q_A(G(X))$ **differ**. In fact,

Proposition . *Under Assumptions 1 and 2,*

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

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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***

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

Proposition . *Under Assumptions 1 and 2,*

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

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Probably some interesting 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***

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

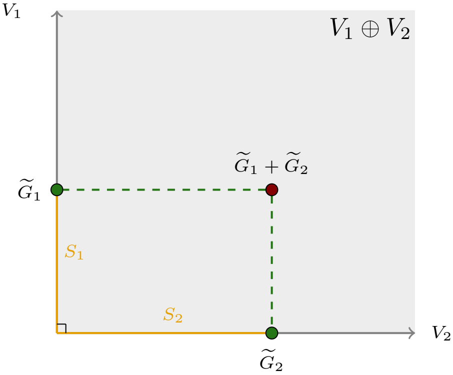
The **correlative effects** represent the part of variance that is due to the correlation between the $G_A(X_A)$.

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

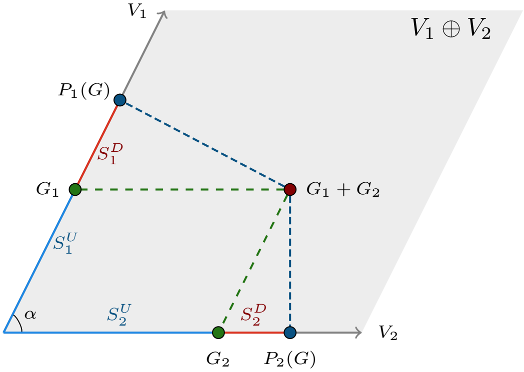
$$S_A^C = \mathcal{C}ov\left(G_A(X_A), \sum_{B \in \mathcal{P}_D : B \neq A} G_B(X_B)\right).$$

Variance decomposition: Intuition

Pure interaction effects



Structural and dependence effects



Conclusion

Main take-aways:

- Hoeffding-like decomposition of function with dependent inputs is **achievable under reasonable assumptions.**
- Mixing **probability, functional analysis (and combinatorics)** lead to an **interesting framework for studying multivariate stochastic problems**.
- We can define **meaningful (i.e., intuitive) decompositions of quantities of interest**, which **intrinsically encompasses the dependence between the inputs**.
- We proposed candidates to separate and quantify **pure interaction** from **dependence effects**.

Perspective

Main challenge: Estimation.

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A few perspectives:

- Links with already-established results (e.g., on copulas).
- Non $\mathbb{R}$-valued output.
- Many methodological questions that seemed unreachable so far, but appear approachable using this framework.

Checkout our pre-print!

To go further + illustrations (HAL/ResearchGate)

Understanding black-box models with dependent inputs through a generalization of Hoeffding's decomposition

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References i

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Thank you for your attention!

Any questions?