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 $\mathbb{V}\left(G(X_1, \ldots, X_d)\right)$?

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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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In this talk:

- **Dive into how cooperative game theory can be useful**, and what the Shapley values are.
- Draw a **link** between **cooperative game theory** and the field of **combinatorics**.
- Open on the **interpretation challenges** of the resulting decomposition.

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Formally, given:

- A **set of players** $D = \{1, \ldots, d\}$, and the subsequent **set of coalitions** $\mathcal{P}(D)$.
- A **value function** $v : \mathcal{P}(D) \to \mathbb{R}$ quantifying the **value produced** by each **coalition**.

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Using **allocations !**

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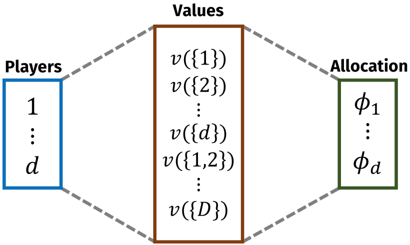
Allocating "the **whole cake** and **nothing but the cake**" is ensured by two criteria:

- **Efficiency**: $\sum_{i=1}^{d} \phi_i = v(D)$ (The whole cake).
- **Nonnegativity**: $\forall i \in D, \quad \phi_i \geq 0$ (Nothing but the cake).



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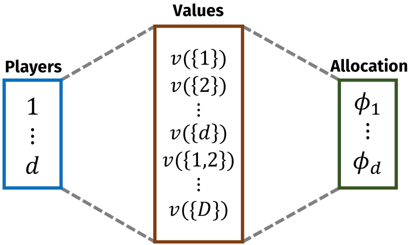

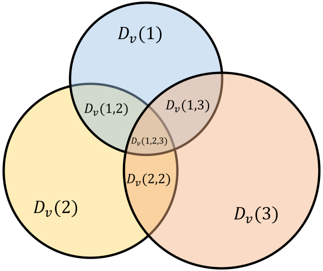

The **Harsanyi (1963) dividends** $\mathcal{D}_v$ of a cooperative game (D, v) are defined, $\forall A \in \mathcal{P}(D)$ as:

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

and can be interpreted as **the surplus due to a coalition of players**: $\sum_{A \in \mathcal{P}(D)} \mathcal{D}_v(A) = v(D)$.

Egalitarian redistribution: Shapley values

The **Shapley (1951) values** are an **egalitarian redistribution of the Harsanyi dividends**, defined, for $i = 1, \dots, d$ as:

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

where $|.|$ denotes the cardinality of sets.

The Harsanyi set

The **Harsanyi set** is the collection of allocations that can be written, for $i = 1, \ldots, d$ as:

$$\phi_i = \sum_{A \in \mathcal{P}(D) : i \in A} \lambda_A(i) \mathcal{D}_v(A).$$

under the constraint that, $\forall A \in \mathcal{P}(D)$,

$$\sum_{i \in D} \lambda_A(i) = 1.$$

These allocations are:

- **Always efficient** (the whole cake).
- If v is monotonic, they are **non-negative** (nothing but the cake).

Monotonicity: A bigger coalition has a greater value than a smaller one:

$$\forall A \in \mathcal{P}(D), \forall B \subseteq A, \quad v(B) \leq v(A).$$

Importance quantification

By **analogy between players and inputs**, Owen (2014) proposed to study the game:

$$(D, S^T), \quad \text{where } \forall A \in \mathcal{P}(D), \quad S^T_A = \frac{\mathbb{E}\left[\mathbb{V}\left(G(X) \mid X_{\overline{A}}\right)\right]}{\mathbb{V}\left(G(X)\right)}.$$

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However, **they do not detect exogenous inputs:**

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

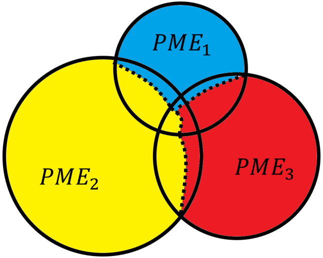
$$\text{Sh}_1 = 0.5 - \rho^2/4, \quad \text{Sh}_2 = 0.5, \quad \text{Sh}_3 = \rho^2/4 > 0 \text{ if } \rho \neq 0.$$

Proportional redistribution and exogeneity detection

The **proportional values** (Ortmann 2000) can be interpreted as a redistribution such that

> "[...] *each player gains in* ***equal proportion*** *to that which could be obtained by each alone."* - B. Feldman (1999)

They are based on a **proportional allocation principle of the Harsanyi dividends**.



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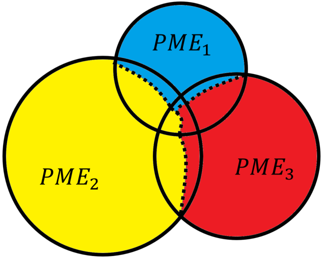

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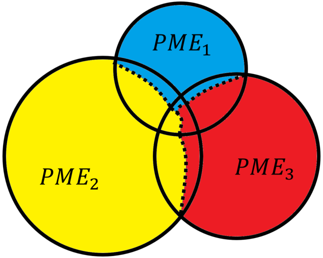

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Proposition *(Exogeneity detection (Herin et al. 2022)). Suppose that any different subset of the inputs cannot be expressed as functions of each other. Then, for any $i \in \{1, \dots, d\}$:*

$$PME_i = 0 \iff X_i \text{ is exogenous.}$$

Estimation

Estimating the PME/Shapley effects $\iff$ Estimating S_A^T for every $A \in \mathcal{P}(D)$.

It can be achieved:

- Via **Monte Carlo sampling**: Requires a number proportional to $d!(d-1)$ model evaluations (Song, Nelson, and Staum 2016).
- **Given-data** (i.i.d. input-output sample) via a **nearest-neighbor procedure**: Requires 2^d estimates (Broto, Bachoc, and Depecker 2020).

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.**

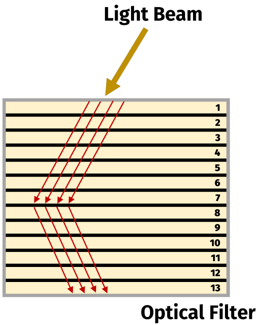
Optical filter transmittance - Feature selection

Quantification of the **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 filter ($\mathcal{U}([-0.05, 0.05])$)

These errors are (highly) correlated due to the manufacturing process (Gaussian copula, $\rho = 0.95$).

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



We can only access an i.i.d. input-output sample ($n = 1000$).

The indices are computed using the nearest-neighbors approach (6 neighbors).

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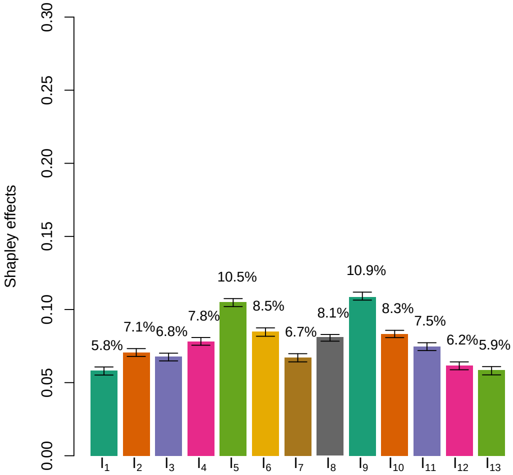

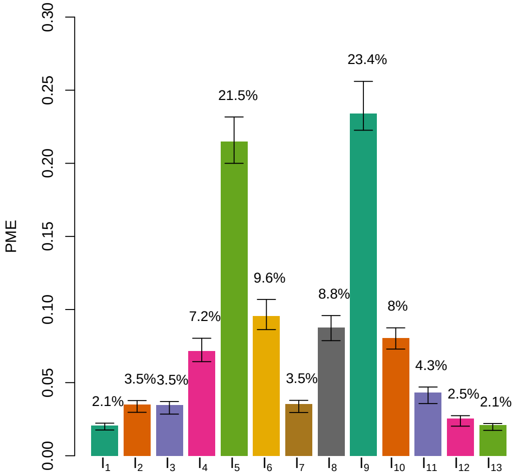

Optical filter transmittance - Feature selection

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:** I_1 and I_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 went through 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.**

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

Let $D = \{1, \ldots, d\}$, and any two set functions:

$$\varphi : \mathcal{P}(D) \to \mathbb{A}, \quad \psi : \mathcal{P}(D) \to \mathbb{A},$$

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

$$\forall A \in \mathcal{P}(D), \quad \varphi(A) = \sum_{B \in \mathcal{P}(A)} \psi(B) \quad \Longleftrightarrow \quad \forall A \in \mathcal{P}(D), \quad \psi(A) = \sum_{B \in \mathcal{P}(A)} (-1)^{|A|-|B|} \varphi(B).$$

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

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

Let, $\forall A \subseteq \{1, 2, 3\}$:

$$v(A) = S_A^T, \quad S(A) = \sum_{B \in \mathcal{P}(A)} (-1)^{|A|-|B|} S_B^T \times \mathbb{V}(G(X))$$

Independent case $(\rho = 0)$

$$\mathcal{D}_v(1) = \mathbb{V}(G(X))/2, \quad \mathcal{D}_v(2) = 0, \quad \mathcal{D}_v(3) = 0,$$
$$\mathcal{D}_v(12) = 0, \quad \mathcal{D}_v(13) = 0,$$
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In both cases $\sum_{A \in \mathcal{P}(D)} \psi(A) = \mathbb{V}(G(X))$.

What is due to the correlation? What is due to the interaction?

Shapley effects with dependent inputs

Hence, **the precise interpretation of**

$$\mathcal{D}_v(A) = \frac{1}{\mathbb{V}(G(X))} \sum_{B \in \mathcal{P}(A)} (-1)^{|A|-|B|} S_B^T$$

is still an open question : it clearly is a **mixture of interaction and dependence effects**.

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

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Choosing $v(A) = S_B^T$, leads to an uncharacterized quantification when the inputs are dependent.

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.
- **Estimation:** VERY time-consuming (but embarrassingly parallel).

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Challenges and open questions:

- **Estimation:** Is it possible to drive the cost down?
- **Interpretation**: Model-centric approach, **FANOVA with dependent inputs**.
- **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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Thank you for your attention!

Any questions?