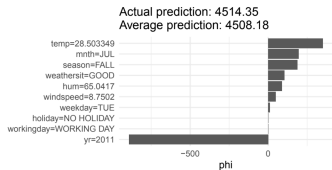


Interpretable Machine Learning

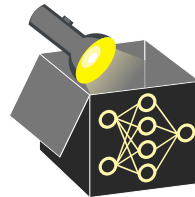
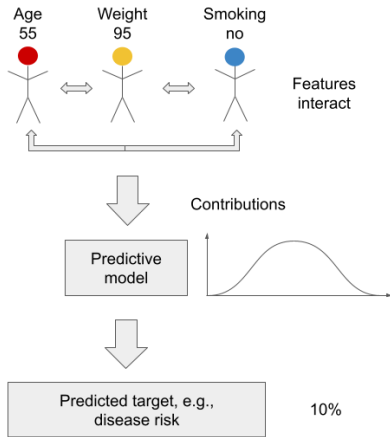
Shapley Values for Local Explanations



Learning goals

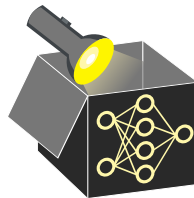
- See model predictions as a cooperative game
- Transfer the Shapley value concept from game theory to machine learning

FROM GAME THEORY TO MACHINE LEARNING



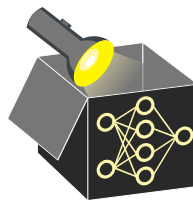
FROM GAME THEORY TO MACHINE LEARNING

- Game: Make prediction $\hat{f}(x_1, x_2, \dots, x_p)$ for a single observation \mathbf{x}



FROM GAME THEORY TO MACHINE LEARNING

- Game: Make prediction $\hat{f}(x_1, x_2, \dots, x_p)$ for a single observation \mathbf{x}
- Players: Features $x_j, j \in \{1, \dots, p\}$ which cooperate to produce a prediction
 \rightsquigarrow How can we make a prediction with a subset of features without changing the model?
 \rightsquigarrow PD function: $\hat{f}_S(\mathbf{x}_S) := \int_{X_{-S}} \hat{f}(\mathbf{x}_S, X_{-S}) d\mathbb{P}_{X_{-S}}$ (“removing” by marginalizing over $-S$)

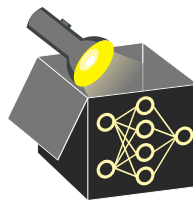
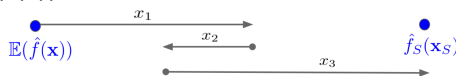


FROM GAME THEORY TO MACHINE LEARNING

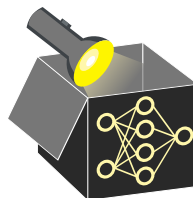
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- Value function / payout of coalition $S \subseteq P$ for observation \mathbf{x} :

$$v(S) = \hat{f}_S(\mathbf{x}_S) - \mathbb{E}_{\mathbf{x}}(\hat{f}(\mathbf{x})), \text{ where } \hat{f}_S : \mathcal{X}_S \mapsto \mathcal{Y}$$

\rightsquigarrow subtraction of $\mathbb{E}_{\mathbf{x}}(\hat{f}(\mathbf{x}))$ ensures that v is a value function with $v(\emptyset) = 0$



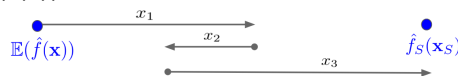
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- Marginal contribution: $v(S \cup \{j\}) - v(S) = \hat{f}_{S \cup \{j\}}(\mathbf{x}_{S \cup \{j\}}) - \hat{f}_S(\mathbf{x}_S)$
 $\rightsquigarrow \mathbb{E}_{\mathbf{x}}(\hat{f}(\mathbf{x}))$ cancels out due to the subtraction of value functions

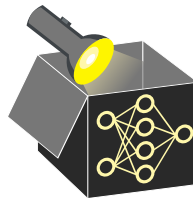
SHAPLEY VALUE - DEFINITION

► Shapley (1953)

► Strumbelj et al. (2014)

Shapley value ϕ_j of feature j for observation \mathbf{x} via **order definition**:

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



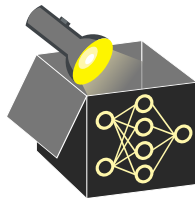
- Interpretation: Feature x_j contributed ϕ_j to difference between $\hat{f}(\mathbf{x})$ and average prediction
 \rightsquigarrow Note: Marginal contributions and Shapley values can be negative
- For exact computation of $\phi_j(\mathbf{x})$, the PD function $\hat{f}_S(\mathbf{x}_S) = \frac{1}{n} \sum_{i=1}^n \hat{f}(\mathbf{x}_S, \mathbf{x}_{-S}^{(i)})$ for any set of features S can be used which yields

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

\rightsquigarrow Note: \hat{f}_S marginalizes over all other features $-S$ using all observations
 $i = 1, \dots, n$

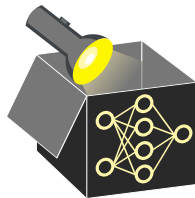
ESTIMATION: A PRACTICAL PROBLEM

- Exact Shapley value computation is problematic for high-dimensional feature spaces
 \rightsquigarrow For 10 features, there are already $|P|! = 10! \approx 3.6$ million possible orders of features



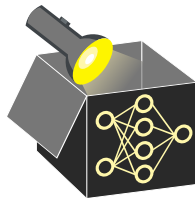
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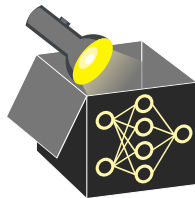
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- Solution to both problems is sampling: Instead of averaging over $|P|! \cdot n$ terms, we approximate it using a limited amount of M random samples of τ to build coalitions S_j^τ
- M is a tradeoff between accuracy of the Shapley value and computational costs
 \rightsquigarrow The higher M , the closer to the exact Shapley values, but the more costly the computation

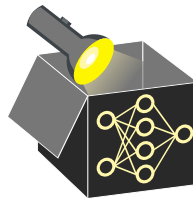


APPROXIMATION ALGORITHM

► Strumbelj et al. (2014)

Estimation of ϕ_j for observation \mathbf{x} of model \hat{f} fitted on data \mathcal{D} using sample size M :

❶ For $m = 1, \dots, M$ do:



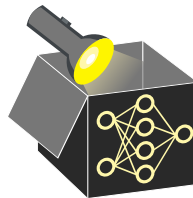
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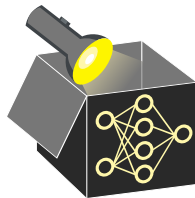
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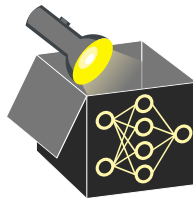
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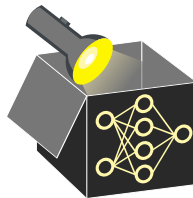
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APPROXIMATION ALGORITHM

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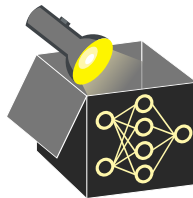
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$$\bullet \mathbf{x}_{+j}^{(m)} = \underbrace{(x_{\tau^{(1)}}, \dots, x_{\tau^{(|S_m|-1)}}, x_j)}_{\mathbf{x}_{S_m \cup \{j\}}} \underbrace{(z_{\tau^{(|S_m|+1)}}, \dots, z_{\tau^{(p)}})}_{\mathbf{z}_{-\{S_m \cup \{j\}\}}^{(m)}} \text{ takes features}$$

$S_m \cup \{j\}$ from \mathbf{x}



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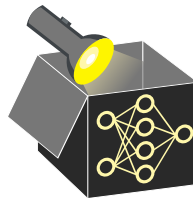
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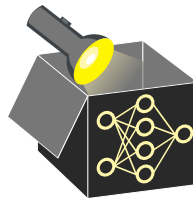
- $\mathbf{x}_{+j}^{(m)} = (\underbrace{x_{\tau^{(1)}}, \dots, x_{\tau^{(|S_m|-1)}}}_{\mathbf{x}_{S_m \cup \{j\}}}, x_j, \underbrace{z_{\tau^{(|S_m|+1)}}, \dots, z_{\tau^{(p)}}}_{\mathbf{z}_{-\{S_m \cup \{j\}\}}^{(m)}})$ takes features

$S_m \cup \{j\}$ from \mathbf{x}

- $\mathbf{x}_{-j}^{(m)} = (\underbrace{x_{\tau^{(1)}}, \dots, x_{\tau^{(|S_m|-1)}}}_{\mathbf{x}_{S_m}}, \underbrace{z_j^{(m)}, z_{\tau^{(|S_m|+1)}}, \dots, z_{\tau^{(p)}}}_{\mathbf{z}_{-S_m}^{(m)}})$ takes features

S_m from \mathbf{x}





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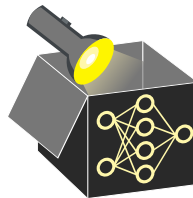
$S_m \cup \{j\}$ from \mathbf{x}

- $\mathbf{x}_{-j}^{(m)} = \underbrace{(x_{\tau^{(1)}}, \dots, x_{\tau^{(|S_m|-1)}})}_{\mathbf{x}_{S_m}}, \underbrace{z_j^{(m)}, z_{\tau^{(|S_m|+1)}}^{(m)}, \dots, z_{\tau^{(p)}}^{(m)}}_{\mathbf{z}_{-S_m}^{(m)}}$ takes features

S_m from \mathbf{x}

- ❺ Compute difference $\phi_j^m = \hat{f}(\mathbf{x}_{+j}^{(m)}) - \hat{f}(\mathbf{x}_{-j}^{(m)})$

$\rightsquigarrow \hat{f}_{S_m}(\mathbf{x}_{S_m})$ is approximated by $\hat{f}(\mathbf{x}_{-j}^{(m)})$ and $\hat{f}_{S_m \cup \{j\}}(\mathbf{x}_{S_m \cup \{j\}})$ by $\hat{f}(\mathbf{x}_{+j}^{(m)})$
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$S_m \cup \{j\}$ from \mathbf{x}

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 over M iters.

❻ Compute Shapley value $\phi_j = \frac{1}{M} \sum_{m=1}^M \phi_j^m$

SHAPLEY VALUE APPROXIMATION - ILLUSTRATION

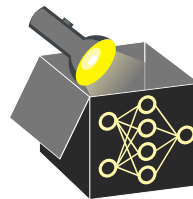
Definition

\mathbf{x} : obs. of interest

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

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

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



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

j

SHAPLEY VALUE APPROXIMATION - ILLUSTRATION

Definition

Contribution of feature j
to coalition S_m

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

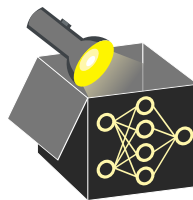
- $\Delta(j, S_m) = \hat{f}(\mathbf{x}_{+j}^{(m)}) - \hat{f}(\mathbf{x}_{-j}^{(m)})$ is the marginal contribution of feature j to coalition S_m
- Here: Feature *year* contributes +700 bike rentals if it joins coalition $S_m = \{\text{temp}, \text{hum}\}$

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

j

\hat{f}

$\Delta(j, S_m)$
marginal contribution

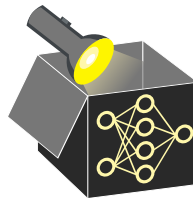


SHAPLEY VALUE APPROXIMATION - ILLUSTRATION

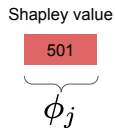
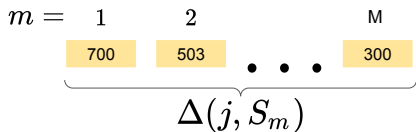
Definition

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 \mathbf{x}

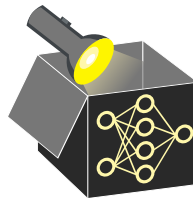


REVISITED: AXIOMS FOR FAIR ATTRIBUTIONS

We take the general axioms for Shapley Values and apply it to predictions:

- **Efficiency:** Shapley values add up to the (centered) prediction:

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



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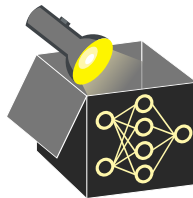
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$$\sum_{j=1}^p \phi_j = \hat{f}(\mathbf{x}) - \mathbb{E}_{\mathbf{x}}(\hat{f}(X))$$

- **Symmetry:** Two features j and k that contribute the same to the prediction get the same payout

\rightsquigarrow interaction effects between features are fairly divided

$$\hat{f}_{S \cup \{j\}}(\mathbf{x}_{S \cup \{j\}}) = \hat{f}_{S \cup \{k\}}(\mathbf{x}_{S \cup \{k\}}) \text{ for all } S \subseteq P \setminus \{j, k\} \text{ then } \phi_j = \phi_k$$



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We take the general axioms for Shapley Values and apply it to predictions:

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

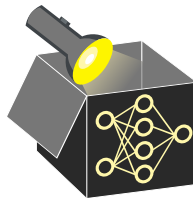
- **Symmetry:** Two features j and k that contribute the same to the prediction get the same payout

\rightsquigarrow interaction effects between features are fairly divided

$$\hat{f}_{S \cup \{j\}}(\mathbf{x}_{S \cup \{j\}}) = \hat{f}_{S \cup \{k\}}(\mathbf{x}_{S \cup \{k\}}) \text{ for all } S \subseteq P \setminus \{j, k\} \text{ then } \phi_j = \phi_k$$

- **Dummy / Null Player:** Shapley value of a feature that does not influence the prediction is zero \rightsquigarrow if a feature was not selected by the model (e.g., tree or LASSO), its Shapley value is zero

$$\hat{f}_{S \cup \{j\}}(\mathbf{x}_{S \cup \{j\}}) = \hat{f}_S(\mathbf{x}_S) \text{ for all } S \subseteq P \text{ then } \phi_j = 0$$



REVISITED: AXIOMS FOR FAIR ATTRIBUTIONS

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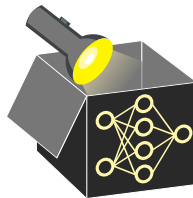
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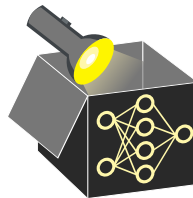
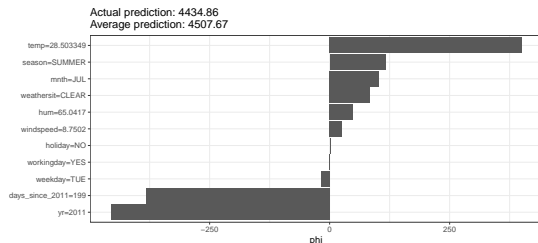
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- **Additivity:** For a prediction with combined payouts, the payout is the sum of payouts: $\phi_j(v_1) + \phi_j(v_2) \rightsquigarrow$ Shapley values for model ensembles can be combined



BIKE SHARING DATASET



- Shapley values of observation $i = 200$ from the bike sharing data
- Difference between model prediction of this observation and the average prediction of the data is fairly distributed among the features (i.e., $4434 - 4507 \approx -73$)
- Feature value $\text{temp} = 28.5$ has the most positive effect, with a contribution (increase of prediction) of about +400

ADVANTAGES AND DISADVANTAGES

Advantages:

- **Solid theoretical foundation** in game theory
- Prediction is **fairly distributed** among the feature values \rightsquigarrow easy to interpret for a user
- **Contrastive explanations** that compare the prediction with the average prediction

Disadvantages:

- Without sampling, Shapley values need a lot of computing time to inspect all possible coalitions
- Like many other IML methods, Shapley values suffer from the inclusion of unrealistic data observations when features are correlated

