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

Context

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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

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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 $E_A = \bigtimes_{i \in A} E_i$.

☞ Let $\widehat{f}$ denote the **black-box ML model**, and $\widehat{f}(X)$ be the **random output**.
A measurable mapping from E to $\mathbb{R}$. $\widehat{f}(X)$ is a **random variable**.

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

Cooperative Game Theory

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Two ingredients:

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

☞ (D, v) formally defines a **cooperative game**
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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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Cooperative game:
Players: the covariates $(X_1, \ldots, X_d)$ (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?

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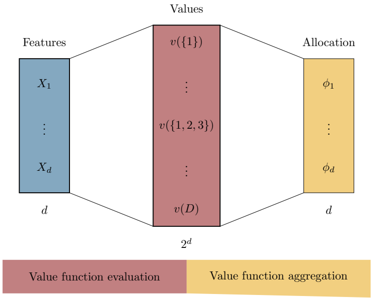

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- Start with a learned model with d input features
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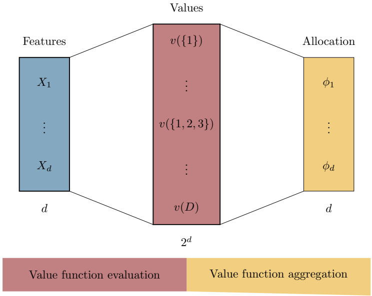

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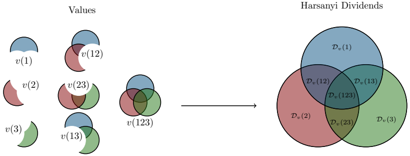
Is there a way to define efficient allocations?

Allocations as a dividend sharing mechanism

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

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



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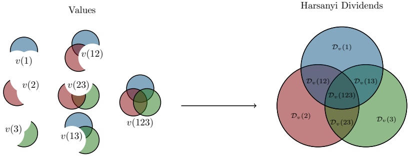

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They are the **Möbius inverse** of the **value function**

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

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

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

(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** $\lambda : D \times \mathcal{P}_D \to \mathbb{R}$

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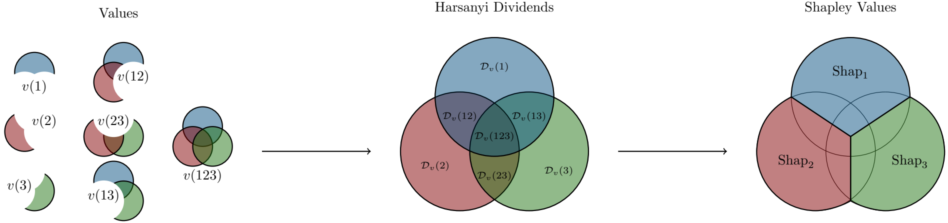
In this setting, the **Shapley values are the egalitarian redistribution**, i.e., $\lambda_i(A) = 1/|A|$



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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

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

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

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

Overall blueprint for using cooperative games for XAI:
(I., 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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e.g., **correlation/concurvity identifiability issues** (Zhang, Martinelli, and John 2024), **lack of purity** (Köhler, Rügamer, and Schmid 2024)...

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Conditional expectation

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

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

$$\mathcal{D}_v(12) = x_1x_2 - \rho(x_1 + x_1^2 + x_2 + x_2^2 - 1)$$

$$\mathrm{Shap}_v(\{1\}) = x_1 + \frac{\rho}{2}(x_1 + x_1^2 - x_2 - x_2^2 - 1) + \frac{x_1x_2}{2}$$

$$\mathrm{Shap}(\{2\}) = x_2 + \frac{\rho}{2}(x_2 + x_2^2 - x_1 - x_1^2 - 1) + \frac{x_1x_2}{2}$$

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

$$\mathcal{D}_v(12) = x_1x_2 - \rho(x_1 + x_1^2 + x_2 + x_2^2 - 1)$$

$$\mathrm{Shap}_v(\{1\}) = x_1 + \frac{\rho}{2}(x_1 + x_1^2 - x_2 - x_2^2 - 1) + \frac{x_1x_2}{2}$$

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Oblique projections

I. et al. (2025a)

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- ☞ For a sub-σ-algebra $\mathcal{B} \subseteq \mathcal{F}$, denote $\mathbb{L}^2(\mathcal{B}) := \mathbb{L}^2\left((\Omega, \mathcal{B}, \mathbb{P})\right)$

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

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

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

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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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How do we pick a ”good” allocation?

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It is still an **open question**:

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

- **Quantity of interest:** $\mathbb{V}\left(f(X)\right)$
- **Value function:** $v(A) = \mathbb{E}\left[\mathbb{V}\left(f(X) \mid X_{D \setminus A}\right)\right]$
- **Allocation:** *Proportional values*

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

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Proposition *(Exogeneity detection)*.

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

Challenge 3:
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Computational aspects - Monte-Carlo type estimates

We need to **evaluate the value function** for the 2^d coalitions

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For certain **value functions**, this implies **fitting** 2^d **regression models**
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Proposition *(I. et al. 2025b)*. Let p be a pmf over $\mathcal{S}_D$. Let $m > 0$ and $\pi_1, \ldots, \pi_m$ 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 $j \in D$,

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

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 memorytrade-off...

Quick illustration - Conformal prediction decomposition

Uncertainty attribution based on conformal prediction (CP) intervals:

1. **Quantity of interest:** Width of the CP interval $\widehat{C}(x)$ at point x
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Synthetic model: The Sobol-Levitan function (Sobol′ and Levitan 1999)

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

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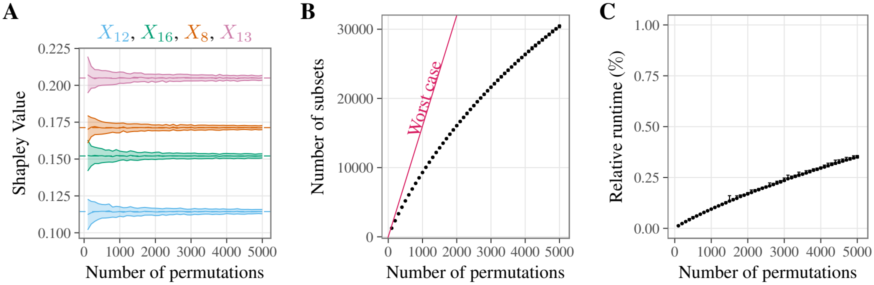

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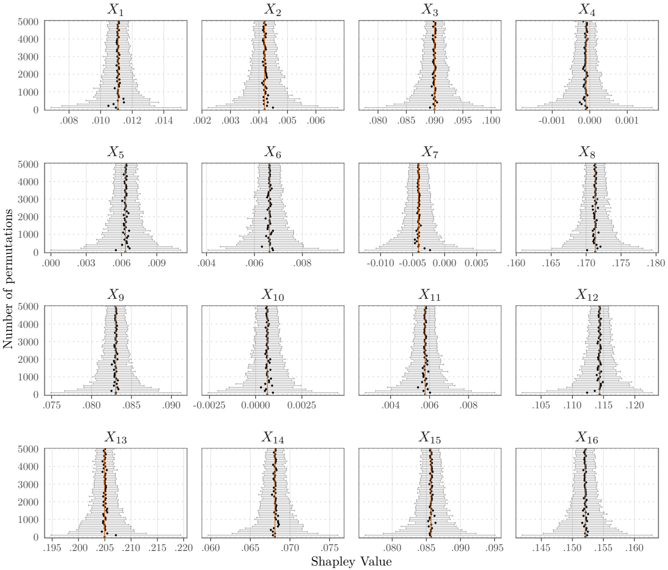

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Dataset	**Description**	n	d	Estimation
`bike`	Bike rental data	17,379	12	Exact
`blog`	Number of comments per blog posts	52,397	238	$m = 50$
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More details in our most recent preprint:

Unveil Sources of Uncertainty: Feature Contribution to Conformal Prediction Intervals

Marouane Il Idrissi[a,b,e], Agathe Fernandes Machado[a], Ewen Gallic[c,d], Arthur Charpentier[a]

Conclusion

Key take-aways:

- **Three ingredients** to using cooperative game for ML interpretability: The **quantity of interest**, the **value function**, and the **allocation**

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Thank you for your attention!

Any questions?

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