Cooperative Game Theory and Importance Quantification

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Context

Given **random inputs** $X_1, \ldots, X_d$ and a **random output** $G(X_1, \ldots, X_d)$, how much each **input contribute** to $\mathbb{V}(G(X_1, \ldots, X_d))$?

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G is a **deterministic black-box model**:

- **Numerical model** (e.g., simulation codes)
- **Learned ML/DL models** (e.g., post-hoc interpretations).

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Goals of the presentation:

- Offer a **different take** on cooperative games for **importance quantification purposes**.
- Propose an **alternative** to the drawbacks of the **Shapley values**.
- Discuss the **fundamental interpretation challenges** related to these methods.

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Cooperative Game Theory

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Let $D = \{1, \ldots, d\}$ 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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Main question:

How to redistribute $v(D)$ to each of the d players?

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Answer:

By using allocations!

Cooperative Game Theory

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- **Efficiency:** $\sum_{i \in D} \psi(i) = v(D)$.
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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.**

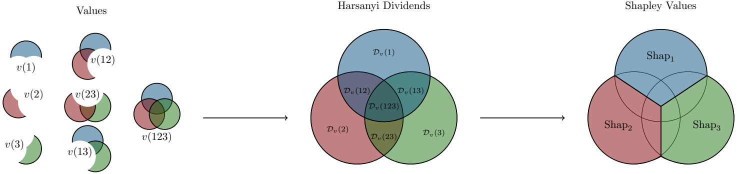
It is the case for $\mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_A\right]\right)$.

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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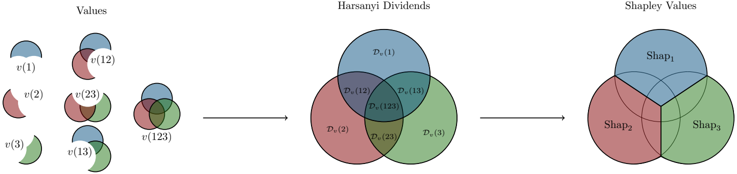

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The Shapley values with the choice $v(A) = \mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_A\right]\right)$.

$$\mathrm{Sh}_i = \sum_{A \in \mathcal{P}(D) : i \in A} \frac{S_A}{|A|},$$

where the **Harsanyi dividends** become S_A : the **Sobol' indices**.

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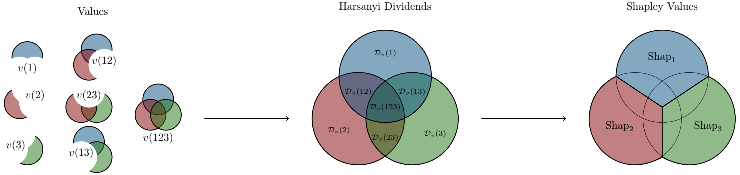

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☞ **They quantify the importance** of **dependent inputs**.

☞ **They have been extensively studied in the GSA literature.**

(Owen and Prieur 2017; Iooss and Prieur 2019; Benoumechiara and Elie-Dit-Cosaque 2019; Plischke, Rabitti, and Borgonovo 2021...)

Exogeneity detection and Shapley's joke

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

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

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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.**

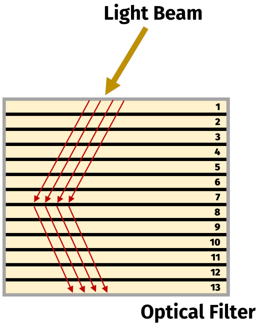
Optical filter transmittance - Feature selection

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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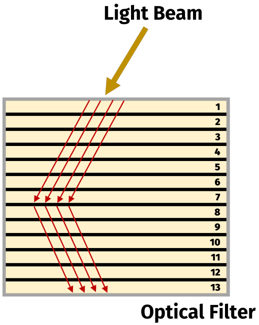

☞ **We only have access to an i.i.d. input-output sample** ($n = 1000$).

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.

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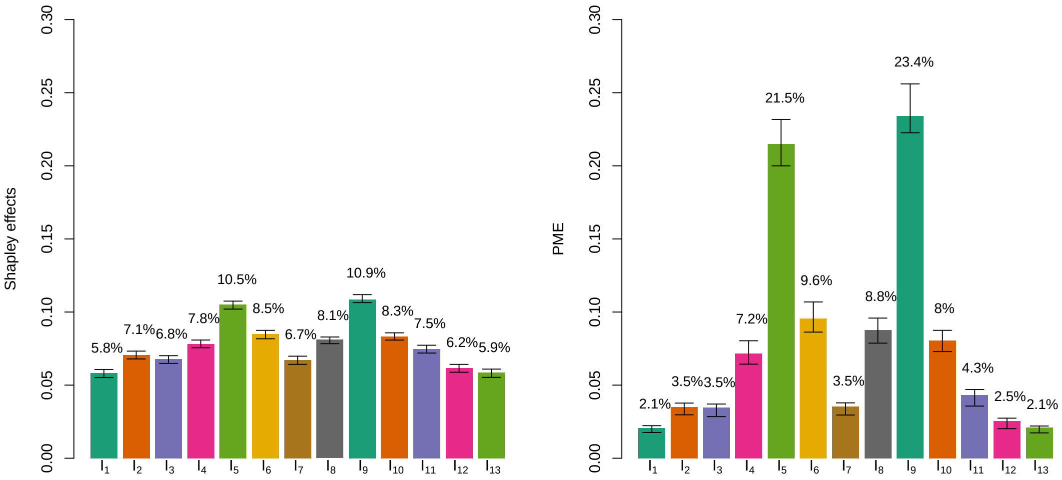

Optical filter transmittance - Feature selection

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.

Links with combinatorics

To define suitable indices, recall that we took the following steps:

1. We **chose of a value function** $v : \mathcal{P}(D) \to \mathbb{R}$.
2. We defined the **Harsanyi dividends** of v as: $\forall A \in \mathcal{P}(D)$, $\mathcal{D}_v(A) = \sum_{B\mathcal{P}(A)} (-1)^{|A|-|B|} v(B)$.

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This approach is **intimately linked to a well-known equivalence in the field of combinatorics.**

Proposition *(Möbius inversion on power-sets (Rota 1964; Kung, Rota, and Hung Yan 2012)).*

For any two set functions $v : \mathcal{P}(D) \to \mathbb{R}$, $\phi : \mathcal{P}(D) \to \mathbb{R}$, the following equivalence holds:

$$\forall A \in \mathcal{P}(D), \quad v(A) = \sum_{B \in \mathcal{P}(A)} \phi(B), \quad \iff \quad \forall A \in \mathcal{P}(D), \quad \phi(A) = \sum_{B \in \mathcal{P}(A)} (-1)^{|A|-|B|} v(B).$$

We went from the **right-hand side** to the **left-hand side** of the equivalence: the **input-centric approach**.

Illustration: Linear model with interaction and Gaussian inputs

Consider the model:

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

and recall that $\mathcal{D}_v(A) = \sum_{B \in \mathcal{P}(A)} (-1)^{|A|-|B|} \mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_B\right]\right)$.

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Traditional FANOVA (normalized)
Independent inputs (**Sobol' indices**)

$$\mathcal{D}_v(1) = 0.5 \quad \mathcal{D}_v(2) = 0, \quad \mathcal{D}_v(3) = 0,$$
$$\mathcal{D}_v(12) = 0, \quad \mathcal{D}_v(13) = 0, \quad \mathcal{D}_v(23) = 0.5,$$
$$\mathcal{D}_v(123) = 0$$

☞ **Sobol' indices** are **"interactions effects" due to** G.

Input-centric approach (normalized)
Dependent inputs

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☞ **Correlated inputs** $\Longrightarrow$ **unclear interpretation**.

Effects due to interaction and effects due to dependence are entangled.

Shapley effects with dependent inputs

Hence, **the precise interpretation of**

$$\mathcal{D}_v(A) = \sum_{B \in \mathcal{P}(A)} (-1)^{|A|-|B|} \mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_B\right]\right)$$

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In conclusion:

The choice $v(A) = \mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_A\right]\right)$, leads to an uncharacterized quantification when the inputs are dependent.

Solution: Generalized Hoeffding decomposition (I. et al. 2024).

Conclusion

Key messages:

- **Cooperative game theory:** Resourceful for building interpretable importance indices.
- **Harsanyi dividends:** Links the field to **combinatorics** through Möbius inversion.
- **Shapley values:** Egalitarian redistribution ($\neq$ fair).
- **PME:** Allow to detect exogenous inputs, more descriminative.
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Challenges and open questions:

- **Estimation:** More efficient estimation schemes.
- **Interpretation**: FANOVA with dependent inputs (I. et al. 2024).
- **Allocations:** Properties of other allocations ? (e.g., weighted Shapley)

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To go further

More on the Proportional Marginal Effects (PME) (HAL/arXiv/ResearchGate)

Proportional marginal effects for global sensitivity analysis

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More about the links with combinatorics (HAL/arXiv/ResearchGate)

On the coalitional decomposition of parameters of interest

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Generalized FANOVA indices for dependent inputs (HAL/arXiv/ResearchGate)

Hoeffding decomposition of black-box models with dependent inputs

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Thank you for your attention!

Any questions?