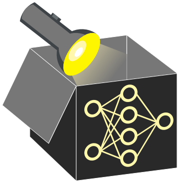
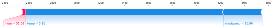
Interpretable Machine Learning



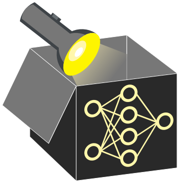
Shapley
SHAP (SHapley Additive exPlanation)



Learning goals

- Recall order- and set-based definitions of Shapley values in ML
- Interpret predictions via additive Shapley decomposition
- Understand SHAP as surrogate-based model
- Understand SHAP properties

SHAPLEY VALUES IN ML - A SHORT RECAP



Shapley values (order definition): Average over marginal contributions across all permutations of feature indices $\tau \in \Pi$:

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

- For each permutation τ, determine coalition : features before j in τ
- In $\hat{f}_S$, features not in S are marginalized (e.g., randomly imputed)
- Compute marginal contribution of adding j to via the difference above
- Average over all $p!$ permutations (in practice, over $M << p!$)

SHAPLEY VALUES IN ML - A SHORT RECAP

Shapley values (order definition): Average over marginal contributions across all permutations of feature indices $\tau \in \Pi$:

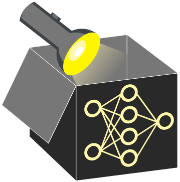
$$\phi_j(\mathbf{x}) = \frac{1}{p!} \sum_{\tau \in \Pi} \underbrace{\hat{f}(\mathbf{x}) - \hat{f}(\mathbf{x})}_{\text{marginal contribution of feature } j}$$

- For each permutation τ, determine coalition : features before j in τ
- In $\hat{f}_S$, features not in S are marginalized (e.g., randomly imputed)
- Compute marginal contribution of adding j to via the difference above
- Average over all $p!$ permutations (in practice, over $M << p!$)

Alternative (set definition): Average marginal contribution over all subsets, weighted by their relative number of appearances in permutations:

$$\phi_j(\mathbf{x}) = \sum_{S \subseteq \{1,\ldots,p\} \setminus \{j\}} \frac{|S|!(p - |S| - 1)!}{p!} \left[\hat{f}_{S \cup \{j\}}(\mathbf{x}_{S \cup \{j\}}) - \hat{f}_S(\mathbf{x}_S) \right].$$

SHAPLEY VALUES IN ML - EXAMPLE



Example (Bike sharing data):

- Train random forest using humidity (hum), temperature (temp), windspeed (ws)
- Consider observation of interest $\mathbf{x}$ with prediction $\hat{f}(\mathbf{x}) = 2573$
- Mean prediction $\mathbb{E}_{\mathbf{x}}[\hat{f}(\mathbf{x})] = 4515$
- Compute exact Shapley value for $\mathbf{x}$ for feature hum:

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	temp, ws, hum	2623	2573	$2/6$

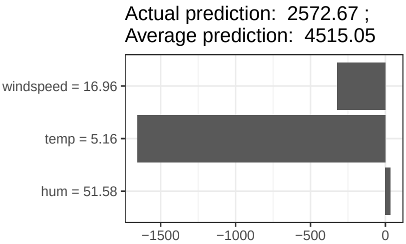
$\Rightarrow \phi_{\text{hum}}(\mathbf{x}) = \frac{2}{6}(4635-4515)+\frac{1}{6}(3060-3087)+\frac{1}{6}(4450-4359)+\frac{2}{6}(2573-2623) = 34$

$\Rightarrow$ Analogously $\phi_{\text{temp}}(\mathbf{x}) = -1654$, $\phi_{\text{ws}}(\mathbf{x}) = -322$

FROM SHAPLEY VALUES TO SHAP

Shapley value interpretation (for x):

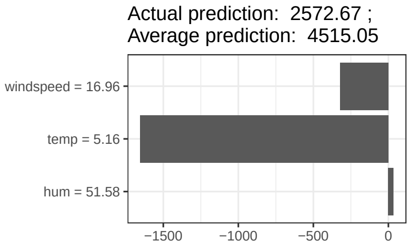
- `hum` $(+34)$ pushes pred. *above* baseline (= average prediction).
- `temp` (-1654) and `ws` (-322) pull prediction *below* baseline.
- Together, they explain full deviation from average prediction.



FROM SHAPLEY VALUES TO SHAP

Shapley value interpretation (for $\mathbf{x}$):

- `hum` $(+34)$ pushes pred. *above* baseline (= average prediction).
- `temp` (-1654) and `ws` (-322) pull prediction *below* baseline.
- Together, they explain full deviation from average prediction.



Shapley-based additive decomposition of prediction for $\mathbf{x}$ gives insights on how features shift prediction from baseline $\mathbb{E}(\hat{f})$:

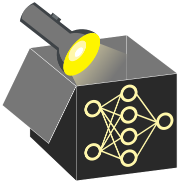
$$\underbrace{\hat{f}(\mathbf{x})}_{\text{actual prediction}} = \underbrace{\phi_0}_{\mathbb{E}_{\mathbf{x}}[\hat{f}(\mathbf{x})]} + \sum\nolimits_{j \in \{\text{hum},\text{temp},\text{ws}\}} \phi_j(\mathbf{x})$$

$$2573 = 4515 + \left(34 - 1654 - 322\right) = 4515 - 1942$$

$\rightsquigarrow$ Like a LM evaluated at $\mathbf{x}$: global intercept ϕ_0 plus per-feature contribs $\phi_j(\mathbf{x})$.

SHAP Motivation: Can we efficiently estimate this Shapley-based additive decomp. of $\hat{f}(\mathbf{x})$ via a surrogate model (while preserving Shapley axioms)?

SHAP FRAMEWORK ▸ LUNDBERG_2017

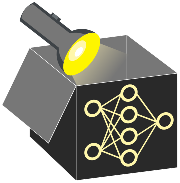


SHAP expresses the prediction of $\mathbf{x}$ as a sum of contribs from each feature:

$$g(\mathbf{z}') = \phi_0 + \sum_{j=1}^{p} \phi_j z'_j$$

- $\mathbf{z}' \in \{0,1\}^p$: simplified binary input referring to a coalition (coal. vector)
- $z'_j = 1$: feature j is "present" $\Rightarrow$ use x_j in model evaluation
- $z'_j = 0$: feature j is "absent"
  $\Rightarrow$ influence of x_j is removed via marginalization over a reference distrib.

SHAP FRAMEWORK ▸ LUNDBERG_2017



SHAP expresses the prediction of **x** as a sum of contribs from each feature:

$$g(\mathbf{z}') = \phi_0 + \sum_{j=1}^{p} \phi_j z'_j$$

- $\mathbf{z}' \in \{0, 1\}^p$: simplified binary input referring to a coalition (coal. vector)
- $z'_j = 1$: feature j is "present" $\Rightarrow$ use x_j in model evaluation
- $z'_j = 0$: feature j is "absent"
  $\Rightarrow$ influence of x_j is removed via marginalization over a reference distrib.

SHAP as a theoretical framework: Fit a surrogate model $g(\mathbf{z}')$ satisfying Shapley axioms and recovering $\hat{f}(\mathbf{x})$ when all features are "present":

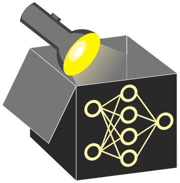
$$\hat{f}(\mathbf{x}) = g(\mathbf{1}) = \phi_0 + \sum_{j=1}^{p} \phi_j$$

Evaluation of $g(\mathbf{z}')$: Let $S = \{j : z'_j = 1\}$ be the active coalition. Then:

- $g(\mathbf{z}') \approx \mathbb{E}[\hat{f}(\mathbf{X}) \mid \mathbf{X}_S = \mathbf{x}_S]$ (conditional expectation)
- $g(\mathbf{z}') \approx \mathbb{E}_{\mathbf{X}_{-S}}[\hat{f}(\mathbf{x}_S, \mathbf{X}_{-S})]$ (marginal expectation, i.e., PD function)
- *Note: Practical implementations (e.g., KernelSHAP) use the marginal expectation, approximated via random imputations from background data.*

SHAP FRAMEWORK ▸ LUNDBERG_2017

SHAP defines an additive surrogate $g(\mathbf{z}')$ over a binary input $\mathbf{z}' \in \{0,1\}^p$:



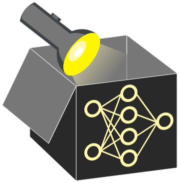
$\mathbf{z}'^{(k)}$: **coalition vector**
subset of features

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

ϕ_j: **feature attribution**
marginal effect of j in coalition

ϕ_0: **baseline** $\mathbb{E}[\hat{f}()]$

SHAP FRAMEWORK ▸ LUNDBERG_2017



SHAP defines an additive surrogate $g(\mathbf{z}')$ over a binary input $\mathbf{z}' \in \{0,1\}^p$:

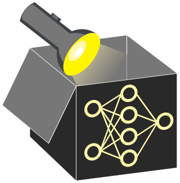
$g(\mathbf{z}'^{(k)})$: **approx. prediction** for coalition

ϕ_j: **Shapley value**

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

Next: How do we estimate the Shapley values ϕ_j efficiently?

PROPERTIES



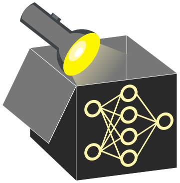
Local Accuracy

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

Intuition: If coalition includes all features ($\mathbf{z}' = (z_1', \ldots, z_p')^\top = (1, \ldots, 1)^\top$), the attributions ϕ_j and the baseline ϕ_0 sum up to the original model output $\hat{f}(\mathbf{x})$

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

PROPERTIES



Local Accuracy

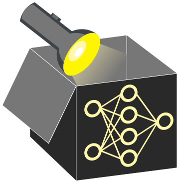
$$\hat{f}(\mathbf{x}) = g\left(\mathbf{z}'\right) = \phi_0 + \sum_{j=1}^{p} \phi_j z_j'$$

Missingness

$$z_j' = 0 \Longrightarrow \phi_j = 0$$

Intuition: A "missing" feature (whose value is imputed) gets zero attribution

PROPERTIES



Local Accuracy

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

Missingness

$$z_j' = 0 \Longrightarrow \phi_j = 0$$

Consistency (Let $\mathbf{z}_{-j}'^{(k)}$ refer to $z_j'^{(k)} = 0$)
For any two models $\hat{f}$ and $\hat{f}'$, if for all inputs $\mathbf{z}'^{(k)} \in \{0, 1\}^p$

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

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

Consistency implies Shapley's axioms of **additivity, dummy, symmetry**.