

BEYOND SHAPLEY VALUES

COOPERATIVE GAMES FOR THE INTERPRETATION OF MACHINE LEARNING MODELS

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Project: *Interpretability of black-box machine learning models*

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

Research interests:

Statistical Learning • XAI • Uncertainty Quantification • Sensitivity Analysis • Probability Theory • Cooperative game theory • Functional analysis



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However, **eXplainable AI (XAI) methods** are often backed by **empirical arguments**

“SOTA” methods, testing on limited benchmarks...

This is **not enough** to convince safety/regulatory authorities...

Our position:

Before choosing an XAI method, we need to understand it theoretically

👉 Understand the method before “explaining” the phenomenon

Context

In this talk:

Revisit **post-hoc model-agnostic** XAI methods based on **cooperative game theory**

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Side quests:

- Understand **what the Shapley values are** and how to go **beyond them**
- Introduce some of **the open questions and challenges** that I will take on during the next two years

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A mapping from Ω to $E_A = \prod_{i \in A} E_i$.

☞ Let $\hat{f}$ denote the **black-box ML model**, and $\hat{f}(X)$ be the **random output**.

A measurable mapping from E to $\mathbb{R}$. $\hat{f}(X)$ is a **random variable**.

Remark . We take a **post-hoc, model-agnostic** approach.

“Cooperative game theory = The art of sharing a cake”



Cooperative Game Theory

“Cooperative game theory = The art of sharing a cake”



Two ingredients:

- $D = \{1, \dots, d\}$, a **set of players**
The power-set $\mathcal{P}_D$ is the **set of coalitions of players**
- $v : \mathcal{P}_D \rightarrow \mathbb{R}$, a **value function**
It **assigns a value to each coalition**

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

☞ $v(D)$ is the value of the “grand coalition” (the cake)

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Main concern of the theory of cooperative games:

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

A famous example - LMG indices

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Players: the covariates $(X_1, \dots, X_d)$ (rather, their indices D)

Coalitions: for $A \in \mathcal{P}_D$, the subset of covariates X_A

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Is it possible to aggregate this information (2^d coefficients) into something more manageable?

Allocations as an aggregation

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It is a mapping $\phi : D \rightarrow \mathbb{R}$, that must ideally respect one criteria:

- **Efficiency:** $\sum_{i \in D} \phi(i) = v(D)$
 - ☞ Ensures that **the we actually redistribute the cake**

Allocations as an aggregation

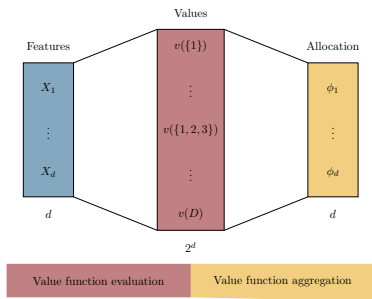
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In a nutshell:

- Start with a learned model with d input features
- Chose a **value function** resulting in 2^d quantities
- Aggregate the 2^d quantities into d quantities using an **efficient allocation**

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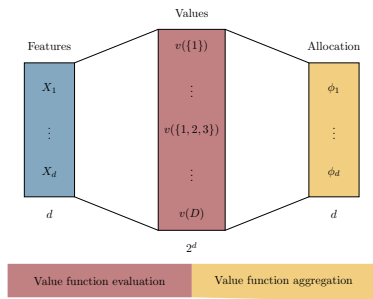
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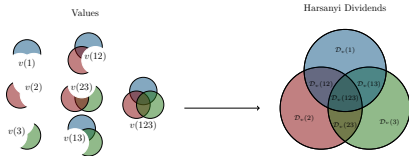
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Is there a way to define efficient **allocations**?

Allocations as a dividend sharing mechanism

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

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



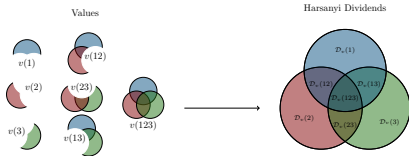
They quantify **the added-value of a coalition**:

$$\mathcal{D}_v(12) = v(12) - v(1) - v(2)$$

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They are the **Möbius inverse** of the **value function**

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

For any two set functions $v : \mathcal{P}_D \rightarrow \mathbb{R}$, $\mathcal{D} : \mathcal{P}_D \rightarrow \mathbb{R}$, the following equivalence holds:

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

(i.e., generalized inclusion-exclusion principle)

Shapley values as the egalitarian dividend sharing mechanism

The **Harsanyi set** is a family of efficient allocations that aggregate of the **Harsanyi dividends**:

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

parametrized by the **weight system** $\lambda : D \times \mathcal{P}_D \rightarrow \mathbb{R}$

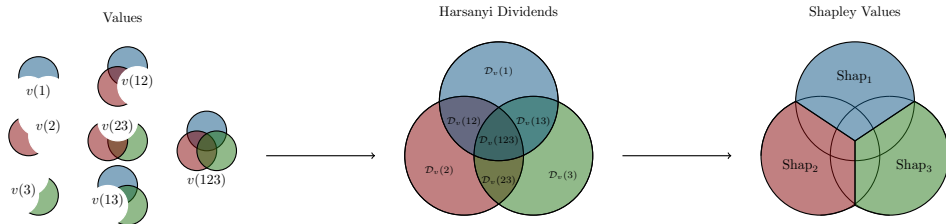
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In this setting, the **Shapley values** are the egalitarian redistribution, i.e., $\lambda_i(A) = 1/|A|$



Allocations using random orders

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For any $i \in D$, denote $\pi(i)$ the **position of player i in the permutation π** (i.e., $\pi_{\pi(i)} = i$)

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The **Weber (1988) set** is a family of **efficient allocations** as an average over the orderings

$$\begin{aligned}\phi(i) &= \mathbb{E}_{\pi \sim p} [v(\{\pi_1, \dots, \pi_{\pi(i)}\}) - v(\{\pi_1, \dots, \pi_{\pi(i)-1}\})] \\ &= \sum_{\pi \in \mathcal{S}_D} p(\pi) [v(\{\pi_1, \dots, \pi_{\pi(i)}\}) - v(\{\pi_1, \dots, \pi_{\pi(i)-1}\})]\end{aligned}$$

parametrized by a **probability mass function** over the permutations $\mathcal{S}_D$.

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parametrized by a **probability mass function** over the permutations $\mathcal{S}_D$.

In this setting, the **Shapley values are the uniform distribution over the permutations**, i.e., $p(\pi) = 1/d!$

$$\text{Shap}(i) = \frac{1}{d!} \sum_{\pi \in \mathcal{S}_D} [v(\{\pi_1, \dots, \pi_{\pi(i)}\}) - v(\{\pi_1, \dots, \pi_{\pi(i)-1}\})]$$

The recipe

Overall blueprint for using cooperative games for XAI:

(l., Charpentier, and Fernandes Machado 2025)

1. **Step 1: Identify a quantity of interest**

Choose **a cake worth cutting**, e.g., point predictions $f(x)$, model variance $\mathbb{V}(f(X))...$

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2. Step 2: Pick a value function v

And make sure that **$v(D)$ is equal to the quantity of interest**, e.g.,

$\mathbb{E}[f(X) \mid X_A = x_A]$ for $f(x)$, $\mathbb{V}(\mathbb{E}[f(X) \mid X_A])$ for $\mathbb{V}(f(X))$...

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3. Step 3: Pick an efficient allocation

In order to summarize the information of the 2^d evaluations of v

☞ Less crucial and can **highlight some model behavior**

CHALLENGE 1:
CHOOSING A VALUE FUNCTION

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A **bad choice** can lead to **misleading insights**

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$$f(X) = X_1 + X_2 + X_1 X_2, \quad X = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \sim \mathcal{N} \left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \right), \quad x = X(\omega), \omega \in \Omega$$

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Conditional expectation

$$v(A) = \mathbb{E}[f(X) \mid X_A = x_A]$$

$$\mathcal{D}_v(1) = x_1 + \rho(x_1 + x_1^2 - 1) \quad \mathcal{D}_v(2) = x_2 + \rho(x_2 + x_2^2 - 1)$$

$$\mathcal{D}_v(12) = x_1 x_2 - \rho(x_1 + x_1^2 + x_2 + x_2^2 - 1)$$

$$\text{Shap}_v(\{1\}) = x_1 + \frac{\rho}{2}(x_1 + x_1^2 - x_2 - x_2^2 - 1) + \frac{x_1 x_2}{2}$$

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Oblique projections

I. et al. (2025a)

$$\mathcal{D}_v(1) = x_1 \quad \mathcal{D}_v(2) = x_2$$

$$\mathcal{D}_v(12) = x_1 x_2$$

$$\text{Shap}_v(\{1\}) = x_1 + \frac{x_1 x_2}{2}$$

$$\text{Shap}(\{2\}) = x_2 + \frac{x_1 x_2}{2}$$

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Theorem (I. et al. [2025a](#)). Under very mild assumptions on X , for every $A \in \mathcal{P}_D$,

$$\mathbb{L}^2(\sigma_A) = \bigoplus_{B \in \mathcal{P}_A} V_B.$$

where $V_\emptyset = \mathbb{L}^2(\sigma_\emptyset)$, and $V_B = \left[\bigoplus_{C \in \mathcal{P}_B, C \neq B} V_C \right]^{\perp_B}$, with $\perp_B$ denoting the orthogonal complement in $\mathbb{L}^2(\sigma_B)$.

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Open question: Great contenders, but **we don't know how to estimate them**

CHALLENGE 2:
PICKING AN ALLOCATION

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Example: Proportional Marginal Effects (Herin et al. 2024)

- **Quantity of interest**: $\mathbb{V}(f(X))$
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- **Allocation**: *Proportional values*

$$p(\pi) = \frac{L(\pi)}{\sum_{\sigma \in \mathcal{S}_D} L(\sigma)}, \quad L(\pi) = \exp \left(- \sum_{j \in D} \log (v(\{\pi_1, \dots, \pi_{\pi(j)}\})) \right)$$

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Proposition (*Exogeneity detection*).

$$PME_i = 0 \iff X_i \text{ is not in the model.}$$

CHALLENGE 3:

COMPUTATIONAL ASPECTS

Computational aspects - Monte-Carlo type estimates

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Proposition (I. et al. 2025b). Let p be a pmf over $\mathcal{S}_D$. Let $m > 0$ and $\pi_1, \dots, \pi_m$ be an i.i.d. sample drawn from p . Assume that $0 < \mathbb{E}_p \left[\left(v(\pi^j) - v(\pi^j \setminus \{j\}) \right)^2 \right] < \infty$. Then, for every $j \in D$,

$$\widehat{\phi}_v(j) = \frac{1}{m} \sum_{i=1}^m \left[v(\pi_i^j) - v(\pi_i^j \setminus \{j\}) \right],$$

is an unbiased, strongly consistent, and asymptotically normal estimators of $\phi_v(j) := \mathbb{E}_p[h(\pi)]$.

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👉 **Worst-case scenario:** $m \times d$ models to train instead of $d!$.

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Open question: Any refinement possible?

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Open question: Other types of computational improvement?

Maximal coalition cardinality, parallel and efficient computing, time and memory trade-off...

Quick illustration - Conformal prediction decomposition

Uncertainty attribution based on conformal prediction (CP) intervals:

1. **Quantity of interest:** Width of the CP interval $\hat{C}(x)$ at point x
2. **Value function:** Width of the CP interval $\hat{C}_A(x)$ only using covariates X_A
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Synthetic model: The Sobol-Levitan function (Sobol' and Levitan 1999)

$$X = (X_1, \dots, X_{16})^\top \sim \mathcal{U}(0, 1)^{\times 16}, \quad \beta \in \mathbb{R}^{16}, \quad \epsilon_Y \sim \mathcal{N}(0, 1), \quad Y = \exp[\beta^\top X] + \prod_{i=1}^{16} \frac{\exp[\beta_i] - 1}{\beta_i} + \epsilon_Y$$

Here, $d = 16$, $d! \approx 2 \times 10^{13}$ and $2^{16} = 65\,536$

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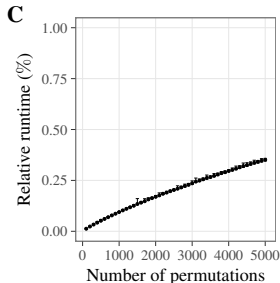
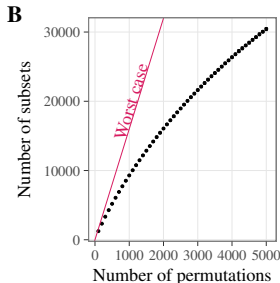
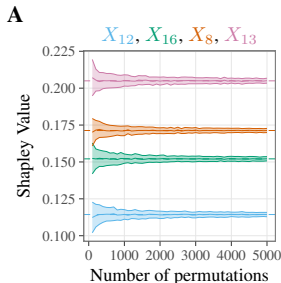
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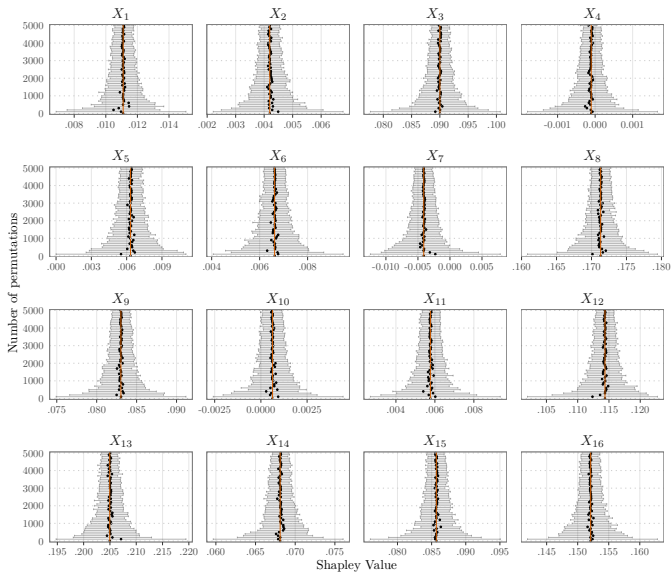
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Dataset	Description	n	d	Estimation
bike	Bike rental data	17,379	12	Exact
blog	Number of comments per blog posts	52,397	238	$m = 50$
casp	Physicochemical properties of proteins	45,730	9	Exact
concrete	Concrete compressive strength	1,030	8	Exact
facebook	Engagement of facebook posts	79,788	37	$m = 200$
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More details in our most recent preprint:

Unveil Sources of Uncertainty: Feature Contribution to Conformal Prediction Intervals

Marouane El Idrissi^{a,b,e}, Agathe Fernandes Machado^a, Ewen Gallic^{c,d}, Arthur Charpentier^a

Conclusion

Key take-aways:

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THANK YOU FOR YOUR ATTENTION!

ANY QUESTIONS?

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