Cooperative Games for the Interpretation of ML Models

Some Methodological and Computational Aspects

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Introduction

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

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In this presentation:

How can we leverage the theory of cooperative games for the interpretation of black-box machine learning models?

Two parts:

1. **Methodological aspects** (Marouane) ☞ Not a lot of new stuff
2. **Computational aspects** (Lucas) ☞ A lot of new stuff

Part I
Methodological aspects

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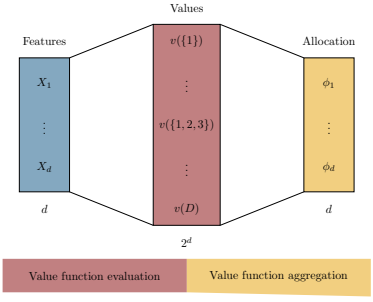

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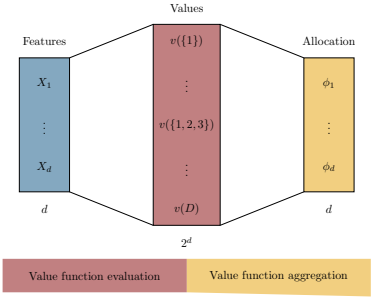

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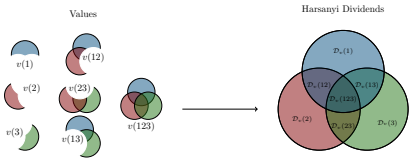
Is there a way to define efficient allocations?

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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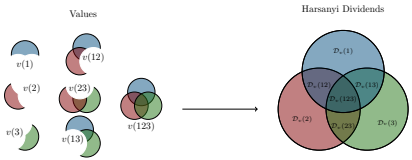

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They are the **Möbius inverse** of the **value function**

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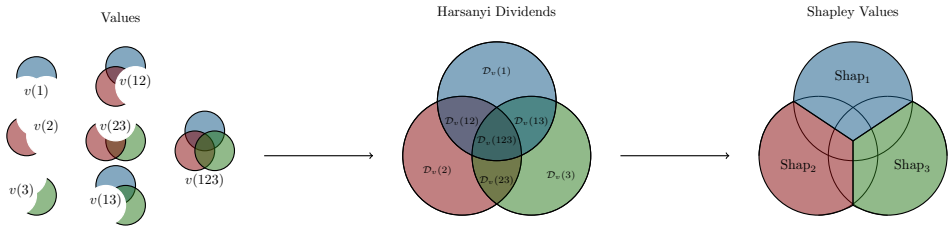
In this setting, the **Shapley values are the egalitarian redistribution**, i.e., $\lambda_i(A) = 1/|A|$



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Let $\mathcal{S}_D$ be the **set of permutations** $\pi = (\pi_1, \ldots, \pi_d)$ (i.e., orders) of players
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

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

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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.,
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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**

Conclusion

Key take-aways:

- **Three ingredients** to using cooperative game for XAI:
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Part II
Computational Aspects

It's always harder in practice

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- **Temporal complexity of the allocations formulas** ☞

$$\begin{cases} \textit{Shapley} : O(d2^d) \\ \textit{Harsanyi} : O(3^d) \\ \textit{Weber} : O(d!) \end{cases}$$

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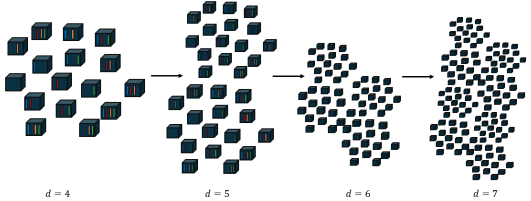
- **Space complexity of the models**

  ☞ For each feature added in the model, we need to double the amount of storage



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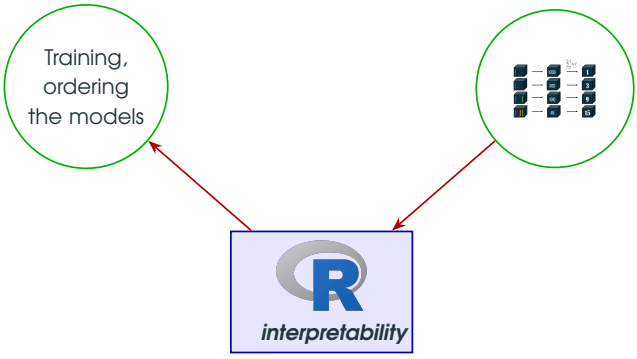

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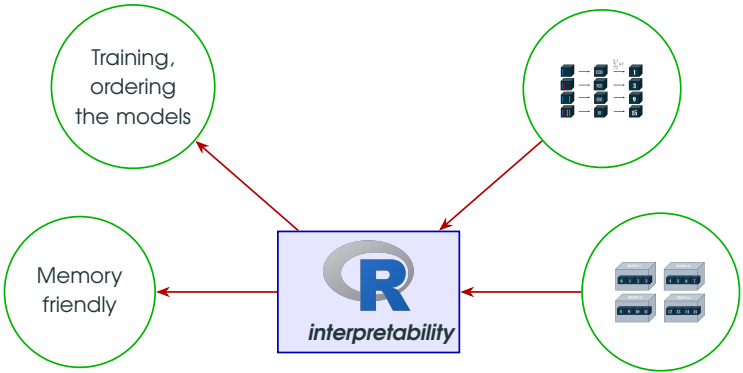

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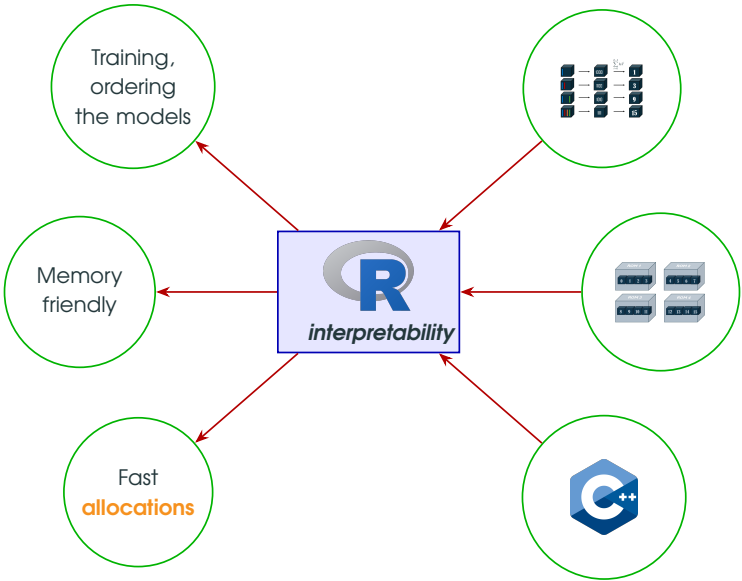

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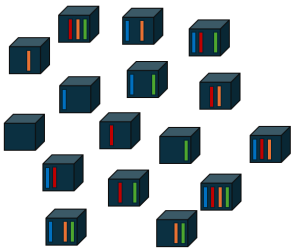

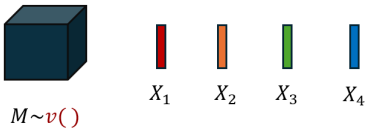

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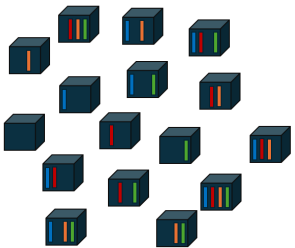

$M \sim v(\,)$

☞ **First question : how to organize that mess ?**

Coalition indexing : bit representation and lexicographical ordering

- **Idea**: map each coalition to an index $i \in \mathbb{N}$

1. **Remark:** It starts from 0 with the null coalition. We invert the order for better comprehension.

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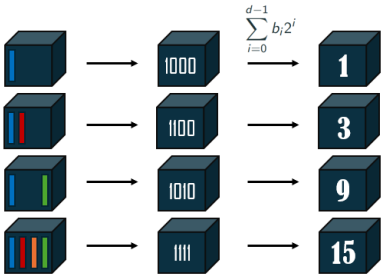

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Memory and parallelization issues

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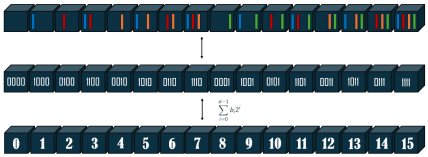

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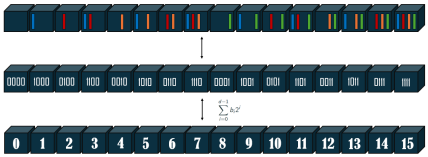

- We can't store on the memory ➢ We switch to disk storage
  ☞ **We only train the 2^d models once and for all**

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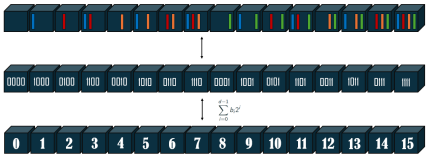

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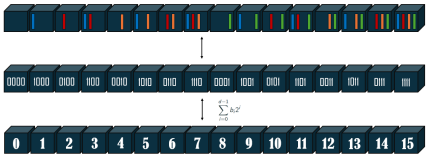

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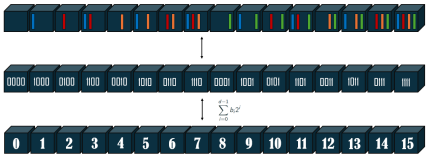

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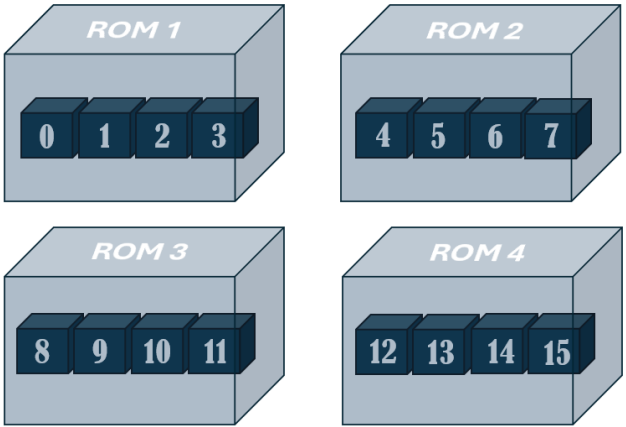
  - Sequential Blocks
  - Coalitional Properties Blocks

Sequential Blocks

- ☞ Natural batching by sequential blocks
- ☞ 2^b blocks for a good balance (but flexible)



Coalitional Properties Blocks

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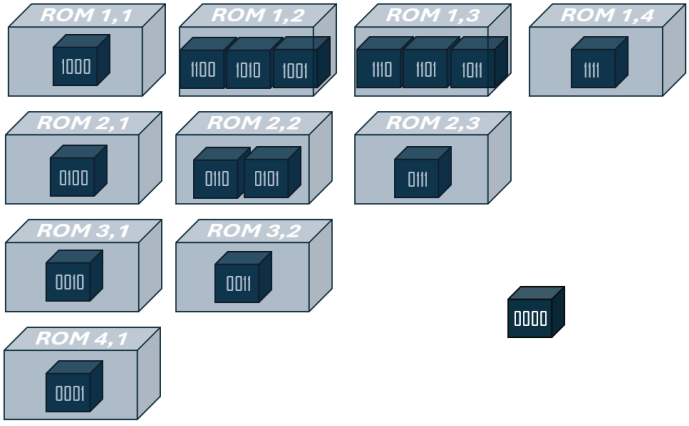

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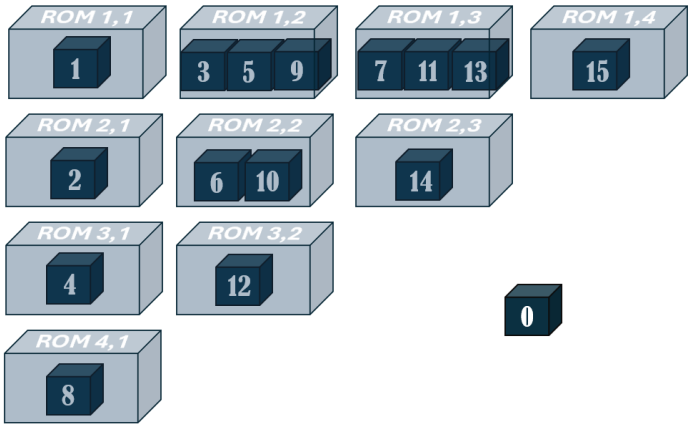
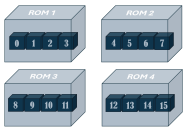


Two efficient ideas

Sequential Blocks



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- Flexible size of blocks and memory managment
- Parallelization is easy to implement

Drawbacks.

- No particular properties inside blocks

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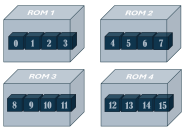

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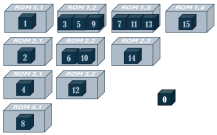

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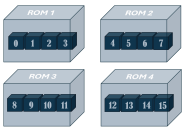

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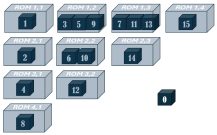

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☞ Now, we need to adapt the formulas so they can work with parallelism

A common formula for Harsanyi, Weber and Shapley

How to parallelize that :

$$\begin{cases} \phi^H(i) = \displaystyle\sum_{A \in \mathcal{P}_D \,:\, i \in A} \lambda_i(A) \sum_{B \in \mathcal{P}_A} (-1)^{|A|-|B|} v(B) \\ \phi^W(i) = \displaystyle\sum_{\pi \in \mathcal{S}_D} p(\pi) \left[v\left(\{\pi_1, \ldots, \pi_{\pi(i)}\}\right) - v\left(\{\pi_1, \ldots, \pi_{\pi(i)-1}\}\right) \right] \end{cases}$$

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  ☞ Above all, this formulation allows us parallelize the computations

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SMC Algorithm.

➢ **For** A **in** $\mathcal{P}_D$

➢ **If** $i \in A : \phi(i) \leftarrow \phi(i) + \beta(i, A) v(A)$

➢ **If** $i \notin A : \phi(i) \leftarrow \phi(i) - \beta(i, A \cup i) v(A)$

Fast Möbius Transform

- "We will see after a solution if λ depends on v"
  - ☞ We need to make $n.d$ Möbius Transforms for the whole sample
    - ☞ We consider back the initial formulation and try to find a "fast" way to compute the Möbius formula : $\mathcal{D}(v) = \sum_{B \in \mathcal{P}_A} (-1)^{|A|-|B|} v(B)$

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FMT Algorithm.

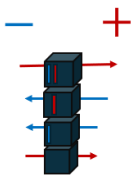
For i **in** D

➢ **For** A **in** $\mathcal{P}_D$

➢ **If** $i \in A$: $v(A) \leftarrow v(A) - v(A \setminus \{i\})$

Fast Möbius Transform : Example

$\mathcal{D}($  $) = v(\{1,2\}) - v(\{2\}) - v(\{1\}) + v(\emptyset) =$



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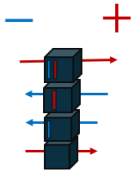

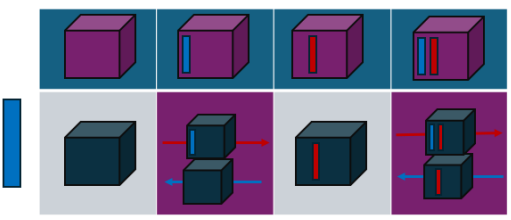

Step 1 : player

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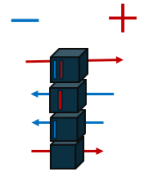

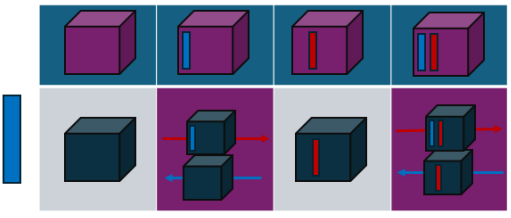

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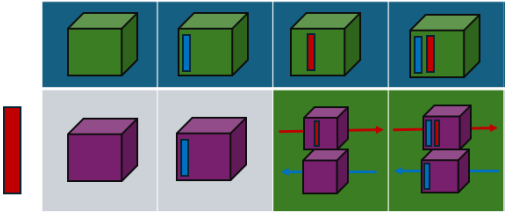

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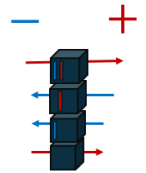

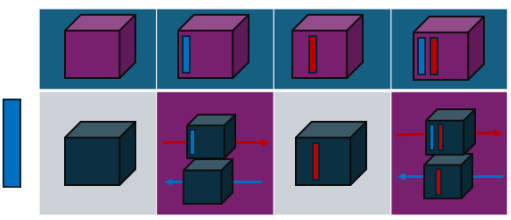

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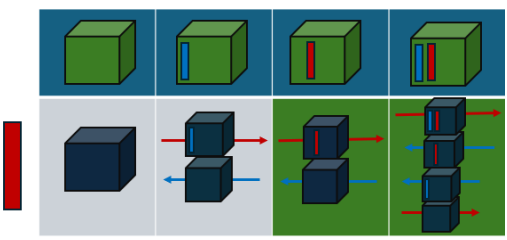

Final Möbius Transform

- We can't flat all the 2^d values

  ☞ **How to adapt this algorithm to our blocks structure ?**

Distributed Fast Möbius Transform

- We can't flat all the 2^d values
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The Solution : Distributed Fast Möbius Transform

- Adapted to the Sequential Blocks structure 
- Allow parallelism
- Memory-safe designed
- The number of blocks B must be a power of 2 ($B = 2^b$)

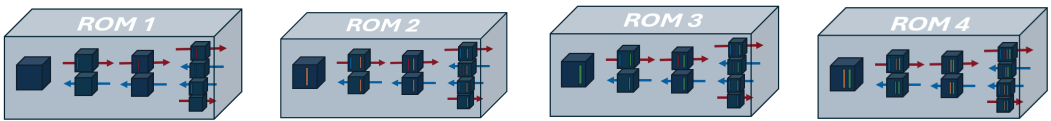
Distributed Fast Möbius Transform

Distributed FMT Algorithm.

Phase 1 : Intra-Blocks

For *bl* **in Blocks** (parallelism)

➢ **DO (scalar)** $\mathbb{R}$**-FMT inside** *bl* (considering lexicographical order inside the block)



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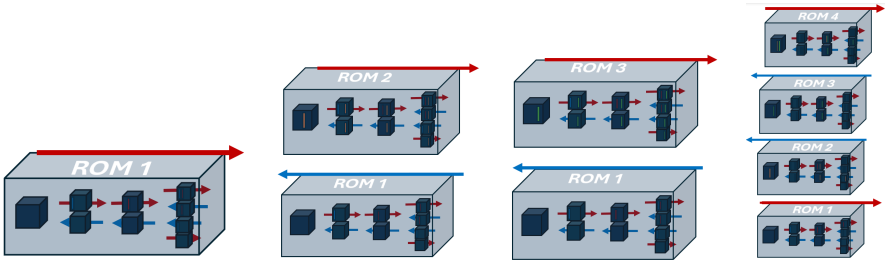
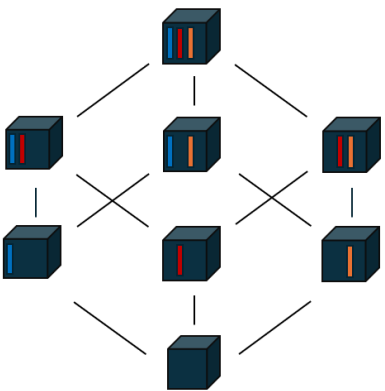
Phase 2 : Inter-Blocks

➢ **DO (vectorial)** $\mathbb{R}^{2^{d-b}}$**-FMT along Blocks** (considering lexicographical order of the blocks)



☞ **Phase 1 :** Möbius Transforms on sub-lattices



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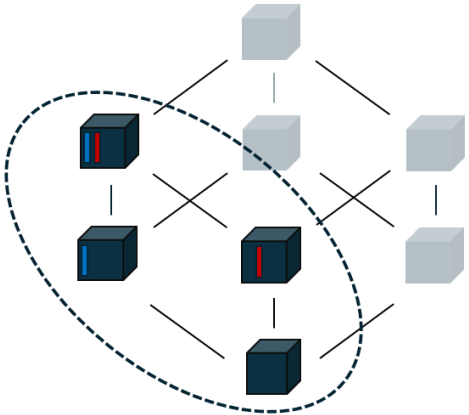

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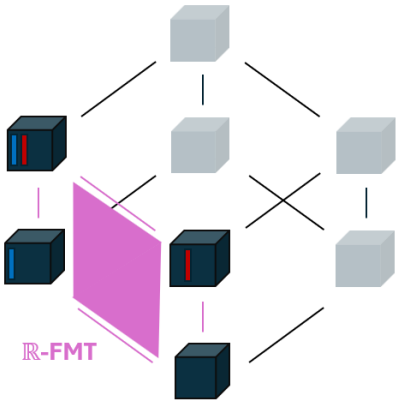

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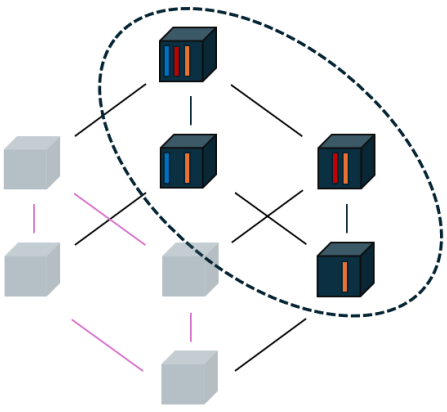
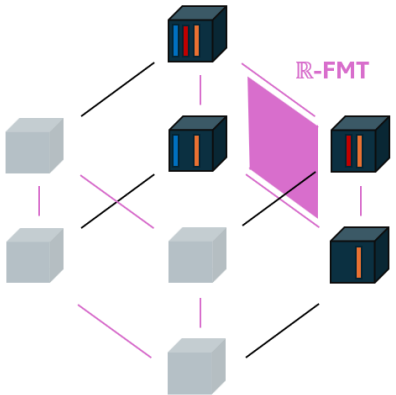


Distributed Fast Möbius Transform as an inversion on the boolean lattice

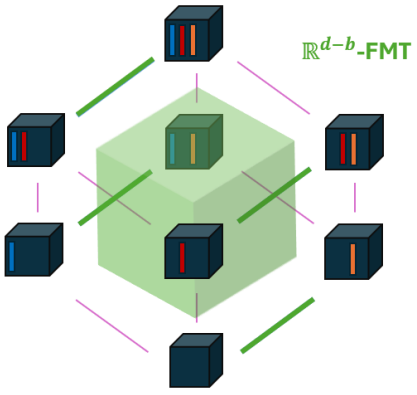
☞ **Phase 1 :** Möbius Transforms on sub-lattices



Distributed Fast Möbius Transform as an inversion on the boolean lattice

☞ **Phase 1 :** Möbius Transforms on sub-lattices

☞ **Phase 2 :** Möbius Transform



Distributed Fast Möbius Transform as a mixed Kronecker matrix-vector product

☞ Mazo and Tournier 2025 :

$$\mathcal{D}(v) = \otimes^d M.v \text{ , with : } M = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}, \ v \in \mathbb{R}^{2^d}$$

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☞ Mixed Kronecker matrix-vector product :

$$(B \otimes A)\,\mathrm{vec}(V) = \mathrm{vec}(A\,V\,B^\top) \text{ with : } V \in \mathbb{R}^{2^b \times 2^{d-b}}$$

$$\mathcal{D}(v) = \otimes^d M.v = \mathrm{vec}\Big(\underbrace{(\otimes^b M)}_{\text{Phase 1, intra-blocks}} \quad V \quad \underbrace{(\otimes^{d-b} M)^\top}_{\text{Phase 2, inter-blocks}} \Big)$$

What did you learn today ?

- **Two data structures**
  ☞ Sequential Blocks, Coalional properties Blocks
- **A new common formula** for Harsanyi, Weber and Shapley
  ☞ Allows independent, parallelized computations
- **New algorithms** adapted to the Sequential Blocks structure
  ☞ Split Marginal Contribution, Fast Möbius Transform, Distributed Fast Möbius Transform

What's next ?

- ☞ Finish and publish ***interpretability***
- ☞ **Theorethically :** Find **closed formulas** for β for specific choices of weight systems λ and permutation distributions p
- ☞ **Computationally :** Find a way to **"compress"** each model (i.e. store the minimum requirement)

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Thank you for your attention!

Any questions?

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