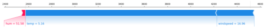
Interpretable Machine Learning

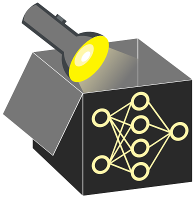
SHAP (SHapley Additive exPlanation) Values



Learning goals

- Get an intuition of additive feature attributions
- Understand the concept of Kernel SHAP
- Ability to interpret SHAP plots
- Global SHAP methods

SHAPLEY VALUES IN ML - A SHORT RECAP



Question: How much does a feat. j contribute to the prediction of a single obs.

Idea: Use Shapley values from cooperative game theory

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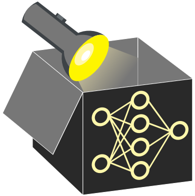

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Procedure:

- Compare "reduced prediction function" of feature coalition S with $S \cup \{j\}$
- Iterate over possible coalitions to calculate marginal contribution of feature j to sample $\mathbf{x}$

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

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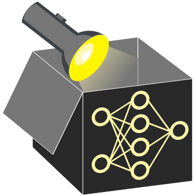

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Remember:

- $\hat{f}$ is the prediction function, p denotes the number of features
- Non-existent feat. in a coalition are replaced by values of random feat. values
- Recall S_j^τ defines the coalition as the set of players before player j in order $\tau = (\tau^{(1)}, \dots, \tau^{(p)})$

$$\underbrace{\boxed{\tau^{(1)}}\boxed{\;\dots\;}\boxed{\tau^{(|S|)}}}_{S_j^\tau\text{ : Players before player } j}\underbrace{\boxed{\tau^{(|S|+1)}}}_{\text{player } j}\underbrace{\boxed{\tau^{(|S|+2)}}\boxed{\;\dots\;}\boxed{\tau^{(p)}}}_{\text{Players after player } j}$$

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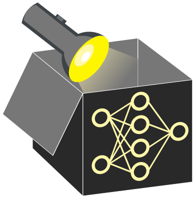

Example:

- Train a random forest on bike sharing data only using features humidity (hum), temperature (temp) and windspeed (ws)
- Calculate Shapley value for an observation **x** with $\hat{f}(\mathbf{x}) = 2573$
- Mean prediction is $\mathbb{E}(\hat{f}) = 4515$

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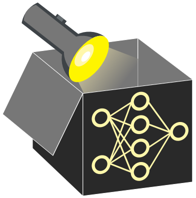

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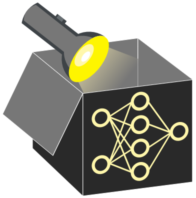
Exact Shapley calculation for humidity:

S	$S \cup \{j\}$	$\hat{f}_S$	$\hat{f}_{S\cup\{j\}}$	weight
$\emptyset$	hum	4515	4635	$2/6$
temp	temp, hum	3087	3060	$1/6$
ws	ws, hum	4359	4450	$1/6$
temp, ws	hum, temp, ws	2623	2573	$2/6$

$$\phi_{hum} = \frac{2}{6}(4635 - 4515) + \frac{1}{6}(3060 - 3087) + \frac{1}{6}(4450 - 4359) + \frac{2}{6}(2573 - 2623) = 34$$

FROM SHAPLEY TO SHAP



Example continued: Same calculation can be done for temperature and windspeed:

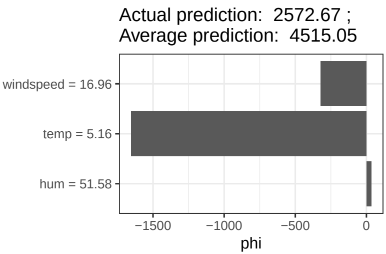
- $\phi_{temp} = \ldots = -1654$
- $\phi_{ws} = \ldots = -323$

Remember: Shapley values explain difference between actual and average pred.:

$$\begin{aligned} 2573 - 4515 &= 34 - 1654 - 323 = -1942 \\ \hat{f}(\mathbf{x}) - \mathbb{E}(\hat{f}) &= \phi_{hum} + \phi_{temp} + \phi_{ws} \end{aligned}$$

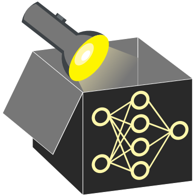
$\leadsto$ can be rewritten to

$$\hat{f}(\mathbf{x}) = \underbrace{\mathbb{E}(\hat{f})}_{\phi_0} + \phi_{hum} + \phi_{temp} + \phi_{ws}$$



SHAP DEFINITION

Lundberg et al. 2017



Aim: Find an additive combination that explains the prediction of an observation $\mathbf{x}$ by computing the contribution of each feature to the prediction using a (more efficient) estimation procedure.

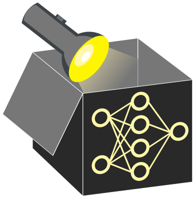
Definition

- Simplified (binary) coalition feat. space $\mathbf{Z}' \in \{0, 1\}^{K \times p}$ with K rows and p cols.
- Rows are referred to as $\mathbf{z}'^{(k)} = \{z_1'^{(k)}, \dots, z_p'^{(k)}\}$ with $k \in \{1, \dots, K\}$ (indexes k-th coalition)
- Cols are referred to as $\mathbf{z}_j$ with $j \in \{1, \dots, p\}$ being the index of the original feat.

Example:

Coalition	$\mathbf{z}'^{(k)}$	hum	temp	ws
$\varnothing$	$\mathbf{z}'^{(1)}$	0	0	0
hum	$\mathbf{z}'^{(2)}$	1	0	0
temp	$\mathbf{z}'^{(3)}$	0	1	0
ws	$\mathbf{z}'^{(4)}$	0	0	1
hum, temp	$\mathbf{z}'^{(5)}$	1	1	0
temp, ws	$\mathbf{z}'^{(6)}$	0	1	1
hum, ws	$\mathbf{z}'^{(7)}$	1	0	1
hum, temp, ws	$\mathbf{z}'^{(8)}$	1	1	1

SHAP DEFINITION ▸ Lundberg et al. 2017



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$\mathbf{z}'^{(k)}$: **Coalition** simplified features

$$g\left(\mathbf{z}'^{(k)}\right) = \phi_0 + \sum_{j=1}^{p} \phi_j z_j'^{(k)}$$

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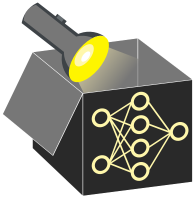

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ϕ_0: **Null Output**
Average Model
Baseline $(\mathbb{E}(\hat{f}))$

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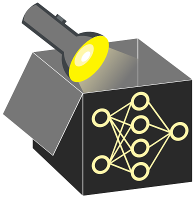

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ϕ_j: **Attribution**
How much does
feature j change the
output for coaltion k

SHAP DEFINITION

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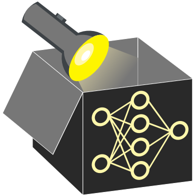


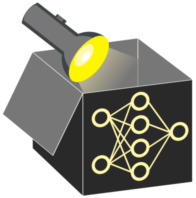
$g(\mathbf{z}'^{(k)})$: **Marginal Contribution**
Contribution of coalition $\mathbf{z}'^{(k)}$ to the prediction

$$\underbrace{g\left(\mathbf{z}'^{(k)}\right) = \phi_0 + \sum_{j=1}^{p} \phi_j z_j'^{(k)}}_{\textbf{Additive Feature Attribution}}$$

ϕ_j: **Shapley Values**

Problem
How do we estimate the Shapley values ϕ_j?

PROPERTIES



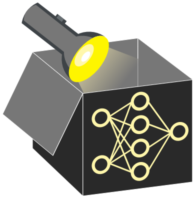
Local Accuracy

$$f(\mathbf{x}) = g\left(\mathbf{x}'\right) = \phi_0 + \sum_{j=1}^{p} \phi_j x_j'$$

Intuition: If the coalition includes all features ($\mathbf{x}' \in \{1\}^p$), the attributions ϕ_j and the null output ϕ_0 sum up to the original model output $f(\mathbf{x})$

Local accuracy corresponds to the **axiom of efficiency** in Shapley game theory

PROPERTIES



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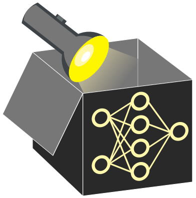
$$f(\mathbf{x}) = g(\mathbf{x}') = \phi_0 + \sum_{j=1}^{p} \phi_j x_j'$$

Missingness

$$x_j' = 0 \Longrightarrow \phi_j = 0$$

Intution: A missing feature gets an attribution of zero

PROPERTIES



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Consistency

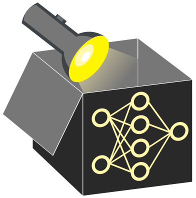
$\hat{f}_x\left(\mathbf{z}'^{(k)}\right) = \hat{f}\left(h_x\left(\mathbf{z}'^{(k)}\right)\right)$ and $\mathbf{z}'^{(k)}_{-j}$ denote setting $z_j'^{(k)} = 0$. For any two models $\hat{f}$ and $\hat{f}'$, if

$$\hat{f}'_x\left(\mathbf{z}'^{(k)}\right) - \hat{f}'_x\left(\mathbf{z}'^{(k)}_{-j}\right) \geq \hat{f}_x\left(\mathbf{z}'^{(k)}\right) - \hat{f}_x\left(\mathbf{z}'^{(k)}_{-j}\right)$$

for all inputs $\mathbf{z}'^{(k)} \in \{0, 1\}^p$, then

$$\phi_j\left(\hat{f}', \mathbf{x}\right) \geq \phi_j(\hat{f}, \mathbf{x})$$

PROPERTIES



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$$\hat{f}_x'\left(\mathbf{z}'^{(k)}\right) - \hat{f}_x'\left(\mathbf{z}_{-j}'^{(k)}\right) \geq \hat{f}_x\left(\mathbf{z}'^{(k)}\right) - \hat{f}_x\left(\mathbf{z}_{-j}'^{(k)}\right) \Longrightarrow \phi_j\left(\hat{f}', \mathbf{x}\right) \geq \phi_j(\hat{f}, \mathbf{x})$$

Intution: If a model changes so that the marginal contribution of a feature value increases or stays the same, the Shapley value also increases or stays the same

From **consistency** the Shapley **axioms of additivity, dummy and symmetry** follow