Beyond Shapley Values

Cooperative Games for the Interpretation of Machine Learning Models

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Institut Intelligence et Données, Université Laval

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:
There needs to be a theoretical justifications to the choice of an XAI method

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How to use cooperative game theory right to extract insights on the behavior of black-box models?

Side quests: Understand **what the Shapley values are** and how to go **beyond them**

Cooperative Game Theory

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Two ingredients:

- $D = \{1, \ldots, d\}$, 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**
☞ $v(D)$ 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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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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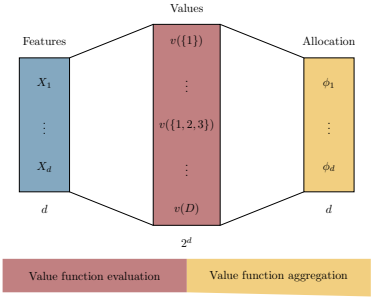

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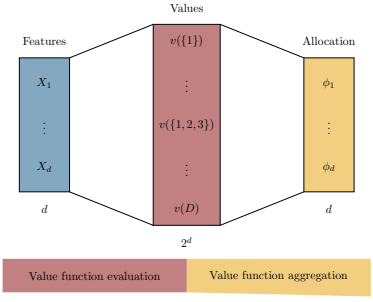

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Is there a way to define efficient allocations?

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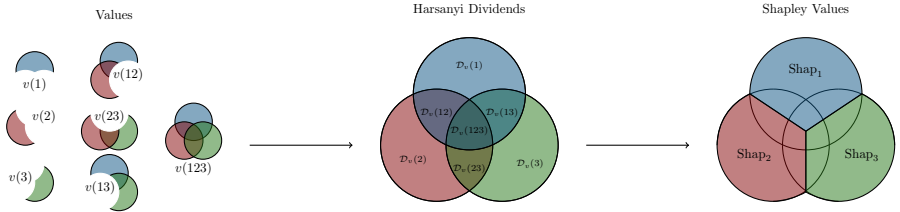
In this setting, the **Shapley values are the egalitarian redistribution**, i.e., $\lambda_i(A) = 1/|A|$



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

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

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

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, but can **highlight some model behavior**

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$$f(X) = X_1 + X_2 + X_1X_2, \quad X = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \right)$$

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Conditional expectation

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

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

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

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

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Oblique projections

I. et al. (2025)

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

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

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

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

Conclusion

Key take-aways:

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

Conclusion

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☞ **Ditch the (arbitrary) Shapley values to propose new goal-oriented XAI method standards**

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Thank you for your attention!

Any questions?

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