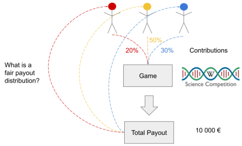
Interpretable Machine Learning

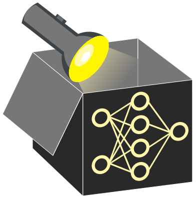
Shapley Values



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

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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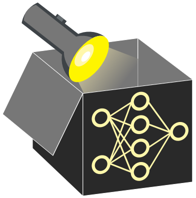

- **Game theory:** Studies strategic interactions among "players" (who act to maximize their utility), where outcomes depend on collective behavior
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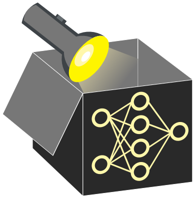
- **Value function:** $v : 2^P \to \mathbb{R}$ assigns each coalition S a payout $v(S)$
  - Convention: $v(\emptyset) = 0 \rightsquigarrow$ Empty coalitions generate no gain
  - $v(P)$: Total achievable payout when all players cooperate
    $\rightsquigarrow$ Forms the game's budget to be fairly distributed
- **Marginal contribution:** Measure how much value player j adds to coalition S by

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

COOPERATIVE GAMES IN GAME THEORY ▸ Shapley (1951)



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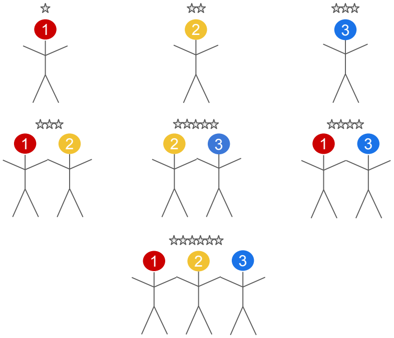
- **Challenge:** Players vary in their contributions & how they influence each other
- **Goal:** Fairly distribute $v(P)$ among players by accounting for player interactions
  $\rightsquigarrow$ Assign each player $j \in P$ a fair share ϕ_j (**Shapley value**)

COOPERATIVE GAMES - NO INTERACTIONS

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



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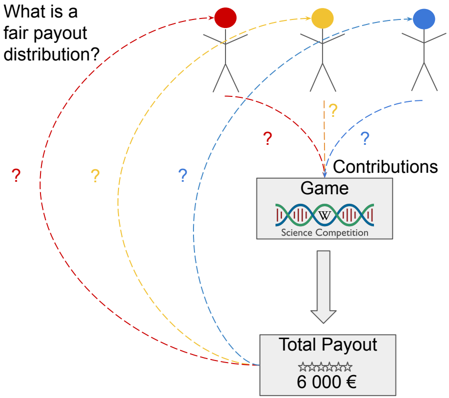

Question: What are the individual marginal contributions and what is a fair payout?

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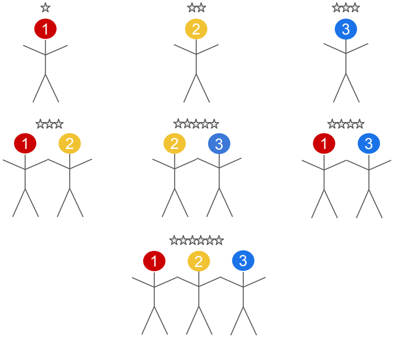

Player	Coalition S	$v(S \cup \{j\})$	$v(S)$	$\Delta(j, S)$
1	$\emptyset$	1000	0	1000
1	$\{2\}$	3000	2000	1000
1	$\{3\}$	4000	3000	1000
1	$\{2, 3\}$	6000	5000	1000
2	$\emptyset$	2000	0	2000
2	$\{1\}$	3000	1000	2000
2	$\{3\}$	5000	3000	2000
2	$\{1, 3\}$	6000	4000	2000
3	$\emptyset$	3000	0	3000
3	$\{1\}$	4000	1000	3000
3	$\{2\}$	5000	2000	3000
3	$\{1, 2\}$	6000	3000	3000

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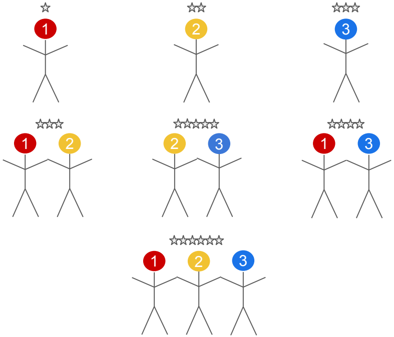
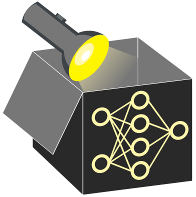


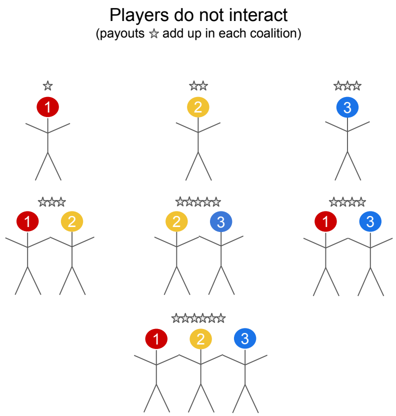
Player	Coalition S	$v(S \cup \{j\})$	$v(S)$	$\Delta(j, S)$
❶	$\emptyset$	1000	0	1000
❶	{❷}	3000	2000	1000
❶	{❸}	4000	3000	1000
❶	{❷, ❸}	6000	5000	1000
❷	$\emptyset$	2000	0	2000
❷	{❶}	3000	1000	2000
❷	{❸}	5000	3000	2000
❷	{❶, ❸}	6000	4000	2000
❸	$\emptyset$	3000	0	3000
❸	{❶}	4000	1000	3000
❸	{❷}	5000	2000	3000
❸	{❶, ❷}	6000	3000	3000

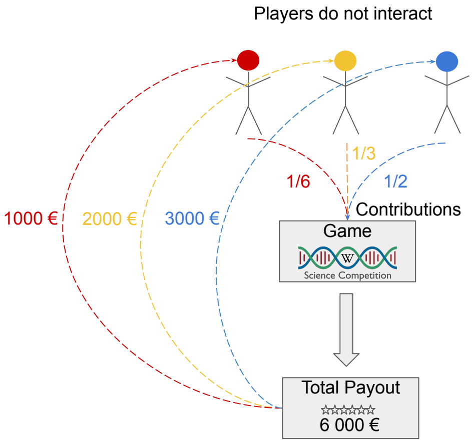


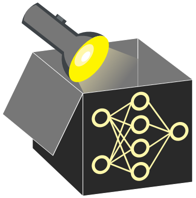
- **No interactions:** Each player contributes the same fixed value to each coalition
  - $\rightsquigarrow$ Player ❶ always adds 1000, ❷ adds 2000, and ❸ adds 3000
  - $\rightsquigarrow$ Marginal contributions are constant across all coalitions S
- **Conclusion:** Fair payout $=$ average marginal contribution across all S
  - $\rightsquigarrow$ Total value $v(P) = 6000$ splits proportionally by individual contributions:

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

COOPERATIVE GAMES - NO INTERACTIONS



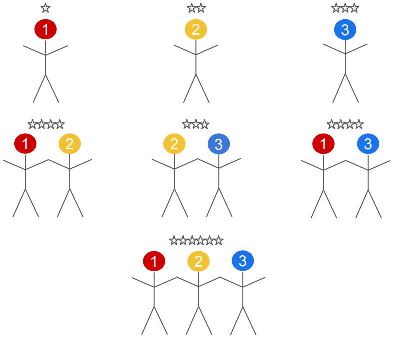


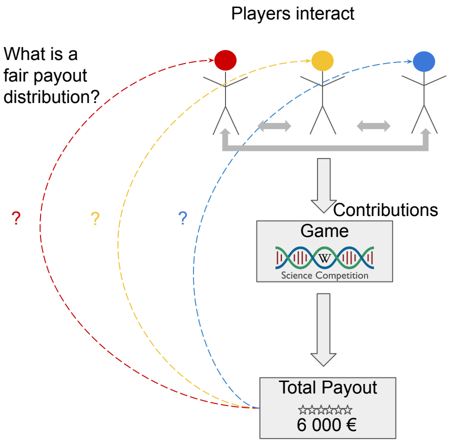


$\Rightarrow$ Fair payouts are trivial without interactions

COOPERATIVE GAMES - INTERACTIONS

Players interact
(payouts ☆ do not add up)





⇒ Unclear how to fairly distribute payouts when players interact

COOPERATIVE GAMES - INTERACTIONS

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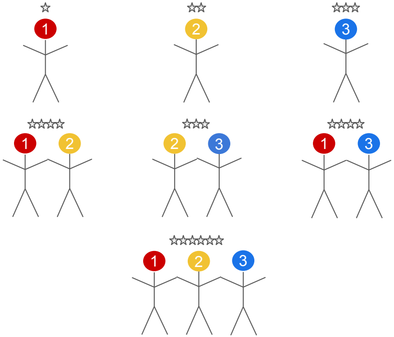

Player	Coalition S	$v(S \cup \{j\})$	$v(S)$	$\Delta(j, S)$
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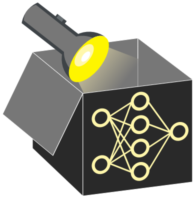
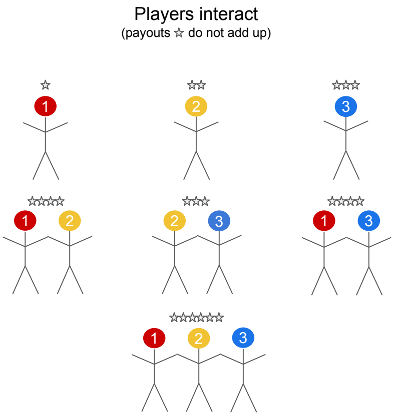


COOPERATIVE GAMES - INTERACTIONS



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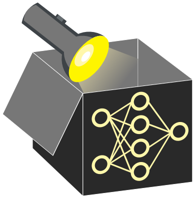
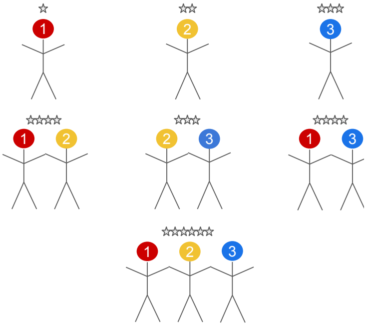
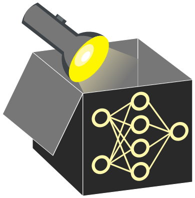


- **With interactions:** Players contribute different amounts depending on coalition
  $\rightsquigarrow$ Marginal contributions vary across coalitions S (e.g., due to overlap, synergy)
- Averaging over subsets does not recover total payout $v(P)$ $\rightsquigarrow$ unfair payout distr.
  $\rightsquigarrow$ 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





Ordering 1: ❸ → ❷ → ❶

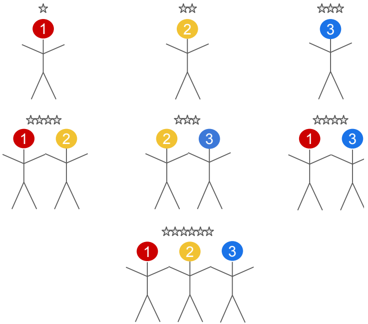
- ❸ joins alone: 3 ☆
- ❷ joins: total = 3 ☆, marginal = 0
- ❶ joins: total = 6 ☆, marginal = +3

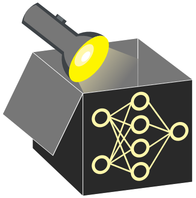
But what if ❶ joins before ❷?

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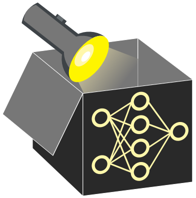
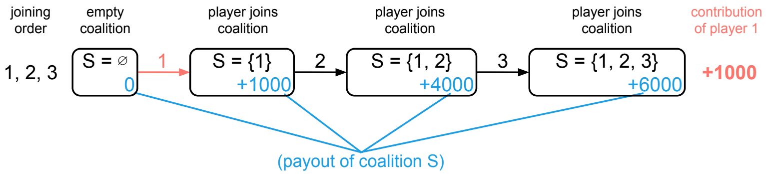
- ❸ joins alone: 3 ☆
- ❶ joins: total = 4 ☆, marginal = +1
- ❷ joins: total = 6 ☆, marginal = +2

- **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)

SHAPLEY VALUES - ILLUSTRATION



- Generate all possible joining orders of players (all permutations of full set P)
- For each order: track player j-th marginal contribution when j joins a coalition



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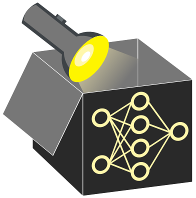
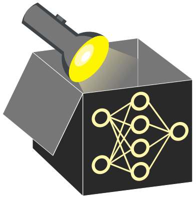


- Generate all possible joining orders of players (all permutations of full set P)
- For each order: track player j-th marginal contribution when j joins a coalition
- Shapley value of j: Average this marginal contribution over all joining orders
- **Example:** Compute payout difference after player 1 enters coalition $\rightsquigarrow$ average

joining order	empty coalition		player joins coalition		player joins coalition		player joins coalition	contribution of player 1
1, 2, 3	$S = \varnothing$ 0	1 →	$S = \{1\}$ +1000	2 →	$S = \{1, 2\}$ +4000	3 →	$S = \{1, 2, 3\}$ +6000	**+1000**
1, 3, 2	$S = \varnothing$ 0	1 →	$S = \{1\}$ +1000	3 →	$S = \{1, 3\}$ +4000	2 →	$S = \{1, 2, 3\}$ +6000	**+1000**
2, 1, 3	$S = \varnothing$ 0	2 →	$S = \{2\}$ +2000	1 →	$S = \{1, 2\}$ +4000	3 →	$S = \{1, 2, 3\}$ +6000	**+2000**
2, 3, 1	$S = \varnothing$ 0	2 →	$S = \{2\}$ +2000	3 →	$S = \{2, 3\}$ +3000	1 →	$S = \{1, 2, 3\}$ +6000	**+3000**
3, 1, 2	$S = \varnothing$ 0	3 →	$S = \{3\}$ +3000	1 →	$S = \{1, 3\}$ +4000	2 →	$S = \{1, 2, 3\}$ +6000	**+1000**
3, 2, 1	$S = \varnothing$ 0	3 →	$S = \{3\}$ +3000	2 →	$S = \{2, 3\}$ +3000	1 →	$S = \{1, 2, 3\}$ +6000	**+3000**

Shapley value of player 1 : +1833.33

SHAPLEY VALUES - ILLUSTRATION

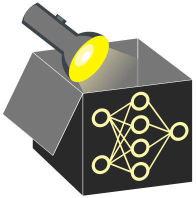


- Generate all possible joining orders of players (all permutations of full set P)
- For each order: track player j-th marginal contribution when j joins a coalition
- Shapley value of j: Average this marginal contribution over all joining orders
- **Example:** Compute payout difference after player 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	$\xrightarrow{1}$	S = {1} +1000	$\xrightarrow{2}$	S = {1, 2} +4000	$\xrightarrow{3}$	S = {1, 2, 3} +6000	**+3000**
1, 3, 2	S = ∅ 0	$\xrightarrow{1}$	S = {1} +1000	$\xrightarrow{3}$	S = {1, 3} +4000	$\xrightarrow{2}$	S = {1, 2, 3} +6000	**+2000**
2, 1, 3	S = ∅ 0	$\xrightarrow{2}$	S = {2} +2000	$\xrightarrow{1}$	S = {1, 2} +4000	$\xrightarrow{3}$	S = {1, 2, 3} +6000	**+2000**
2, 3, 1	S = ∅ 0	$\xrightarrow{2}$	S = {2} +2000	$\xrightarrow{3}$	S = {2, 3} +3000	$\xrightarrow{1}$	S = {1, 2, 3} +6000	**+2000**
3, 1, 2	S = ∅ 0	$\xrightarrow{3}$	S = {3} +3000	$\xrightarrow{1}$	S = {1, 3} +4000	$\xrightarrow{2}$	S = {1, 2, 3} +6000	**+2000**
3, 2, 1	S = ∅ 0	$\xrightarrow{3}$	S = {3} +3000	$\xrightarrow{2}$	S = {2, 3} +3000	$\xrightarrow{1}$	S = {1, 2, 3} +6000	**+0**

Shapley value of player 2 : +1833.33

SHAPLEY VALUES - ILLUSTRATION

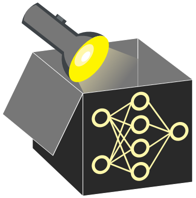


- Generate all possible joining orders of players (all permutations of full set P)
- For each order: track player j-th marginal contribution when j joins a coalition
- Shapley value of j: Average this marginal contribution over all joining orders
- **Example:** Compute payout difference after player 3 enters coalition $\rightsquigarrow$ average

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

Shapley value of player 3 : +2333.33

SHAPLEY VALUES - ILLUSTRATION



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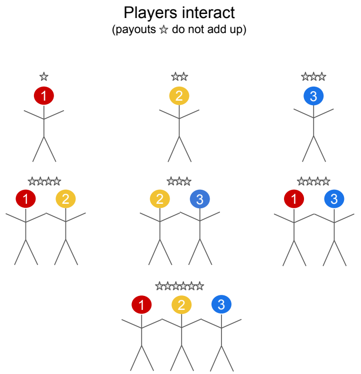
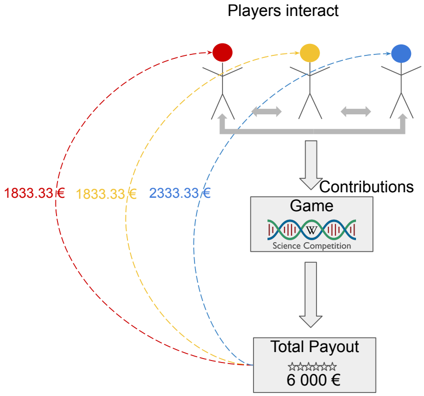
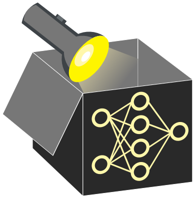




SHAPLEY VALUE - ORDER DEFINITION



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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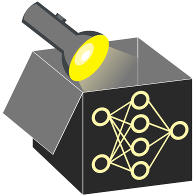

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- Π: Set of all permutations (joining orders) of the players – there are $|P|!$ in total
- S_j^τ: Set of players before j joins, for each ordering $\tau = (\tau^{(1)}, \dots, \tau^{(p)})$
  E.g.: $\Pi = \{(❶, ❷, ❸), (❶, ❸, ❷), (❷, ❶, ❸), (❷, ❸, ❶), (❸, ❶, ❷), (❸, ❷, ❶)\}$
  $\rightsquigarrow$ For joining order $\tau = (❷, ❶, ❸)$ and player $j = ❸ \Rightarrow S_j^\tau = \{❷, ❶\}$
  $\rightsquigarrow$ For joining order $\tau = (❸, ❶, ❷)$ and player $j = ❶ \Rightarrow S_j^\tau = \{❸\}$

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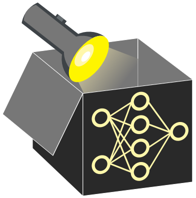
- Π: Set of all permutations (joining orders) of the players – there are $|P|!$ in total
- S_j^τ: Set of players before j joins, for each ordering $\tau = (\tau^{(1)}, \dots, \tau^{(p)})$
  E.g.: $\Pi = \{$(❶, ❷, ❸), (❶, ❸, ❷), (❷, ❶, ❸), (❷, ❸, ❶), (❸, ❶, ❷), (❸, ❷, ❶)$\}$
  $\rightsquigarrow$ For joining order $\tau =$ (❷, ❶, ❸) and player $j =$ ❸ $\Rightarrow S_j^\tau = \{$❷, ❶$\}$
  $\rightsquigarrow$ For joining order $\tau =$ (❸, ❶, ❷) and player $j =$ ❶ $\Rightarrow S_j^\tau = \{$❸$\}$
- Order definition allows to approximate Shapley values by sampling permutations
  $\rightsquigarrow$ Sample a fixed number $M \ll |P|!$ of random permutations and average:

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

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

FROM ORDER DEFINITION TO SET DEFINITION

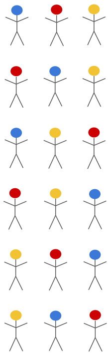


- **Note:** The same subset S_j^{τ} can occur in multiple permutations (joining orders)
  $\rightsquigarrow$ Its marginal contribution is included multiple times in the sum in ϕ_j
- **Example (for set of players $P = \{$❶, ❷, ❸$\}$, player of interest $j =$ ❸):**
  $\Pi = \{$(❶, ❷, ❸), (❶, ❸, ❷), (❷, ❶, ❸), (❷, ❸, ❶), (❸, ❶, ❷), (❸, ❷, ❶)$\}$
  $\rightsquigarrow$ In both (❶, ❷, ❸) and (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

|P|! = 6 orders



- **Order view:** Each of the $|P|!$ permutations contributes one term with weight $\frac{1}{|P|!}$
- Same subset $S \subseteq P \setminus \{j\}$ can appear before j in multiple orders
  $\rightsquigarrow$ e.g., S = {●, ●} = {●, ●}
- **Set view:** Group by unique subsets S, not permutations
- Each S occurs in $|S|!(|P| - |S| - 1)!$ orderings $\rightsquigarrow$ Weight: $\frac{|S|!(|P|-|S|-1)!}{|P|!}$

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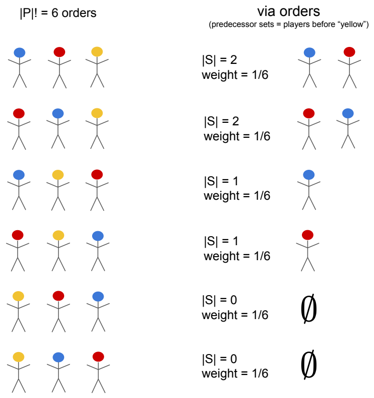

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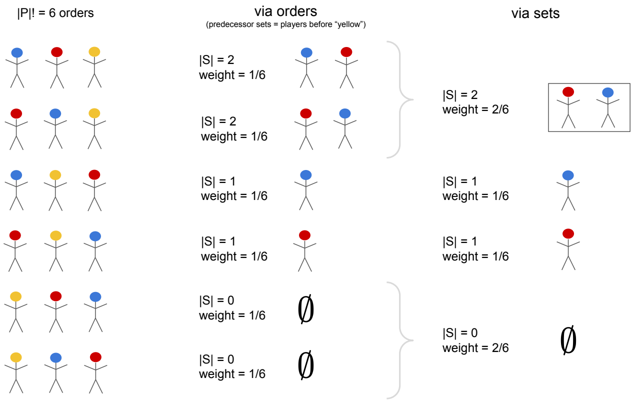

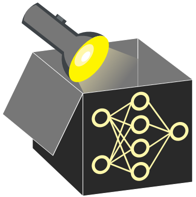

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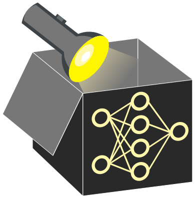
SHAPLEY VALUE - SET DEFINITION



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.

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

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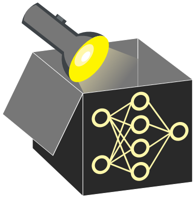

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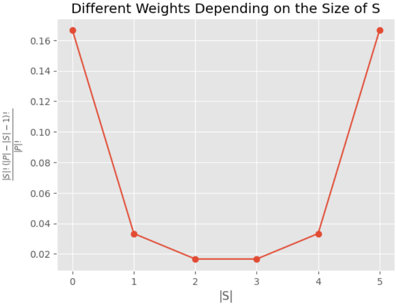
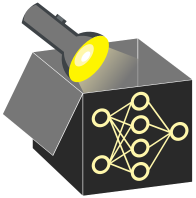


- $|S| = 0$: player j joins first
  $\Rightarrow$ many permutations $\Rightarrow$ high weight
- $|S| = |P| - 1$: player j joins last
  $\Rightarrow$ many permutations $\Rightarrow$ high weight
- Middle-sized $|S|$: fewer exact matches
  $\Rightarrow$ lower weight
- Result: U-shaped weight distribution

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:

- **Efficiency**: Total payout $v(P)$ is fully allocated to players:

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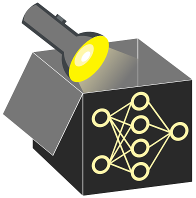

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$$\text{If } v(S \cup \{j\}) = v(S \cup \{k\}) \text{ for all } S \subseteq P \setminus \{j, k\}, \text{ then } \phi_j = \phi_k$$

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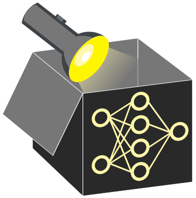

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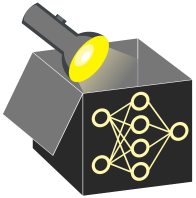

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- **Additivity**: For two separate games with value functions v_1, v_2, define a combined game with $v(S) = v_1(S) + v_2(S)$ for all $S \subseteq P$. Then:

$$\phi_{j, v_1 + v_2} = \phi_{j, v_1} + \phi_{j, v_2}$$

$\rightsquigarrow$ Payout of combined game = payout of the two separate games