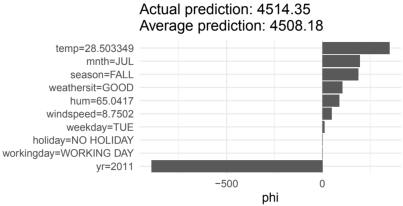
Interpretable Machine Learning

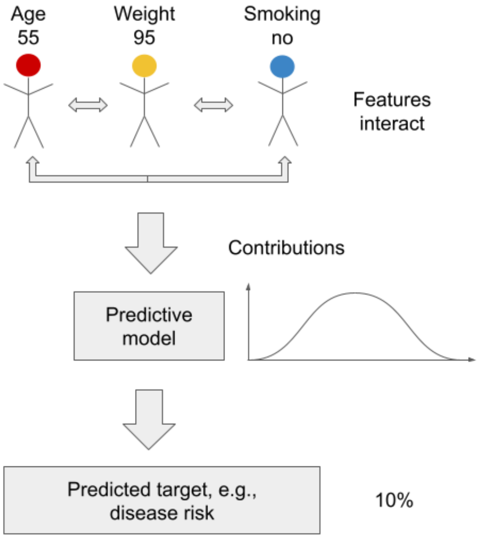
Shapley Values for Local Explanations



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



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  $\rightsquigarrow$ 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 $-S$)

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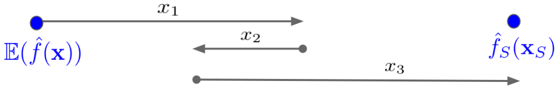
- Value function / payout of coalition $S \subseteq P$ for observation $\mathbf{x}$:

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

$\rightsquigarrow$ 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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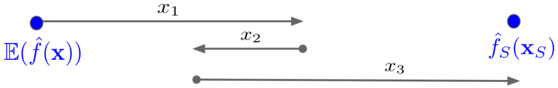

- Marginal contribution: $v(S \cup \{j\}) - v(S) = \hat{f}_{S \cup \{j\}}(\mathbf{x}_{S \cup \{j\}}) - \hat{f}_S(\mathbf{x}_S)$
  $\leadsto$ $\mathbb{E}_{\mathbf{x}}(\hat{f}(\mathbf{x}))$ cancels out due to the subtraction of value functions

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
  $\leadsto$ 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

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

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

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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- 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:

1. For $m = 1, \ldots, M$ **do**:

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

SHAPLEY VALUE APPROXIMATION - ILLUSTRATION

Definition

x: obs. of interest

x with feature values in S_m (other are replaced)

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

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

	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

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

Contribution of feature j to coalition 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 $S_m = \{temp, hum\}$

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

700

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 $S_1, \ldots, S_m$
- 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 $\mathbf{x}$

$$m = \quad 1 \quad 2 \quad \ldots \quad \text{M}$$

$$\underbrace{700 \quad 503 \quad \ldots \quad 300}_{\Delta(j, S_m)} \qquad \overset{\text{Shapley value}}{\underbrace{501}_{\phi_j}}$$

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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  $\rightsquigarrow$ interaction effects between features are fairly divided
  $\hat{f}_{S \cup \{j\}}(\mathbf{x}_{S \cup \{j\}}) = \hat{f}_{S \cup \{k\}}(\mathbf{x}_{S \cup \{k\}})$ for all $S \subseteq P \setminus \{j, k\}$ then $\phi_j = \phi_k$

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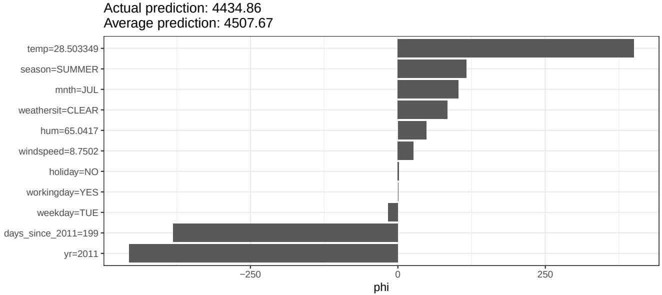
- **Additivity**: For a prediction with combined payouts, the payout is the sum of payouts:
  $\phi_j(v_1) + \phi_j(v_2)$ $\rightsquigarrow$ Shapley values for model ensembles can be combined

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 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