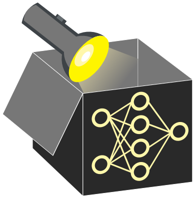
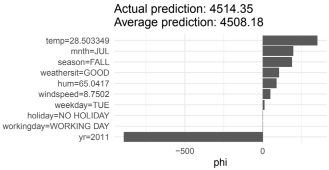
Interpretable Machine Learning

Shapley Values for Local Explanations

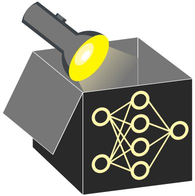




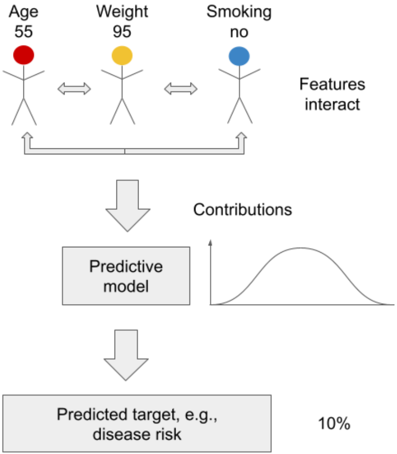
Learning goals

- See model predictions as a cooperative game
- Transfer the Shapley value concept from game theory to machine learning

FROM GAME THEORY TO MACHINE LEARNING



- Model prediction depends on feature interactions for a specific observation
- **Goal:** Decompose prediction into **individual feature contributions**
- **Idea:** Treat features as players jointly producing a prediction
- How to fairly assign credit to features?
  $\Rightarrow$ Shapley values



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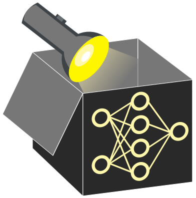

- **Game:** Predict $\hat{f}(x_1, x_2, \dots, x_p)$ for a single observation $\mathbf{x}$
- **Players:** Features $x_j, j \in \{1, \dots, p\}$, cooperate to produce a prediction
- **Value function:** Defines payout of coalition $S \subseteq P$ for observation $\mathbf{x}$ by

$$v(S) = \hat{f}_S(\mathbf{x}_S) - \hat{f}_\emptyset, \text{ where}$$

  - $\hat{f}_S : \mathcal{X}_S \mapsto \mathcal{Y}$ is the PD function $\hat{f}_S(\mathbf{x}_S) := \int \hat{f}(\mathbf{x}_S, X_{-S})\, d\mathbb{P}_{X_{-S}}$
    $\rightsquigarrow$ "Removes" features in $-S$ by marginalizing, keeping $\hat{f}$ fixed
  - Mean prediction $\hat{f}_\emptyset := \mathbb{E}_{\mathbf{x}}(\hat{f}(\mathbf{x}))$ is subtracted to ensure $v(\emptyset) = 0$
- **Goal:** Distribute total payout $v(P) = \hat{f}(\mathbf{x}) - \hat{f}_\emptyset$ fairly among features

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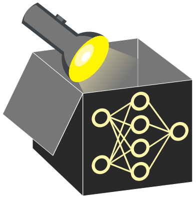

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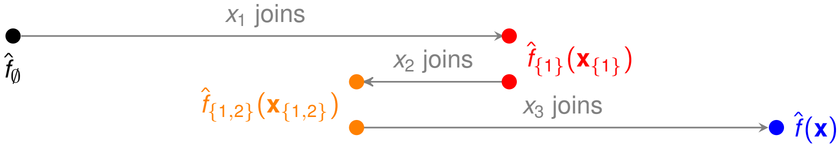
- **Marginal contribution of feature j joining coalition S** ($\hat{f}_\emptyset$ cancels):

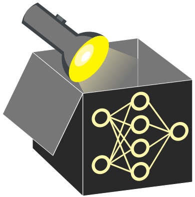
$$\Delta(j, S) = v(S \cup \{j\}) - v(S) = \hat{f}_{S \cup \{j\}}(\mathbf{x}_{S \cup \{j\}}) - \hat{f}_S(\mathbf{x}_S)$$

- **Example (3 features):** Feature contributions for joining order $x_1 \rightarrow x_2 \rightarrow x_3$ toward total payout $v(P) = \hat{f}(\mathbf{x}) - \hat{f}_\emptyset$, each step reflects a marginal contribution



SHAPLEY VALUE - DEFINITION

▸ Shapley (1953) ▸ Strumbelj et al. (2014)



Order definition: Shapley value $\phi_j(\mathbf{x})$ quantifies contribution of x_j via

$$\phi_j(\mathbf{x}) = \frac{1}{|P|!} \sum_{\tau \in \Pi} \underbrace{\hat{f}_{S_j^\tau \cup \{j\}}(\mathbf{x}_{S_j^\tau \cup \{j\}}) - \hat{f}_{S_j^\tau}(\mathbf{x}_{S_j^\tau})}_{\Delta(j, S_j^\tau) \text{ marginal contribution of feature } j}$$

- **Interpretation:** $\phi_j(\mathbf{x})$ quantifies how much feature x_j contributes to the difference between $\hat{f}(\mathbf{x})$ and the mean prediction $\hat{f}_\emptyset$
  $\rightsquigarrow$ Marginal contributions and Shapley values can be negative
- **Exact computation of ϕ_j:** Using PD function $\hat{f}_S(\mathbf{x}_S) = \frac{1}{n}\sum_{i=1}^n \hat{f}(\mathbf{x}_S, \mathbf{x}_{-S}^{(i)})$ yields

$$\phi_j(\mathbf{x}) = \frac{1}{|P|!} \sum_{\tau \in \Pi} \frac{1}{n} \sum_{i=1}^{n} \hat{f}(\mathbf{x}_{S_j^\tau \cup \{j\}}, \mathbf{x}^{(i)}_{-\{S_j^\tau \cup \{j\}\}}) - \hat{f}(\mathbf{x}_{S_j^\tau}, \mathbf{x}^{(i)}_{-S_j^\tau})$$

$\rightsquigarrow$ $\hat{f}_S$ marginalizes over all features not in S using all observations $i = 1, \dots, n$
$\rightsquigarrow$ Exact computation requires $|P|! \cdot n$ marginal contribution terms

ESTIMATION: A PRACTICAL PROBLEM

- **Exact computation is infeasible for many features:**
  For $|P| = 10$, the number of permutations is $10! \approx 3.6$ million
  $\rightsquigarrow$ Complexity grows factorially with feature count

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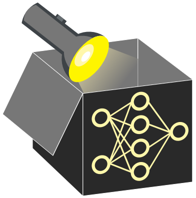

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  Each permutation τ defines a coalition S_j^τ needing its own estimate of $\hat{f}_{S_j^\tau}(\mathbf{x}_{S_j^\tau})$
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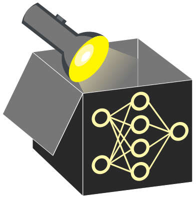

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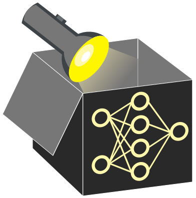

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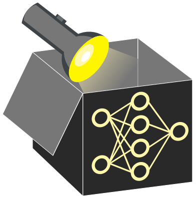
- **Tradeoff: Accuracy vs. Efficiency**
  Larger M improves Shapley approximation
  $\rightsquigarrow$ Higher cost, but better fidelity to the exact value

APPROXIMATION ALGORITHM ▸ Strumbelj et al. (2014)



Estimate Shapley value ϕ_j of observation $\mathbf{x}$ for feature j:

- **Input:** $\mathbf{x}$ obs. of interest, j feat. of interest, $\hat{f}$ model, $\mathcal{D}$ data, M iterations

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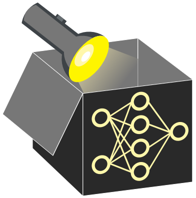

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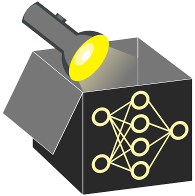

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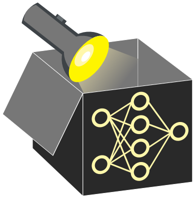

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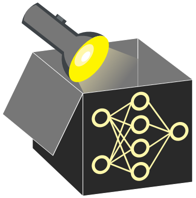

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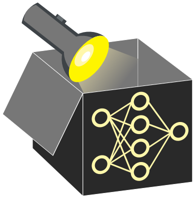

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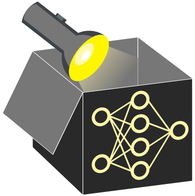

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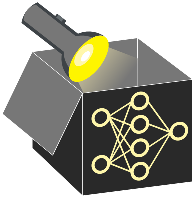

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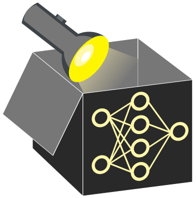

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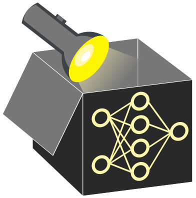

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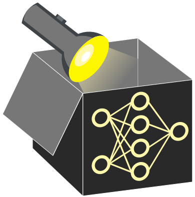

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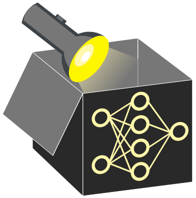
2. Compute Shapley value $\phi_j = \frac{1}{M} \sum_{m=1}^{M} \Delta(j, S_m)$

$\rightsquigarrow$ Over M iterations, the PD functions $\hat{f}_{S_m}(\mathbf{x}_{S_m})$ and $\hat{f}_{S_m \cup \{j\}}(\mathbf{x}_{S_m \cup \{j\}})$ are approximated by $\hat{f}(\mathbf{x}_{-j}^{(m)})$ and $\hat{f}(\mathbf{x}_{+j}^{(m)})$, where features not in the coalition (to be marginalized) are imputed with values from the random data points $\mathbf{z}^{(m)}$

SHAPLEY VALUE APPROXIMATION - ILLUSTRATION



Definition

x: obs. of interest

x with feature values in $\mathbf{x}_{S_m}$ (other are replaced)

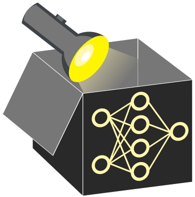
$$\phi_j(\mathbf{x}) = \frac{1}{M}\sum_{m=1}^{M}\left[\hat{f}(\mathbf{x}_{+j}{}^{(m)}) - \hat{f}(\mathbf{x}_{-j}{}^{(m)})\right]$$

x with feature values in $\mathbf{x}_{S_m \cup \{j\}}$

	Temperature	Humidity	Windspeed	Year
x	10.66	56	11	2012
x_{+j}	10.66	56	$random : z^{(m)}_{windspeed}$	2012
x_{-j}	10.66	56	$random : z^{(m)}_{windspeed}$	$random : z^{(m)}_{year}$

j

SHAPLEY VALUE APPROXIMATION - ILLUSTRATION



Definition

Contribution of feature j to coalition S_m

$$\phi_j(\mathbf{x}) = \frac{1}{M}\sum_{m=1}^{M} \underbrace{\left[\hat{f}(\mathbf{x}_{+j}{}^{(m)}) - \hat{f}(\mathbf{x}_{-j}{}^{(m)})\right]}_{:= \Delta(j, S_m)}$$

- $\Delta(j, S_m) = \hat{f}(\mathbf{x}_{+j}^{(m)}) - \hat{f}(\mathbf{x}_{-j}^{(m)})$ is marginal contribution of feature j to coalition S_m
- Here: Feature *year* contributes +700 bike rentals if it joins coalition $S_m = \{temp, hum\}$

	Temperature	Humidity	Windspeed	Year	Count	
x	10.66	56	11	2012		
x_{+j}	10.66	56	$random : z_{windspeed}^{(m)}$	2012	5600	700
x_{-j}	10.66	56	$random : z_{windspeed}^{(m)}$	$random : z_{year}^{(m)}$	4900	

j $\hat{f}$ $\Delta(j, S_m)$ marginal contribution

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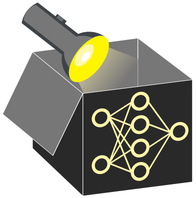


Definition

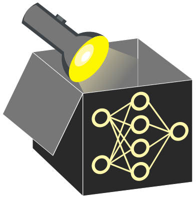
average the contributions of feature j

$$\phi_j(\mathbf{x}) = \frac{1}{M} \sum_{m=1}^{M} \left[\hat{f}(\mathbf{x}_{+j}{}^{(m)}) - \hat{f}(\mathbf{x}_{-j}{}^{(m)}) \right]$$

- Compute marginal contribution of feature j towards the prediction across all randomly drawn feature coalitions $S_1, \dots, S_m$
- Average all M marginal contributions of feature j
- Shapley value ϕ_j is the payout of feature j, i.e., how much feature *year* contributed to the overall prediction in bicycle counts of a specific observation **x**

$$m = \underbrace{\begin{array}{cccc} 1 & 2 & & \text{M} \\ \boxed{700} & \boxed{503} & \cdots & \boxed{300} \end{array}}_{\Delta(j, S_m)} \qquad \underbrace{\begin{array}{c} \text{Shapley value} \\ \boxed{501} \end{array}}_{\phi_j}$$

REVISITED: AXIOMS FOR FAIR ATTRIBUTIONS



We adapt the classic Shapley axioms to the setting of model predictions:

- **Efficiency**: Sum of Shapley values adds up to the centered prediction:

$$\sum_{j=1}^{p} \phi_j(\mathbf{x}) = \hat{f}(\mathbf{x}) - \mathbb{E}_{\mathbf{x}}[\hat{f}(\mathbf{x})]$$

$\rightsquigarrow$ All predictive contribution is fully distributed among features

- **Symmetry**: Identical contributors receive equal value:

$$\hat{f}_{S\cup\{j\}}(\mathbf{x}_{S\cup\{j\}}) = \hat{f}_{S\cup\{k\}}(\mathbf{x}_{S\cup\{k\}})\ \forall S \subseteq P \setminus \{j,k\} \Rightarrow \phi_j = \phi_k$$

$\rightsquigarrow$ Interaction effects are shared equitably

- **Dummy (Null Player)**: Irrelevant features receive zero attribution:

$$\hat{f}_{S\cup\{j\}}(\mathbf{x}_{S\cup\{j\}}) = \hat{f}_{S}(\mathbf{x}_{S})\ \forall S \subseteq P \Rightarrow \phi_j = 0$$

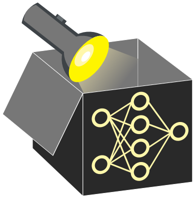
$\rightsquigarrow$ Shapley value is zero for unused features (e.g., trees or LASSO)

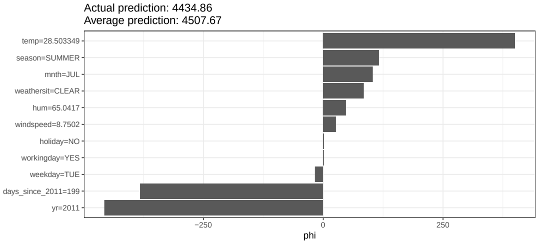
- **Additivity**: Attributions are additive across models:

$$\phi_j(v_1 + v_2) = \phi_j(v_1) + \phi_j(v_2)$$

$\rightsquigarrow$ Enables combining Shapley values for model ensembles

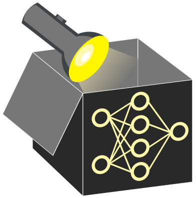
BIKE SHARING DATASET





- Shapley decomposition for a single prediction in bike sharing dataset
- Model prediction: $\hat{f}(\mathbf{x}^{(200)}) =$ **4434.86** vs. dataset average: $\mathbb{E}_{\mathbf{x}}[\hat{f}(\mathbf{x})] =$ **4507.67**
- Total feature attribution: $\sum_j \phi_j =$ **-72.81**
  $\rightsquigarrow$ Explain downward shift from mean prediction
- Temperature (with value 28.5°C) is the strongest positive contributor: $+400$
- Features `yr = 2011` and `days_since_2011 = 199` strongly reduce prediction
  $\rightsquigarrow$ Model captures lower bike demand in 2011 compared to 2012

ADVANTAGES AND DISADVANTAGES



Advantages:

- **Strong theoretical foundation** from cooperative game theory
- **Fair attribution:** Prediction is additively distributed across features
  $\rightsquigarrow$ Easy to interpret for users
- **Contrastive explanations:** Quantify each feature's role in deviating from the average prediction

Disadvantages:

- **Computational cost:** Exact computation scales factorially with feature count
  $\rightsquigarrow$ Without sampling, all 2^p coalitions (or $p!$ permutations) must be evaluated
- **Issue with correlated features:** Shapley values may evaluate the model on feature combinations that do not occur in the real data