SOBOL' INDICES, SHAPLEY EFFECTS

AND A (NEW) PATH TOWARDS HANDLING DEPENDENT INPUTS

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Sensitivity Analysis Discord Group
Online
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Marouane IL IDRISSI

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

EDF R&D - Institut de Mathématiques de Toulouse

Nicolas Bousquet, Fabrice Gamboa, Bertrand Iooss, Jean-Michel Loubes

Interpretability methods for certifying machine learning models applied to critical systems

☞ **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*

Introduction

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How to go beyond mutually independent inputs

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Quick outline:

- ☞ **From Hoeffding's decomposition to Sobol' indices**
- ☞ **Shapley effects and the "cooperative games" solution**
- ☞ **Generalized Hoeffding decomposition: disentangling interaction and dependence**

Hoeffding's decomposition

- ☞ Let $D = \{1, \ldots, d\}$ and let $\mathcal{P}_D$ denote the **power-set** of D
- ☞ Let $X = (X_1, \ldots, X_d)$ be a random vector of **mutually independent inputs**
- ☞ For every $A \in \mathcal{P}_D$, $A \neq \emptyset$, let X_A be a **subset of the inputs**
- ☞ Let G be a **given "black-box" model** such that $\mathbb{V}(G(X)) < \infty$

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Hoeffding (1948): We can **uniquely** write

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

where $G_\emptyset$ is a constant, and the **representants** are all **pairwise orthogonal**, i.e.,

$$\forall A, B \in \mathcal{P}_D, A \neq B, \quad \mathbb{E}\left[G_A(X_A) G_B(X_B)\right] = 0$$

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Moreover, we can characterize

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

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In this case, we have that

$$G_1(X_1) = X_1 \quad G_2(X_2) = 0, \quad G_3(X_3) = 0,$$
$$G_{12}(X_{12}) = 0, \quad G_{13}(X_{13}) = 0, \quad G_{23}(X_{23}) = X_2X_3,$$
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We can retrieve the full model by only having access to the **representants**

Sobol' indices

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An input is important $\iff$ It **contributes** to the model's **uncertainty**

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Sobol (2001) proposed to use

$$S_A = \frac{\mathbb{V}\left(G_A(X_A)\right)}{\mathbb{V}\left(G(X)\right)} = \frac{1}{\mathbb{V}\left(G(X)\right)} \times \sum_{B \in \mathcal{P}_A} (-1)^{|A|-|B|} \mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_B\right]\right)$$

based on the rationale of **Hoeffding's decomposition**

$$\mathbb{V}\left(G(X)\right) = \mathbb{V}\left(\sum_{A \in \mathcal{P}_D} G_A(X_A)\right) \overset{\perp}{=} \sum_{A \in \mathcal{P}_D} \mathbb{V}\left(G_A(X_A)\right)$$

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The model's uncertainty is equal to the sum of its representant's uncertainty

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If we **keep the same formula** : $S_A = \frac{1}{\mathbb{V}(G(X))} \times \sum_{B \in \mathcal{P}_A} (-1)^{|A|-|B|} \mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_B\right]\right)$

$$G(X) = X_1 + X_2 X_3, \quad X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & \rho \\ 0 & 1 & 0 \\ \rho & 0 & 1 \end{pmatrix}\right)$$

Mutually independent case ($\rho = 0$)

$$S_1 = 0.5 \quad S_2 = 0, \quad S_3 = 0,$$
$$S_{12} = 0, \quad S_{13} = 0, \quad S_{23} = 0.5,$$
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Correlated case ($\rho \neq 0$)

$$S_1 = 0.5 \quad S_2 = 0, \quad S_3 = \rho^2/2,$$
$$S_{12} = \rho^2/2, \quad S_{13} = -\rho^2/2, \quad S_{23} = 0.5,$$
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☞ They still **sum to 1** but they can be **negative**

But their overall interpretation as (pure) interaction effects does not hold anymore...

Sobol' indices computed on dependent inputs

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1. **Negative effects** (dependence)
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But, there are solutions!

1. **Cooperative games' allocations** (e.g., Shapley values)
2. **Beyond Hoeffding's original decomposition**

Shapley effects

The Shapley effects (Owen 2014): **Egalitarian redistribution of the Sobol' indices.**

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But let's take a step back...

Cooperative game theory

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"Cooperative game theory = The art of cutting a cake"

Let $D = \{1, \dots, d\}$ be a **set of players**, and $\mathcal{P}_D$ the **set of coalitions**

Let $v : \mathcal{P}_D \to \mathbb{R}$ be a **chosen value function**

☞ (D, v) formally defines a **cooperative game**

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Hint: by using an **allocation**

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How can we define efficient and nonnegative allocations?

The Harsanyi set

The **Harsanyi (1963) dividends** of a cooperative game (D, v) are defined as:

$$\mathcal{D}_v(A) = \sum_{B \in \mathcal{P}_A} (-1)^{|A|-|B|} v(B)$$

It is a mapping $\mathcal{D}_v(A) : \mathcal{P}_D \to \mathbb{R}$

☞ They can be interpreted as the **added value** produced by each **coalition**

☞ They **always** sum-up to $v(D)$:

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The **Harsanyi set of allocations** (Vasil'ev and Laan 2001) are **aggregations of the Harsanyi dividends**:

$$\psi(i) = \sum_{A \in \mathcal{P}_D \,:\, i \in A} \lambda_i(A) \mathcal{D}_v(A), \quad \text{where} \quad \begin{cases} \forall i \in D, \forall A \in \mathcal{P}_D, \ \lambda_i(A) \geq 0, \\ \forall A \in \mathcal{P}_D, \ \sum_{i \in D} \lambda_i(A) = 1 \end{cases}$$

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☞ **They are always efficient**

☞ **Nonnegative if v is monotonic**

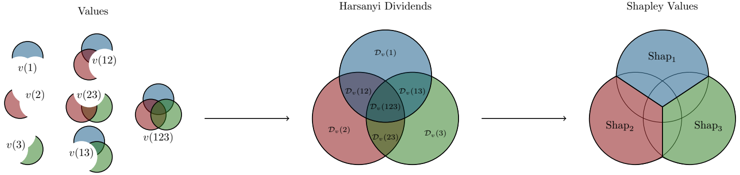
It is the case for $\mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_A\right]\right)$

Egalitarian redistribution: the Shapley values

The **Shapley (1951) values** are the **egalitarian redistribution of the dividends**.

For a player $i \in D$,

$$\mathrm{Shap}_i = \sum_{A \in \mathcal{P}_D : i \in A} \frac{\mathcal{D}_v(A)}{|A|}.$$



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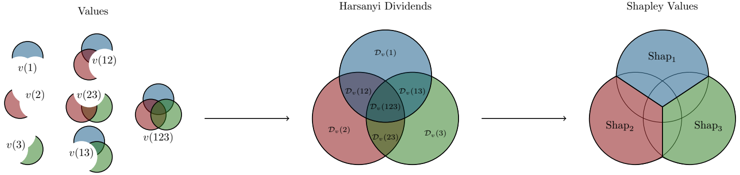

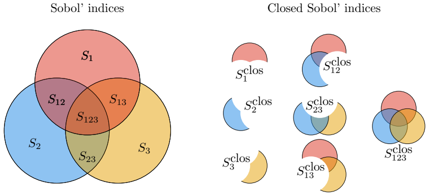

Shapley effects (Owen 2014):

Shapley values with $v(A) = \mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_A\right]\right) = S_A^{\mathrm{clos}}$

$$\mathrm{Sh}_i = \sum_{A \in \mathcal{P}_D : i \in A} \frac{S_A}{|A|}$$

The **Harsanyi dividends** become S_A: the **Sobol' indices**

Exogeneity detection and Shapley's joke

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An **exogenous input** can have a **non-zero share of importance**.

We call it **Shapley's joke** (Iooss and Prieur 2019)

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To solve this issue, we proposed to use **a proportional redistribution of the dividends** (Ortmann 2000)

It led to the definition of the **proportional marginal effects (PME)** (Herin et al. 2023)

Exogeneity detection and Shapley's joke

However, the **Shapley effects** have a **practical drawback**

An **exogenous input** can have a **non-zero share of importance**.

We call it **Shapley's joke** (Iooss and Prieur 2019)

$$G(X) = X_1 + X_2, \quad X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & \rho \\ 0 & 1 & 0 \\ \rho & 0 & 1 \end{pmatrix} \right)$$

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> **Proposition** *(Exogeneity detection)*. Under mild assumptions on the probabilistic structure of X,
>
> $$PME_i = 0 \iff X_i \text{ is exogenous.}$$

In practice, they tend to **"discriminate more" than the Shapley values** when the inputs are **highly correlated**

Estimation

Estimating the PME/Shapley effects $\iff$ Estimating $v(A)$ for every $A \in \mathcal{P}_D$.

Two settings:

- **You can sample your model at will (Monte Carlo)**: Requires a number proportional to $d!(d-1)$ model evaluations (Song, Nelson, and Staum 2016).
  The estimation cost can be substantially lowered by giving-up precision.
- **You only have access to an i.i.d. sample (Given-data)**: **The nearest-neighbor procedure** requires 2^d estimates (Broto, Bachoc, and Depecker 2020a).

These methods are time-consuming and scale exponentially with the number of inputs, but the **estimates can be recycled to compute both indices at once.**
But there are many strategies to drive the computational burden down at the expense of precision

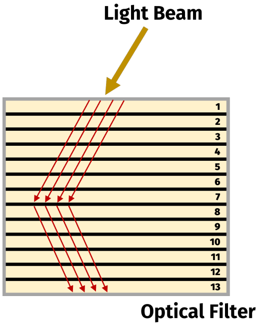
Optical filter transmittance - Feature selection

Transmittance performance of an **optical filter** composed of 13 consecutive layers (Vasseur et al. 2010).

The inputs $I_1, \ldots, I_{13}$ represent the **refractive index error** of each layer.

These errors are (highly) correlated due to the manufacturing process.

The numerical model computes the **transmittance error w.r.t. the "perfect filter"** over several wavelengths.



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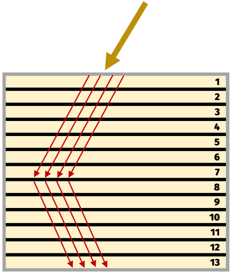


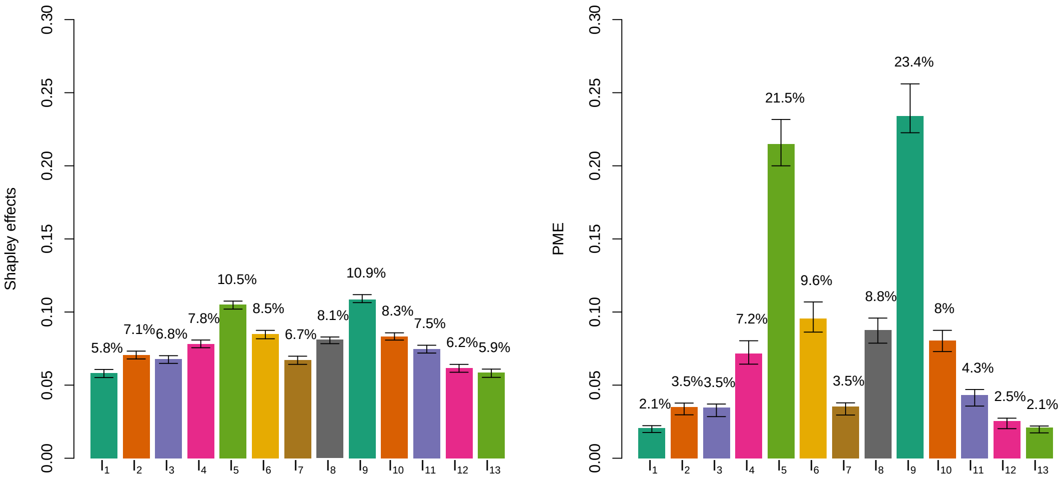
☞ **We only have access to an i.i.d. input-output sample** ($n = 1000$).

The indices are computed using a **nearest-neighbors approach** (Broto, Bachoc, and Depecker 2020b).

Parallelized implementation using the R package `sensitivity` ($\sim$ 4min runtine, 8 cores).

Arbitrarily chosen number of neighbors: 6.

Optical filter transmittance - Feature selection



Optical filter transmittance - Feature selection

Scenario: We want to build a surrogate model (Gaussian process*) of this numerical model.

Using the whole dataset: $Q^2 = 99.48\%$.

Feature selection:

- First threshold: 2.5% importance.
  - **Shapley effects:** No features removed.
  - **PME:** l_1 and l_3 are removed, $Q^2 = 99.14\%$.
- Second threshold: 5% importance.
  - **Shapley effects:** No features removed.
  - **PME:** 7 inputs are removed, $Q^2 = 98.79\%$.

* $5/2$ Matérn covariance kernel, constant trend.

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But what about the second issue?

Generalizing Hoeffding's decomposition to dependent inputs

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But we believe we found an interesting approach to tackle it!

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We do this by imposing two assumptions:

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- Non-perfect functional dependence between the inputs
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Under these two assumptions **we can actually decompose the space of outputs**

Consequences

Under these two assumptions, any real-valued **random output** $G(X)$ with finite second moment can be **uniquely** decomposed:

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

where $G_A(X_A)$ are **hierarchically orthogonal**

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They can be characterized using **oblique projections** $\mathbb{M}_A[G(X)]$ which **change w.r.t. the dependence structure**:

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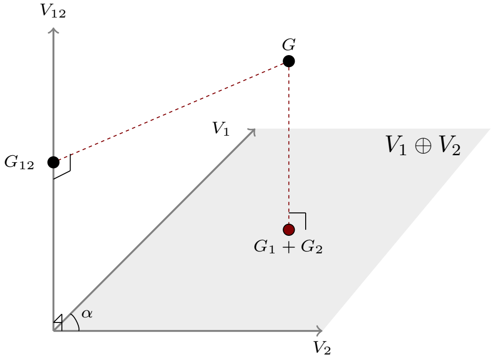
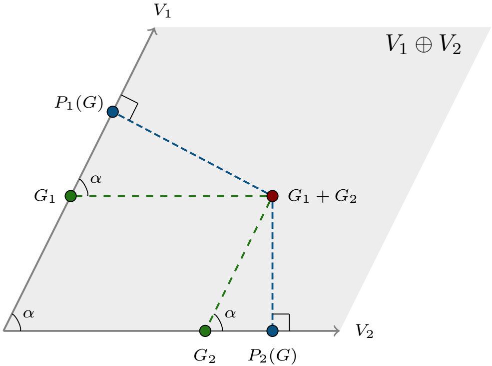
☞ **We recover Hoeffding's classical decomposition**

Illustration*: bivariate function





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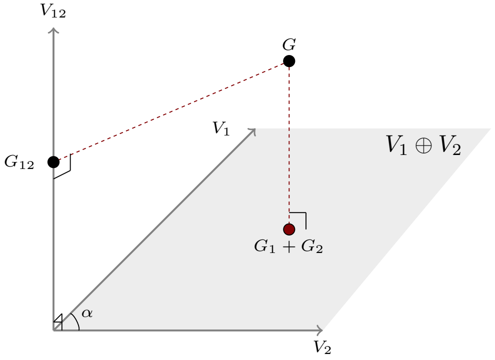

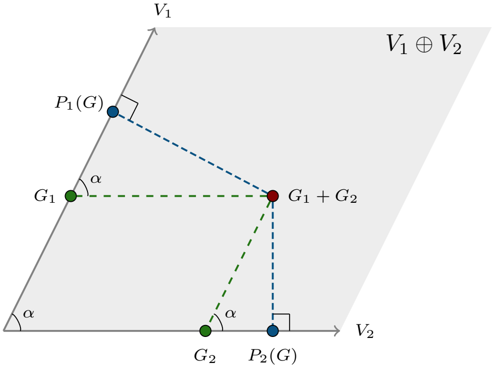

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Variance decomposition

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We propose **two complementary approaches** for decomposing $\mathbb{V}(G(X))$ based on this generalized decomposition, **inspired from the existing literature**

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

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

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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.

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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

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Probably the *overall effect of the dependence on the model's uncertainty*!

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 representants $G_A(X_A)$

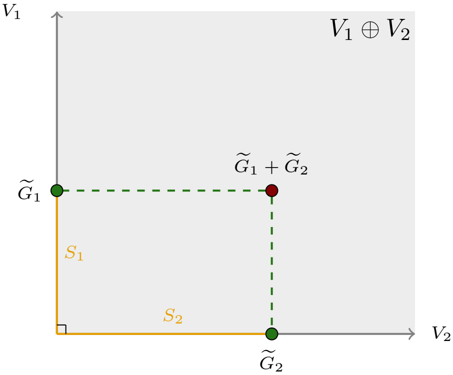
Definition *(Correlative effects)*.

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



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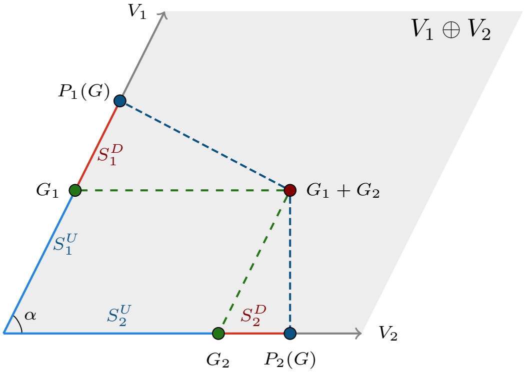

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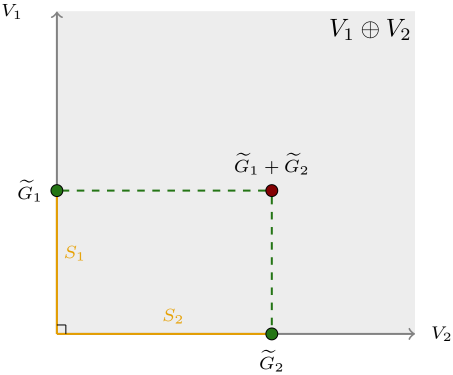

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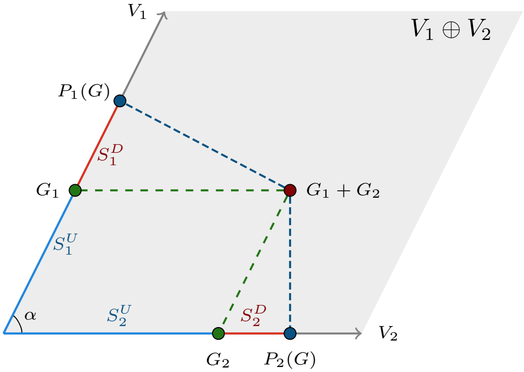

☞ **Maybe a good candidate to solve our second issue!**

Some perspectives

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Global and local sensitivity analysis, theoretically-grounded XAI, fairness assessment...

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☞ **Beyond hierarchical orthogonality**

e.g., Köhler, Rügamer, and Schmid (2024) with "stacked orthogonality" conditions

Broto, B., F. Bachoc, and M. Depecker. 2020a. "Variance reduction for estimation of Shapley effects and adaptation to unknown input distribution." *SIAM/ASA Journal on Uncertainty Quantification* 8:693–716.

———. 2020b. "Variance Reduction for Estimation of Shapley Effects and Adaptation to Unknown Input Distribution." *SIAM/ASA Journal on Uncertainty Quantification* 8 (2): 693–716. ISSN: 2166-2525. https://doi.org/10.1137/18M1234631. https://epubs.siam.org/doi/10.1137/18M1234631.

Chastaing, G., F. Gamboa, and C. Prieur. 2012. "Generalized Hoeffding-Sobol decomposition for dependent variables - application to sensitivity analysis." Publisher: Institute of Mathematical Statistics and Bernoulli Society, *Electronic Journal of Statistics* 6, no. none (January): 2420–2448. ISSN: 1935-7524, 1935-7524. https://doi.org/10.1214/12-EJS749. https://projecteuclid.org/journals/electronic-journal-of-statistics/volume-6/issue-none/Generalized-Hoeffding-Sobol-decomposition-for-dependent-variables---application/10.1214/12-EJS749.full.

Da Veiga, S., F. Gamboa, B. Iooss, and C. Prieur. 2021. *Basics and Trends in Sensitivity Analysis. Theory and Practice in R.* SIAM. Computational Science / Engineering.

Harsanyi, J. C. 1963. "A Simplified Bargaining Model for the n-Person Cooperative Game." Publisher: [Economics Department of the University of Pennsylvania, Wiley, Institute of Social and Economic Research, Osaka University], *International Economic Review* 4 (2): 194–220. ISSN: 0020-6598. https://doi.org/10.2307/2525487. https://www.jstor.org/stable/2525487.

Hart, J., and P. A. Gremaud. 2018. "An approximation theoretic perspective of Sobol' indices with dependent variables" [in English]. Publisher: Begel House Inc. *International Journal for Uncertainty Quantification* 8 (6). ISSN: 2152-5080, 2152-5099. https://doi.org/10.1615/Int.J.UncertaintyQuantification.2018026498. https://www.dl.begellhouse.com/journals/52034eb04b657aea,23dc16a4645b89c9,61d464a51b6bf191.html.

Herin, M., M. I., V. Chabridon, and B. Iooss. 2023. "Proportional marginal effects for global sensitivity analysis." Preprint. https://hal.science/hal-03825935.

Hoeffding, W. 1948. "A Class of Statistics with Asymptotically Normal Distribution." *The Annals of Mathematical Statistics* 19 (3): 293–325. ISSN: 0003-4851, 2168-8990. https://doi.org/10.1214/aoms/1177730196. https://projecteuclid.org/journals/annals-of-mathematical-statistics/volume-19/issue-3/A-Class-of-Statistics-with-Asymptotically-Normal-Distribution/10.1214/aoms/1177730196.full.

Hooker, G. 2007. "Generalized Functional ANOVA Diagnostics for High-Dimensional Functions of Dependent Variables" [in en]. *Journal of Computational and Graphical Statistics* 16 (3): 709–732. http://www.jstor.org/stable/27594267.

Iooss, B., and C. Prieur. 2019. "Shapley effects for Sensitivity Analysis with correlated inputs : Comparisons with Sobol' Indices, Numerical Estimation and Applications." *International Journal for Uncertainty Quantification* 9 (5): 493–514.

Kuo, F. Y., I. H. Sloan, G. W. Wasilkowski, and H. Woźniakowski. 2009. "On decompositions of multivariate functions" [in en]. *Mathematics of Computation* 79, no. 270 (November): 953–966. ISSN: 0025-5718. https://doi.org/10.1090/S0025-5718-09-02319-9. http://www.ams.org/journal-getitem?pii=S0025-5718-09-02319-9.

Köhler, D., D. Rügamer, and M. Schmid. 2024. *Achieving interpretable machine learning by functional decomposition of black-box models into explainable predictor effects.* ArXiv:2407.18650 [cs, stat], July. Accessed August 26, 2024. http://arxiv.org/abs/2407.18650.

Lebrun, R., and A. Dutfoy. 2009a. "A generalization of the Nataf transformation to distributions with elliptical copula." *Probabilistic Engineering Mechanics* 24 (2): 172–178. ISSN: 0266-8920. https://doi.org/10.1016/j.probengmech.2008.05.001. https://www.sciencedirect.com/science/article/pii/S0266892008000507.

———. 2009b. "Do Rosenblatt and Nataf isoprobabilistic transformations really differ?" *Probabilistic Engineering Mechanics* 24 (4): 577–584. ISSN: 0266-8920. https://doi.org/10.1016/j.probengmech.2009.04.006. https://www.sciencedirect.com/science/article/pii/S0266892009000307.

Mara, Thierry A., Stefano Tarantola, and Paola Annoni. 2015. "Non-parametric methods for global sensitivity analysis of model output with dependent inputs" [in en]. *Environmental Modelling & Software* 72 (October): 173–183. ISSN: 13648152. https://doi.org/10.1016/j.envsoft.2015.07.010. https://linkinghub.elsevier.com/retrieve/pii/S1364815215300153.

Ortmann, K. M. 2000. "The proportional value for positive cooperative games." *Mathematical Methods of Operations Research (ZOR)* 51 (2): 235–248.

Owen, A. B. 2014. "Sobol' Indices and Shapley Value." *SIAM/ASA Journal on Uncertainty Quantification* 2 (1): 245–251. ISSN: 2166-2525. https://doi.org/10.1137/130936233. http://epubs.siam.org/doi/10.1137/130936233.

Peccati, Giovanni. 2004. "Hoeffding-ANOVA decompositions for symmetric statistics of exchangeable observations." Publisher: Institute of Mathematical Statistics, *The Annals of Probability* 32 (3): 1796–1829. ISSN: 0091-1798, 2168-894X. https://doi.org/10.1214/009117904000000405. https://projecteuclid.org/journals/annals-of-probability/volume-32/issue-3/Hoeffding-ANOVA-decompositions-for-symmetric-statistics-of-exchangeable-observations/10.1214/009117904000000405.full.

Rabitz, H., and O. Aliş. 1999. "General foundations of high-dimensional model representations" [in en]. *Journal of Mathematical Chemistry* 25 (2): 197–233. ISSN: 1572-8897. https://doi.org/10.1023/A:1019188517934. https://doi.org/10.1023/A:1019188517934.

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

Sobol, I.M. 2001. "Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates." *Mathematics and Computers in Simulation* 55 (1): 271–280. ISSN: 03784754.

Song, E., B.L. Nelson, and J. Staum. 2016. "Shapley effects for global sensitivity analysis: Theory and computation." *SIAM/ASA Journal on Uncertainty Quantification* 4:1060–1083.

Vasil'ev, V., and G. van der Laan. 2001. *The Harsanyi Set for Cooperative TU-Games.* Working Paper 01-004/1. Tinbergen Institute Discussion Paper. https://www.econstor.eu/handle/10419/85790.

References v

Vasseur, O., M. Claeys-Bruno, M. Cathelinaud, and M. Sergent. 2010. "High-dimensional sensitivity analysis of complex optronic systems by experimental design: applications to the case of the design and the robustness of optical coatings." *Chinese Optics Letters* 8(s1):21–24.

Thank you for your attention!

Any questions?