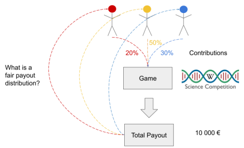
Interpretable Machine Learning

Shapley Values



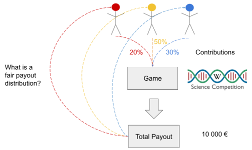
Learning goals

- Learn cooperative games and value functions
- Define the marginal contribution of a player
- Study Shapley value as a fair payout solution
- Compare order and set definitions

Interpretable Machine Learning

Shapley

Shapley Values



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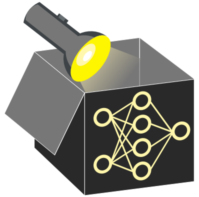
COOPERATIVE GAMES IN GAME THEORY

▸ Shapley (1951)



- **Game theory:** Studies strategic interactions among "players" (who act to maximize their utility), where outcomes depend on collective behavior
- **Cooperative games:** Any subset $S \subseteq P = \{1, \ldots, p\}$ can form a coalition to cooperate in a game, each achieving a payout $v(S)$

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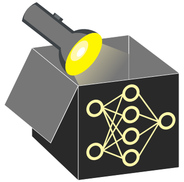

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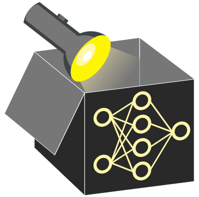

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- **Value function:** $v : 2^P \to \mathbb{R}$ assigns each coalition S a payout $v(S)$
  - Convention: $v(\emptyset) = 0 \rightsquigarrow$ Empty coalitions generate no gain
  - $v(P)$: Total achievable payout when all players cooperate
    $\rightsquigarrow$ Forms the game's budget to be fairly distributed
- **Marginal contribution:** Measure how much value player j adds to coalition S by

$$\Delta(j, S) := v(S \cup \{j\}) - v(S) \qquad \text{(for all } j \in P\ S \subseteq P \setminus \{j\})$$

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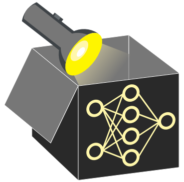

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COOPERATIVE GAMES IN GAME THEORY

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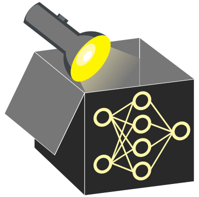

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- **Challenge:** Players vary in their contributions & how they influence each other
- **Goal:** Fairly distribute $v(P)$ among players by accounting for player interactions
  $\rightsquigarrow$ Assign each player $j \in P$ a fair share ϕ_j (**Shapley value**)

COOPERATIVE GAMES IN GAME THEORY

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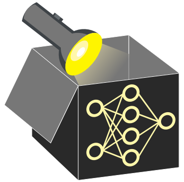

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- **Challenge:** Players vary in their contrib. & how they influence each other
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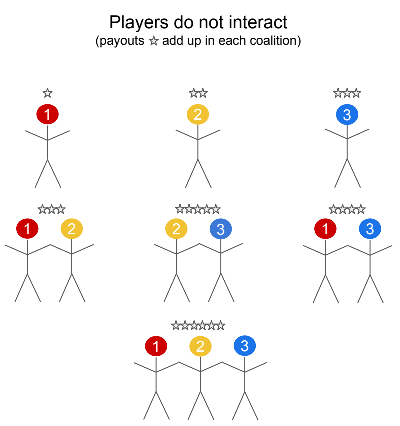
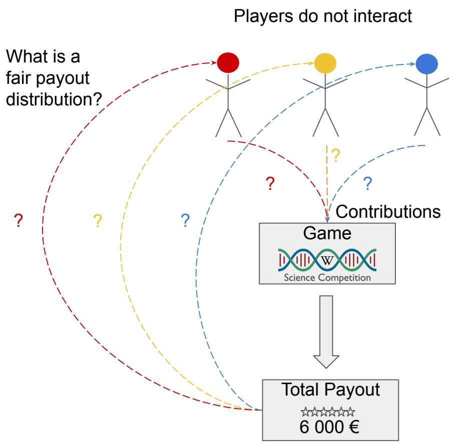
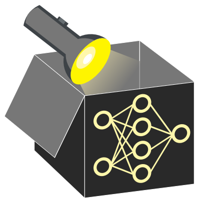
COOPERATIVE GAMES - NO INTERACTIONS

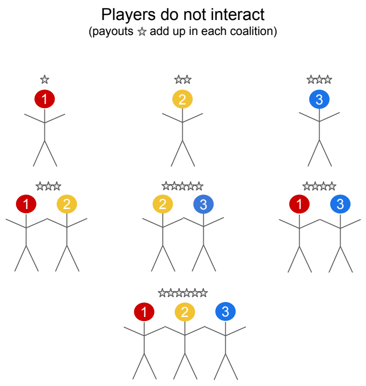


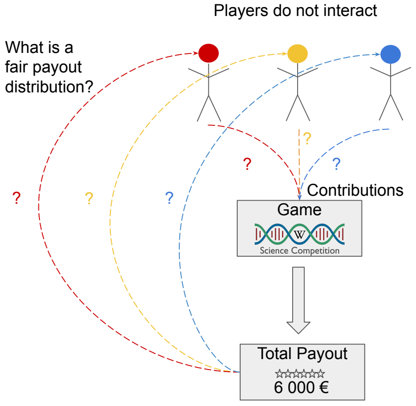


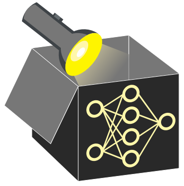


Question: What are the individual marginal contributions and what is a fair payout?

COOPERATIVE GAMES - NO INTERACTIONS







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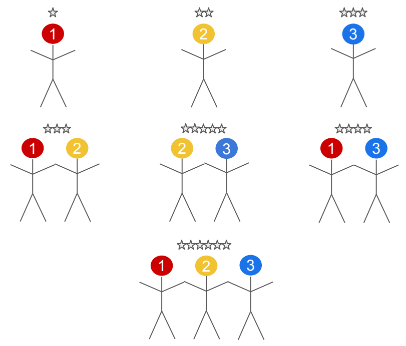
COOPERATIVE GAMES - NO INTERACTIONS

Players do not interact
(payouts ☆ add up in each coalition)



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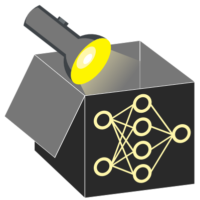

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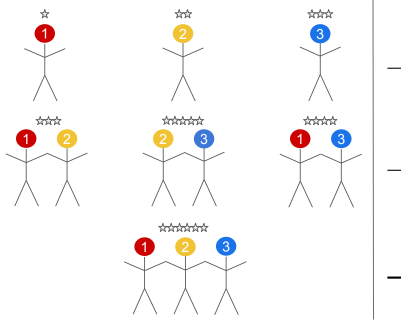

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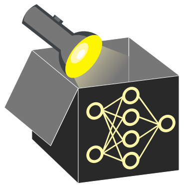

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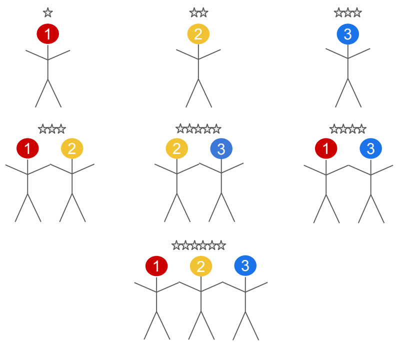

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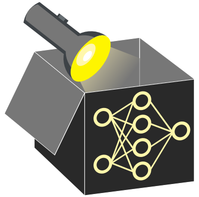

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  - ⇝ Player ❶ always adds 1000, ❷ adds 2000, and ❸ adds 3000
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- **Conclusion:** Fair payout $=$ average marginal contribution across all S
  - ⇝ Total value $v(P) = 6000$ splits proportionally by individual contributions:

$$❶ = \tfrac{1}{6}, \quad ❷ = \tfrac{1}{3}, \quad ❸ = \tfrac{1}{2}$$

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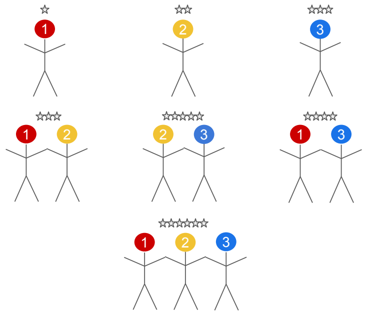

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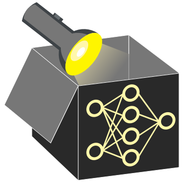

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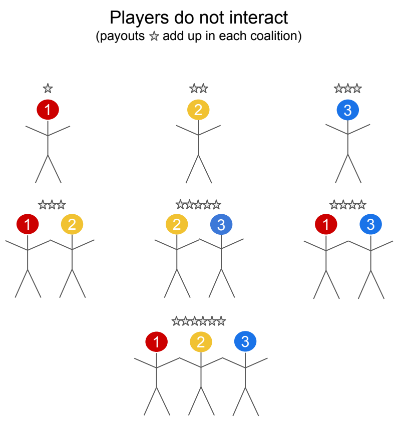
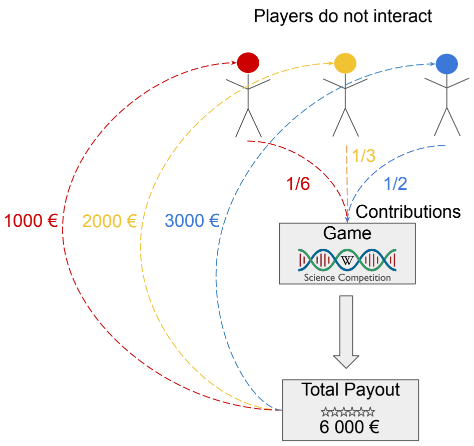
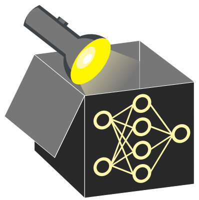
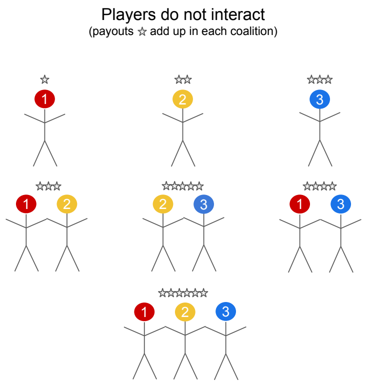


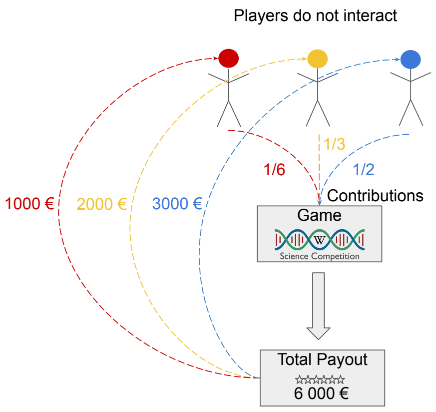


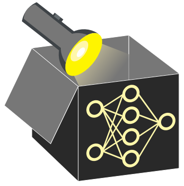


⇒ Fair payouts are trivial without interactions

COOPERATIVE GAMES - NO INTERACTIONS







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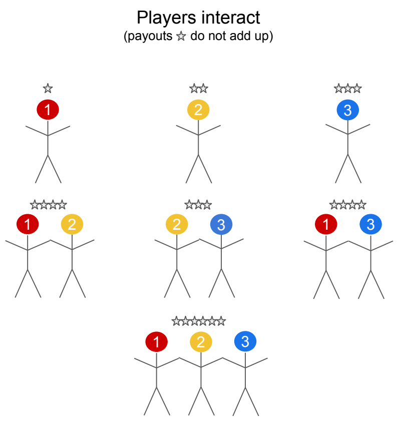
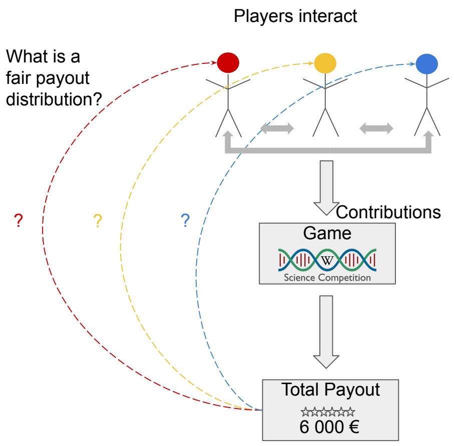
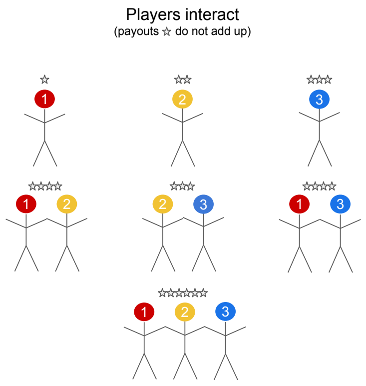
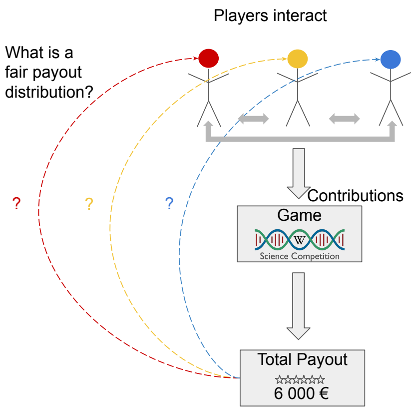




⇒ Unclear how to fairly distribute payouts when players interact

COOPERATIVE GAMES - INTERACTIONS





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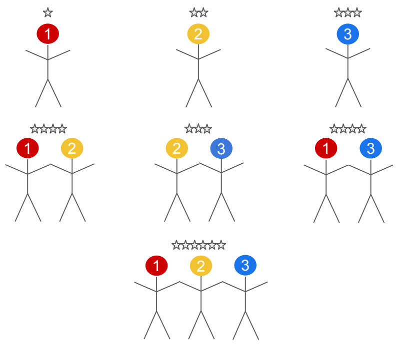
COOPERATIVE GAMES - INTERACTIONS

Players interact
(payouts ☆ do not add up)



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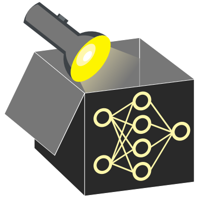

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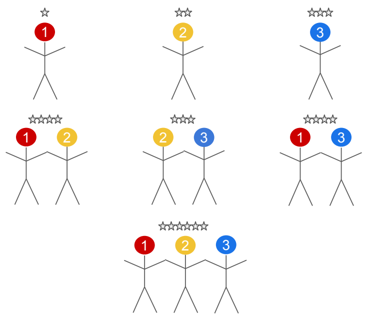

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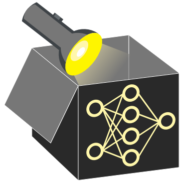

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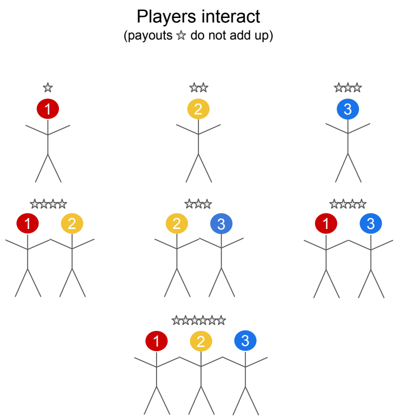
COOPERATIVE GAMES - INTERACTIONS



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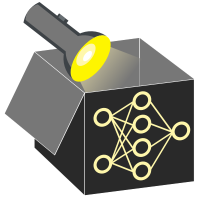
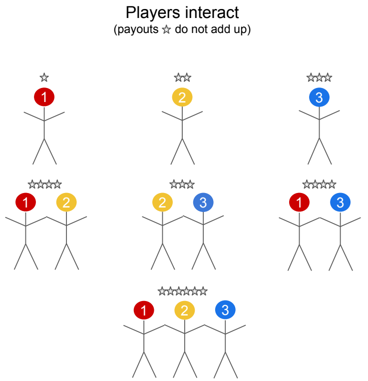


- **With interactions:** Players contribute different amounts depending on coalition
  $\rightsquigarrow$ Marginal contributions vary across coalitions S (e.g., due to overlap, synergy)
- Averaging over subsets does not recover total payout $v(P)$ $\rightsquigarrow$ unfair payout distr.
  $\rightsquigarrow$ average contrib. ❶ = 1750, ❷ = 1750, ❸ = 2250 do not sum to $v(P) = 6000$
- Value a player adds depends on joining order, not just who else is in the coalition
  $\rightsquigarrow$ Shapley values fairly average over all possible joining orders

COOPERATIVE GAMES - INTERACTIONS



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❸	{❷}	3000	2000	1000
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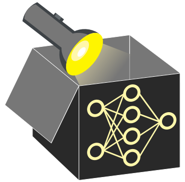

- **With interactions:** Players contribute differently depending on coalition
  $\rightsquigarrow$ Marginal contribs vary across coalitions S (e.g. overlap, synergy)
- Averaging over subsets does not recover total payout $v(P)$
  $\rightsquigarrow$ unfair payout distribution
  $\rightsquigarrow$ avg. contrib. ❶ = 1750 ❷ = 1750 ❸ = 2250 don't sum to $v(P) = 6000$
- Value a player adds depends on joining order, not just who's in coalition
  $\rightsquigarrow$ Shapley values fairly average over all possible joining orders

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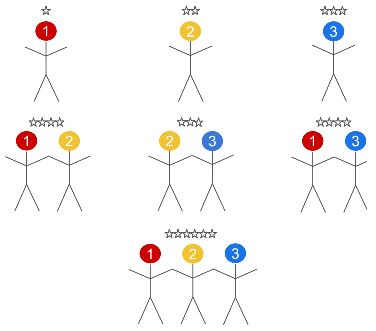
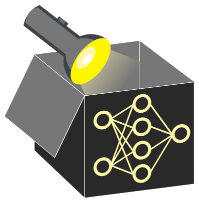
COOPERATIVE GAMES - INTERACTIONS





Ordering 1: ❸ → ❷ → ❶

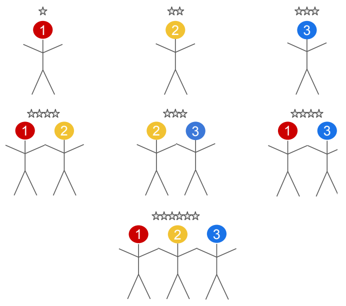
- ❸ joins alone: 3 ☆
- ❷ joins: total = 3 ☆, marginal = 0
- ❶ joins: total = 6 ☆, marginal = +3

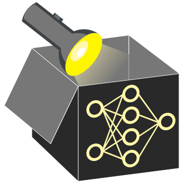
But what if ❶ joins before ❷?

Ordering 2: ❸ → ❶ → ❷

- ❸ joins alone: 3 ☆
- ❶ joins: total = 4 ☆, marginal = +1
- ❷ joins: total = 6 ☆, marginal = +2

COOPERATIVE GAMES - INTERACTIONS





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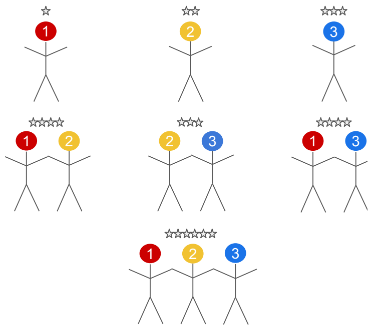

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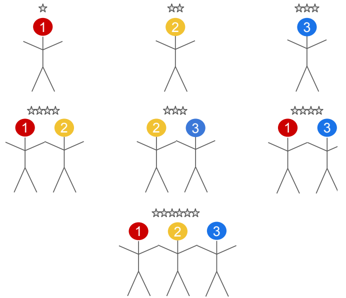
- **Order sensitivity:** A player's marginal contribution depends on when they join S
- **Shapley value:** Averages each player's contribution over all possible join orders
  - ⇝ Resolves redundancy (e.g., ❸'s contribution/skill overlaps with ❷'s)
  - ⇝ Accounts for order sensitivity (e.g., ❶ brings more value if added last)
  - ⇝ Ensures fairness (no player is advantaged or penalized by order of joining)

COOPERATIVE GAMES - INTERACTIONS



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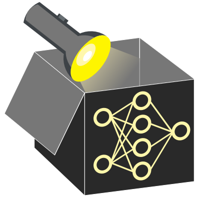
SHAPLEY VALUES - ILLUSTRATION



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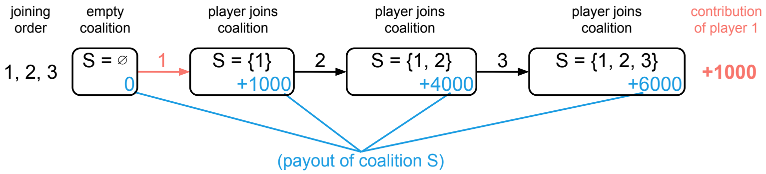
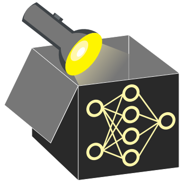
- For each order: track player *j*-th marginal contribution when *j* joins a coalition



SHAPLEY VALUES - ILLUSTRATION



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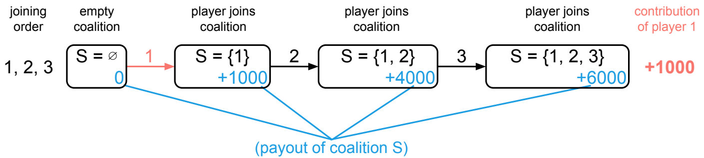

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SHAPLEY VALUES - ILLUSTRATION

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- **Example:** Compute payout difference after player 1 enters coalition ⇝ average

joining order	empty coalition		player joins coalition		player joins coalition		player joins coalition	contribution of player 1
1, 2, 3	S = ∅ 0	1	S = {1} +1000	2	S = {1, 2} +4000	3	S = {1, 2, 3} +6000	+1000
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Shapley value of player 1: +1833.33

SHAPLEY VALUES - ILLUSTRATION

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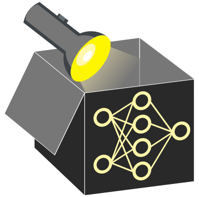

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- For each order: track player j-th marginal contribution when j joins a coalition
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- **Example:** Compute payout difference after player 2 enters coalition $\rightsquigarrow$ average

joining order	empty coalition		player joins coalition		player joins coalition		player joins coalition	contribution of player 2
1, 2, 3	S = ∅ 0	1	S = {1} +1000	2	S = {1, 2} +4000	3	S = {1, 2, 3} +6000	+3000
1, 3, 2	S = ∅ 0	1	S = {1} +1000	3	S = {1, 3} +4000	2	S = {1, 2, 3} +6000	+2000
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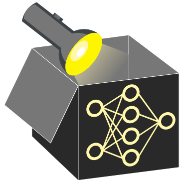
Shapley value of player 2: **+1833.33**

SHAPLEY VALUES - ILLUSTRATION



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SHAPLEY VALUES - ILLUSTRATION

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joining order	empty coalition		player joins coalition		player joins coalition		player joins coalition	contribution of player 3
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Shapley value of player 3: **+2333.33**

SHAPLEY VALUES - ILLUSTRATION

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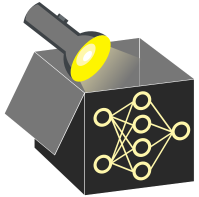
SHAPLEY VALUES - ILLUSTRATION



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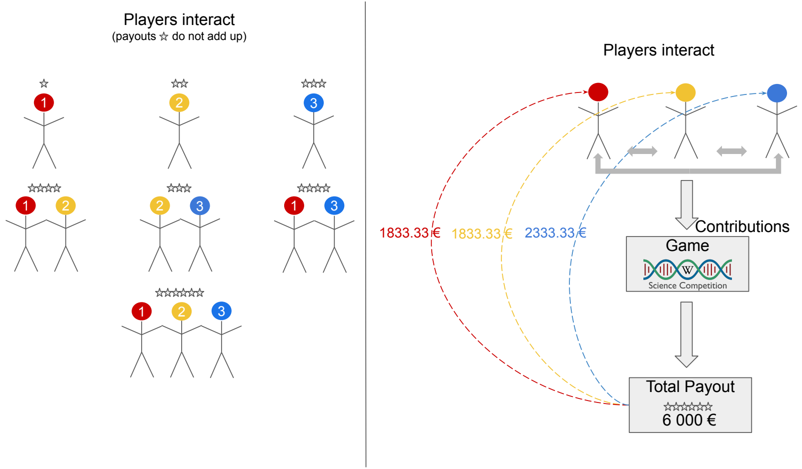

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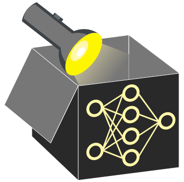

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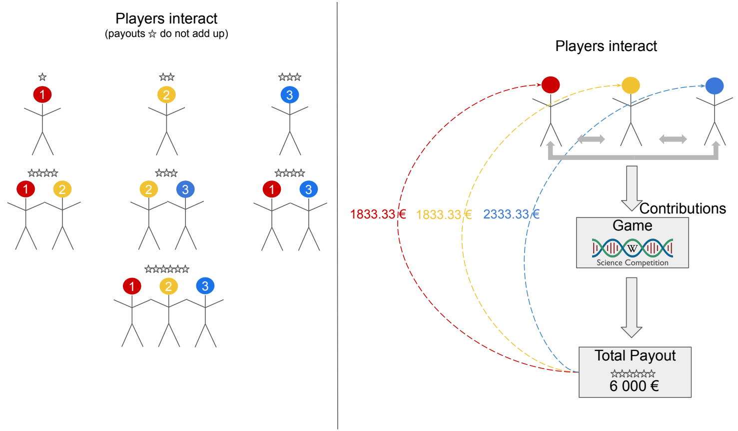

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SHAPLEY VALUE - ORDER DEFINITION

The Shapley value order definition averages the marginal contribution of a player across all possible player orderings:

$$\phi_j = \frac{1}{|P|!} \sum_{\tau \in \Pi} (v(S_j^\tau \cup \{j\}) - v(S_j^\tau))$$

- Π: Set of all permutations (joining orders) of the players – there are $|P|!$ in total

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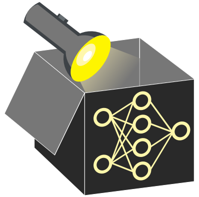

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  E.g.: $\Pi = \{(1, 2, 3), (1, 3, 2), (2, 1, 3), (2, 3, 1), (3, 1, 2), (3, 2, 1)\}$
  $\leadsto$ For joining order $\tau = (2, 1, 3)$ and player $j = 3 \Rightarrow S_j^\tau = \{2, 1\}$
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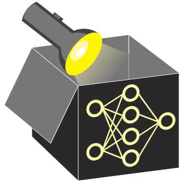

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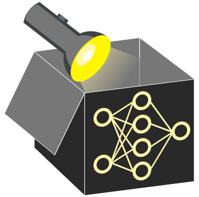

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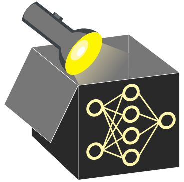
- Order definition allows to approximate Shapley values by sampling permutations
  $\rightsquigarrow$ Sample a fixed number $M \ll |P|!$ of random permutations and average:

$$\phi_j \approx \frac{1}{M} \sum_{\tau \in \Pi_M} (v(S_j^\tau \cup \{j\}) - v(S_j^\tau))$$

where $\Pi_M \subset \Pi$ is the random sample of M player orderings

SHAPLEY VALUE - ORDER DEFINITION



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FROM ORDER DEFINITION TO SET DEFINITION

- **Note:** The same subset S_j^τ can occur in multiple permutations (joining orders)
  $\rightsquigarrow$ Its marginal contribution is included multiple times in the sum in ϕ_j
- **Example (for set of players $P = \{❶, ❷, ❸\}$, player of interest $j = ❸$):**
  $\Pi = \{\underline{(❶, ❷, ❸)}, (❶, ❸, ❷), \underline{(❷, ❶, ❸)}, (❷, ❸, ❶), (❸, ❶, ❷), (❸, ❷, ❶)\}$
  $\rightsquigarrow$ In both $\underline{(❶, ❷, ❸)}$ and $\underline{(❷, ❶, ❸)}$, player ❸ joins after coalition $S_j^\tau = \{❶, ❷\}$
  $\Rightarrow$ Marginal contribution $v(\{❶, ❷, ❸\}) - v(\{❶, ❷\})$ occurs twice in ϕ_j
- **Reason:** Each subset S appears in $|S|!(|P| - |S| - 1)!$ orderings before j joins
  $\Rightarrow$ There are $|S|!$ possible orders of players within coalition S
  $\Rightarrow$ There are $(|P| - |S| - 1)!$ possible orders of players without S and j

$$\underbrace{\overbrace{\tau^{(1)} \mid \ldots \mid \tau^{(|S|)}}^{|S|!\text{ permutations}}}_{\text{Players before player } j} \mid \underbrace{\tau^{(|S|+1)}}_{\text{player } j} \mid \underbrace{\overbrace{\tau^{(|S|+2)} \mid \ldots \mid \tau^{(p)}}^{(|P|-|S|-1)!\text{ permutations}}}_{\text{Players after player } j}$$

FROM ORDER DEFINITION TO SET DEFINITION

- **Note:** The same subset S_j^τ can occur in multiple permutations
  $\rightsquigarrow$ Its marginal contribution is included multiple times in the sum in ϕ_j
- **Example Π (for players $P = \{❶, ❷, ❸\}$, player of interest $j = ❸$):**
  $\{\underline{(❶, ❷, ❸)}, (❶, ❸, ❷), \underline{(❷, ❶, ❸)}, (❷, ❸, ❶), (❸, ❶, ❷), (❸, ❷, ❶)\}$
  $\rightsquigarrow$ In $\underline{(❶, ❷, ❸)}$ and $\underline{(❷, ❶, ❸)}$, player ❸ joins after coal. $S_j^\tau = \{❶, ❷\}$
  $\Rightarrow$ Marginal contribution $v(\{❶, ❷, ❸\}) - v(\{❶, ❷\})$ occurs twice in ϕ_j
- **Reason:** Each subset S appears in $|S|!(|P| - |S| - 1)!$ orderings before j joins
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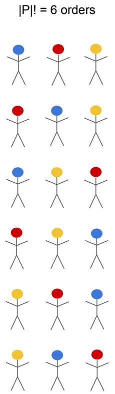

- **Order view:** Each of the $|P|!$ permutations contributes one term with weight $\frac{1}{|P|!}$
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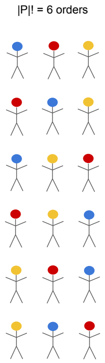

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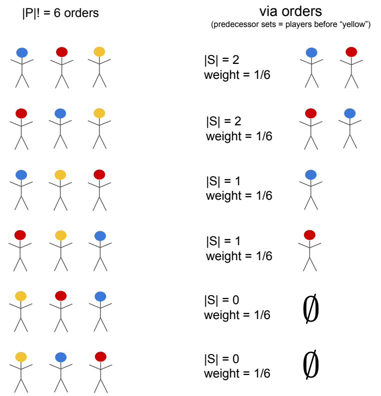

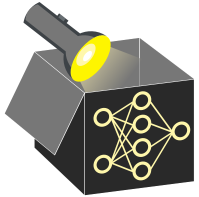

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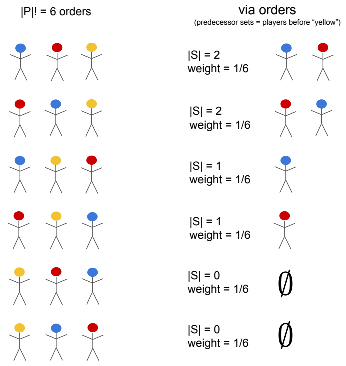

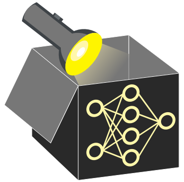

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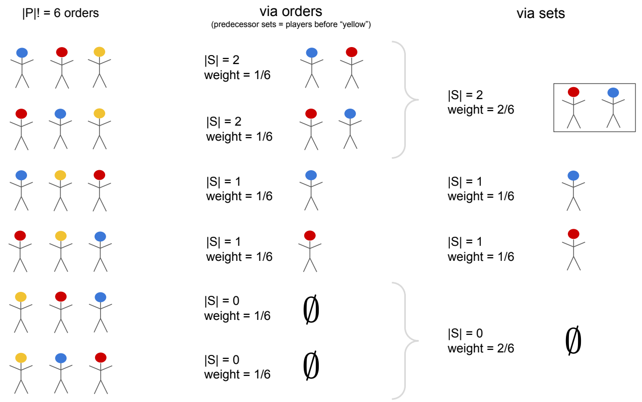

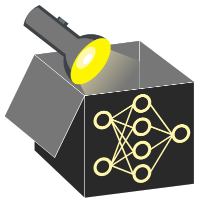

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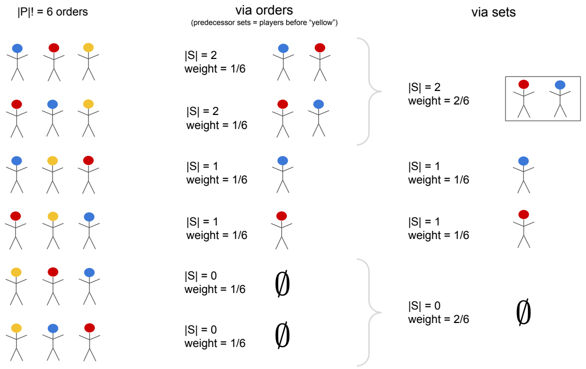

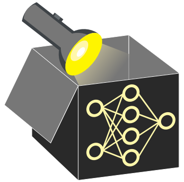

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SHAPLEY VALUE - SET DEFINITION

Shapley value via **set definition** (weighting via multinomial coefficient):

$$\phi_j = \sum_{S \subseteq P \setminus \{j\}} \frac{|S|!(|P| - |S| - 1)!}{|P|!} (v(S \cup \{j\}) - v(S))$$

The coefficient gives the probability that, when randomly arranging all $|P|$ players, the exact set S appears before player j, and the remaining players appear afterward.

$$\underbrace{\boxed{\tau^{(1)}}\boxed{\ldots}\boxed{\tau^{(|S|)}}}_{|S|!\text{ permutations}}\underbrace{\boxed{\tau^{(|S|+1)}}}_{\text{player } j}\underbrace{\boxed{\tau^{(|S|+2)}}\boxed{\ldots}\boxed{\tau^{(|P|)}}}_{(|P|-|S|-1)!\text{ permutations}}$$

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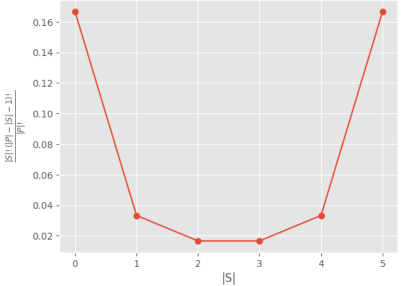
Different Weights Depending on the Size of S



- $|S| = 0$: player j joins first
  $\Rightarrow$ many permutations $\Rightarrow$ high weight
- $|S| = |P| - 1$: player j joins last
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- Result: U-shaped weight distribution

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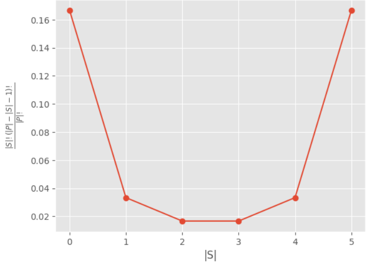

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AXIOMS OF FAIR PAYOUTS

What makes a payout fair? The Shapley value provides a fair payout ϕ_j for each player $j \in P$ and uniquely satisfies the following axioms for any value function v:

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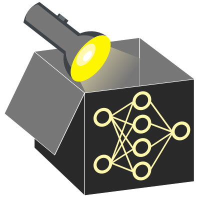

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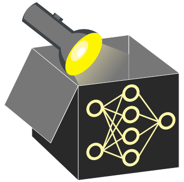

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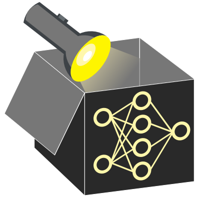

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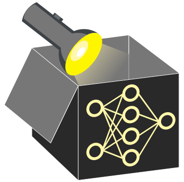

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