

# Interpretable Machine Learning

## Shapley Additive Global Importance (SAGE)

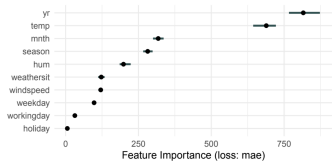


Figure: Bike Sharing Dataset

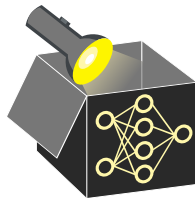
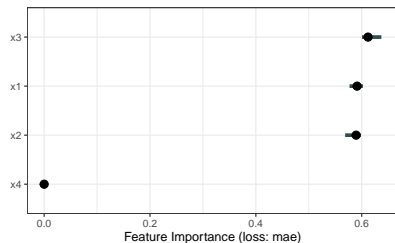
### Learning goals

- How SAGE fairly distributes importance
- Definition of SAGE value function
- Difference SAGE value function and SAGE values
- Marginal and Conditional SAGE

# CHALLENGE: FAIR ATTRIBUTION OF IMPORTANCE

## Recap:

- Data:  $x_1, \dots, x_4$  uniformly sampled from  $[-1, 1]$
- DGP:  $y := x_1 x_2 + x_3 + \epsilon_Y$  with  $\epsilon_Y \sim N(0, 1)$
- Model:  $\hat{f}(x) \approx x_1 x_2 + x_3$



Although  $x_3$  alone contributes as much to the prediction as  $x_1$  and  $x_2$  jointly, all three are considered equally relevant by PFI.

**Reason:** PFI assesses importance given that all remaining features are preserved. If we first permute  $x_1$  and then  $x_2$ , permutation of  $x_2$  would have no effect on the performance (and vice versa).

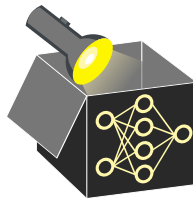
**SAGE:** Use Shapley values to compute a fair attribution of importance (via model performance)

## Idea:

- Feature importance attribution can be regarded as cooperative game  
     $\rightsquigarrow$  features jointly contribute to achieve a certain model performance
- Players: features
- Payoff to be fairly distributed: model performance
- Surplus contribution of a feature depends on the coalition of features that are already accessible by the model

## Note:

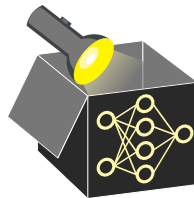
- Same idea (called SFIMP) was proposed in ► Casalicchio et al. (2018)
- Definition based on model refits was proposed in context of feature selection in  
    ► Cohen et al. (2007)



# SAGE - VALUE FUNCTION

**Removal Idea:** To deprive information of the non-coalition features  $-S$  from the model, marginalize the prediction function over the features  $-S$  to be “dropped”.

$$\hat{f}_S(x_S) = \mathbb{E}[\hat{f}(x) | X_S = x_S]$$



# SAGE - VALUE FUNCTION

**Removal Idea:** To deprive information of the non-coalition features –  $S$  from the model, marginalize the prediction function over the features –  $S$  to be “dropped”.

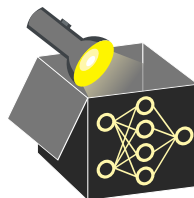
$$\hat{f}_S(x_S) = \mathbb{E}[\hat{f}(x)|X_S = x_S]$$

**SAGE value function:**

$$v_{\hat{f}}(S) = \mathcal{R}(\hat{f}_{\emptyset}) - \mathcal{R}(\hat{f}_S), \text{ where } \mathcal{R}(\hat{f}_S) = \mathbb{E}_{Y, X_S}[L(y, \hat{f}_S(x_S))]$$

~> Quantify the predictive power of a coalition  $S$  in terms of reduction in risk

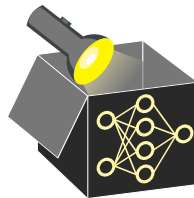
~> Risk of predictor  $\hat{f}_S(x_S)$  is compared to the risk of the mean prediction  $\hat{f}_{\emptyset}$



# SAGE - VALUE FUNCTION

**Removal Idea:** To deprive information of the non-coalition features –  $S$  from the model, marginalize the prediction function over the features –  $S$  to be “dropped”.

$$\hat{f}_S(x_S) = \mathbb{E}[\hat{f}(x)|X_S = x_S]$$



**SAGE value function:**

$$v_{\hat{f}}(S) = \mathcal{R}(\hat{f}_{\emptyset}) - \mathcal{R}(\hat{f}_S), \text{ where } \mathcal{R}(\hat{f}_S) = \mathbb{E}_{Y, X_S}[L(y, \hat{f}_S(x_S))]$$

↪ Quantify the predictive power of a coalition  $S$  in terms of reduction in risk

↪ Risk of predictor  $\hat{f}_S(x_S)$  is compared to the risk of the mean prediction  $\hat{f}_{\emptyset}$

**Surplus contribution of feature  $x_j$  over coalition  $x_S$ :**

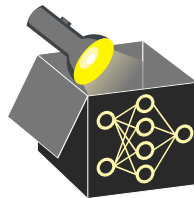
$$v_{\hat{f}}(S \cup \{j\}) - v_{\hat{f}}(S) = \mathcal{R}(\hat{f}_S) - \mathcal{R}(\hat{f}_{S \cup \{j\}})$$

↪ Quantifies the added value of feature  $j$  when it is added to coalition  $S$

# SAGE - MARGINAL AND CONDITIONAL SAMPLING

When computing the marginalized prediction  $\hat{f}_S(x_S)$ , the “dropped” features can be sampled from

- the marginal distribution  $\mathbb{P}(x_{-S}) \Rightarrow$  marginal SAGE
- the conditional distribution  $\mathbb{P}(x_{-S}|x_S) \Rightarrow$  conditional SAGE



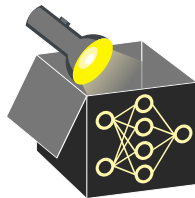
# SAGE - MARGINAL AND CONDITIONAL SAMPLING

When computing the marginalized prediction  $\hat{f}_S(x_S)$ , the “dropped” features can be sampled from

- the marginal distribution  $\mathbb{P}(x_{-S}) \Rightarrow$  marginal SAGE
- the conditional distribution  $\mathbb{P}(x_{-S}|x_S) \Rightarrow$  conditional SAGE

**Interpretation marginal sampling:**  $v(S)$  quantifies the reliance of the model on features  $x_S$

- features  $x_S$  not being causal for the prediction  $\Rightarrow v(S) = 0$

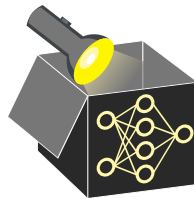




# SAGE - MARGINAL AND CONDITIONAL SAMPLING

When computing the marginalized prediction  $\hat{f}_S(x_S)$ , the “dropped” features can be sampled from

- the marginal distribution  $\mathbb{P}(x_{-S}) \Rightarrow$  marginal SAGE
- the conditional distribution  $\mathbb{P}(x_{-S}|x_S) \Rightarrow$  conditional SAGE



**Interpretation marginal sampling:**  $v(S)$  quantifies the reliance of the model on features  $x_S$

- features  $x_S$  not being causal for the prediction  $\Rightarrow v(S) = 0$

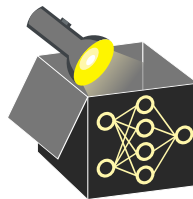
**Interpretation conditional sampling:**  $v(S)$  quantifies whether variables  $x_S$  contain prediction-relevant information (e.g.  $y \not\perp x_S$ ) that is (directly or indirectly) exploited by the model

- features  $x_S$  not being causal for the prediction  $\nRightarrow v(S) = 0$ 
  - e.g., if  $x_1$  and  $x_2$  are perfectly correlated, even if only  $x_1$  has a nonzero coefficient, both are considered equally important
- under model optimality, links to mutual information or the conditional variance exist

# SAGE - MARGINAL AND CONDITIONAL SAMPLING

## Example:

- $y = x_3 + \epsilon_y$   
 $x_1 = \epsilon_1$   
 $x_2 = x_1 + \epsilon_2$   
 $x_3 = x_2 + \epsilon_3$  (all  $\epsilon_j$  i.i.d.)
- Causal DAG:  
 $x_1 \rightarrow x_2 \rightarrow x_3 \rightarrow y$
- Fitted LM:  
 $\hat{f} \approx 0.95x_3 + 0.05x_2$



# SAGE - MARGINAL AND CONDITIONAL SAMPLING

## Example:

- $y = x_3 + \epsilon_y$   
 $x_1 = \epsilon_1$   
 $x_2 = x_1 + \epsilon_2$   
 $x_3 = x_2 + \epsilon_3$  (all  $\epsilon_j$  i.i.d.)

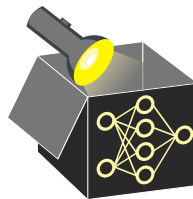
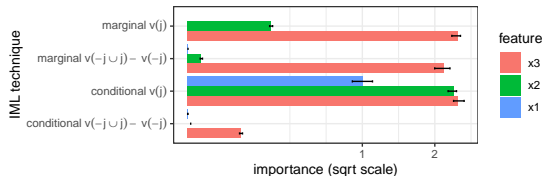
- Causal DAG:

$$x_1 \rightarrow x_2 \rightarrow x_3 \rightarrow y$$

- Fitted LM:

$$\hat{f} \approx 0.95x_3 + 0.05x_2$$

- Marginal  $v(j)$  are only nonzero for features that are used by  $\hat{f}$
- Conditional  $v(j)$  are also nonzero for features that are not used by  $\hat{f}$  (e.g., due to correlation)
- For conditional value function  $v$ , the difference  $v(-j \cup j) - v(-j)$  quantifies the unique contribution of  $x_j$  over remaining features  $x_{-j}$   
 $\Rightarrow$  Since  $y \perp\!\!\!\perp x_1, x_2 | x_3$ , only  $v(\{1, 2, 3\}) - v(\{1, 2\})$  is nonzero (i.e., for feature  $j = 3$ )



# SAGE VALUE FUNCTIONS VERSUS SAGE VALUES

**SAGE value function**  $v(S)$ : measure contribution of a specific feature set over the empty coalition



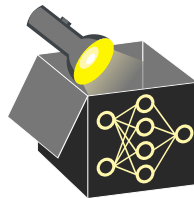
# SAGE VALUE FUNCTIONS VERSUS SAGE VALUES

**SAGE value function**  $v(S)$ : measure contribution of a specific feature set over the empty coalition

**SAGE values**  $\phi_j$ : fair attribution of importance

- can be computed by averaging the contribution of  $x_j$  over all feature orderings
- for feature permutation  $\tau$ , the contribution of  $j$  in the set  $S_j^\tau$  is given as  $v(S_j^\tau \cup \{j\}) - v(S_j^\tau)$

Note:  $S_j^\tau$  is the set of features preceding  $j$  in permutation  $\tau$



# SAGE VALUE FUNCTIONS VERSUS SAGE VALUES

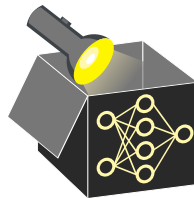
**SAGE value function**  $v(S)$ : measure contribution of a specific feature set over the empty coalition

**SAGE values**  $\phi_j$ : fair attribution of importance

- can be computed by averaging the contribution of  $x_j$  over all feature orderings
- for feature permutation  $\tau$ , the contribution of  $j$  in the set  $S_j^\tau$  is given as  $v(S_j^\tau \cup \{j\}) - v(S_j^\tau)$   
Note:  $S_j^\tau$  is the set of features preceding  $j$  in permutation  $\tau$

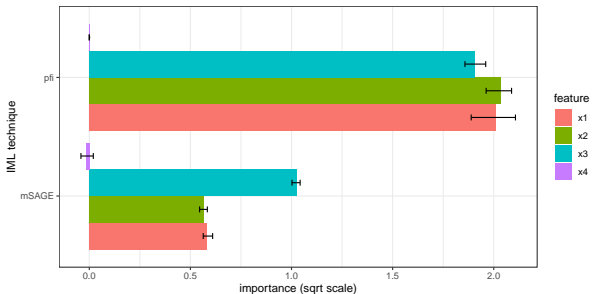
**SAGE value approximation:** Average over the contributions for  $M$  randomly sampled permutations

$$\phi_j = \frac{1}{M} \sum_{m=1}^M v(S_j^{\tau_m} \cup \{j\}) - v(S_j^{\tau_m})$$

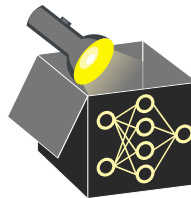


# INTERACTION EXAMPLE REVISITED

**Recap:** Data:  $x_1, \dots, x_4$  uniformly sampled from  $\{-1, 1\}$  and  $y := x_1 x_2 + x_3 + \epsilon_Y$  with  $\epsilon_Y \sim N(0, 1)$ . Model:  $\hat{f}(x) \approx x_1 x_2 + x_3$ .



- PFI regards  $x_1, x_2$  to be equally important as  $x_3$
- Marginal SAGE fairly divides the contribution of the interaction  $x_1$  and  $x_2$



# SAGE LOSS FUNCTIONS

When the loss-optimal model  $f^*$  is inspected using *conditional-sampling* based SAGE value functions, interesting links exist.



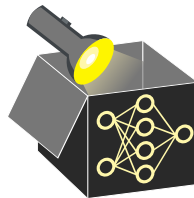


# SAGE LOSS FUNCTIONS

When the loss-optimal model  $f^*$  is inspected using *conditional-sampling* based SAGE value functions, interesting links exist.

## For cross-entropy loss:

- value function is the mutual information:  $v_{f^*}(S) = I(y; x_S)$
- surplus contribution of a feature  $x_j$  is the conditional mutual information:  
$$v_{f^*}(S \cup \{j\}) - v_{f^*}(S) = I(y, x_j | x_S)$$



# SAGE LOSS FUNCTIONS

When the loss-optimal model  $f^*$  is inspected using *conditional-sampling* based SAGE value functions, interesting links exist.



## For cross-entropy loss:

- value function is the mutual information:  $v_{f^*}(S) = I(y; x_S)$
- surplus contribution of a feature  $x_j$  is the conditional mutual information:  
$$v_{f^*}(S \cup \{j\}) - v_{f^*}(S) = I(y, x_j | x_S)$$

## For MSE loss:

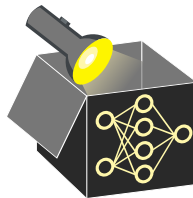
- value function is the expected reduction in variance given knowledge of the features  $x_S$ :  $v_{f^*}(S) = \text{Var}(y) - \mathbb{E}[\text{Var}(y | x_S)]$
- surplus contribution is the respective reduction over  $x_S$ :  
$$v_{f^*}(S \cup \{j\}) - v_{f^*}(S) = \mathbb{E}[\text{Var}(y | x_S)] - \mathbb{E}[\text{Var}(y | x_{S \cup j})]$$

# IMPLICATIONS MARGINAL SAGE VALUES

Can we gain insight into whether the ...

❶ feature  $x_j$  is causal for the prediction?

- for all coalitions  $S$ ,  $v(j \cup S) - v(S)$  can only be nonzero if  $x_j \rightarrow \hat{f}(x)$  (as for PFI)  
 $\rightsquigarrow \phi_j$  is only nonzero if  $x_j$  is causal for the prediction
- $v(j \cup S) - v(S)$  may be zero due to independence  $x_j \perp\!\!\!\perp y | x_S$  (as for PFI)  
 $\rightsquigarrow \phi_j$  may be zero although the feature is causal for the prediction



# IMPLICATIONS MARGINAL SAGE VALUES

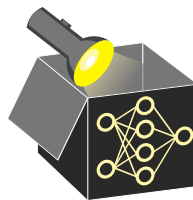
Can we gain insight into whether the ...



- ② feature  $x_j$  contains prediction-relevant information about  $y$ 
  - value functions may be nonzero despite independence due to extrapolation (as for PFI)
    - $\rightsquigarrow \phi_j$  may be nonzero without  $x_j$  being dependent with  $y$
  - value functions may be zero despite  $x_j$  containing prediction-relevant information due to underfitting (as for PFI)
    - $\rightsquigarrow \phi_j$  may be zero although prediction-relevant information contained

# IMPLICATIONS MARGINAL SAGE VALUES

Can we gain insight into whether the ...



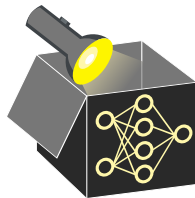
- ③ model requires access to  $x_j$  to achieve it's prediction performance?
  - like PFI, in general marginal value functions do not allow insight into unique contribution  $\rightsquigarrow$  no insight from  $\phi_j$

# IMPLICATIONS CONDITIONAL SAGE VALUES

Can we gain insight into whether the ...

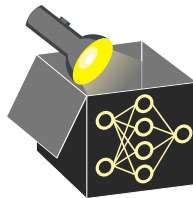
❶ feature  $\mathbf{x}_j$  is causal for the prediction?

- value functions may be nonzero although feature is not directly used by  $\hat{f}$   
 $\rightsquigarrow$  nonzero  $\phi_j$  does not imply  $\mathbf{x}_j \rightarrow \hat{y}$
- value functions may be zero although feature may be used by the model,  
e.g. if feature is independent with  $y$  and all other features  
 $\rightsquigarrow$  zero  $\phi_j$  does not imply  $\mathbf{x}_j \not\rightarrow \hat{y}$



# IMPLICATIONS CONDITIONAL SAGE VALUES

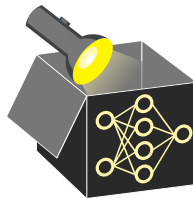
Can we gain insight into whether the ...



- ② feature  $\mathbf{x}_j$  contains prediction-relevant information about  $y$ 
  - e.g. for cross-entropy optimal  $\hat{f}$ ,  $v(j)$  measures mutual information  $I(y; x_j)$   
 $\rightsquigarrow$  prediction-relevance implies nonzero  $\phi_j$
  - $x_j \perp\!\!\!\perp y$  does not imply  $x_j \perp\!\!\!\perp y|x_S$  and consequently does not imply  $v(j \cup S) - v(S) = 0 \rightsquigarrow \phi_j$  may be nonzero although  $\mathbf{x}_j \perp\!\!\!\perp y$

# IMPLICATIONS CONDITIONAL SAGE VALUES

Can we gain insight into whether the ...

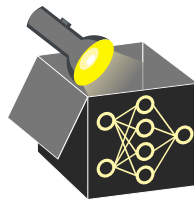


- ③ model requires access to  $x_j$  to achieve it's prediction performance?
  - e.g. for cross-entropy optimal  $\hat{f}$ , the surplus contribution  $v(j \cup -j) - v(-j)$  captures the conditional mutual information  $I(y; x_j | x_{-j})$ 
    - $\rightsquigarrow \phi_j$  is nonzero for features with unique contribution
  - $x_j \perp\!\!\!\perp y | x_{-j}$  does not imply  $x_j \perp\!\!\!\perp y | x_S$  (cond. w.r.t. to arbitrary coalitions  $S$ )
    - $\rightsquigarrow \phi_j$  may be nonzero although the features has no unique contribution



# DEEP DIVE: SHAPLEY AXIOMS FOR SAGE

The Shapley axioms can be translated into properties of SAGE. The interpretation depends on whether conditional or marginal sampling is used.



Shapley property $\implies$	conditional SAGE property
efficiency	$\sum_{i=1}^p \phi_j(\nu) = \mathcal{R}(\hat{f}_\emptyset) - \mathcal{R}(\hat{f})$
symmetry	$x_j = x_i \implies \phi_i = \phi_j$
linearity	$\phi_j$ expectation of per-instance conditional SHAP applied to model loss
monotonicity	given models $f, f'$ , if $\forall S$ : $v_f(S \cup j) - v_f(S) \geq v_{f'}(S \cup j) - v_{f'}(S)$ then $\phi_j(v_f) \geq \phi_j(v_{f'})$
dummy	if $\forall S : \hat{f}(x) \perp\!\!\!\perp x_j   x_S \Rightarrow \phi_j = 0$

# DEEP DIVE: SHAPLEY AXIOMS FOR SAGE

The Shapley axioms can be translated into properties of SAGE. The interpretation depends on whether conditional or marginal sampling is used.



Shapley property $\implies$	marginal SAGE property
efficiency	$\sum_{i=1}^p \phi_j(v) = \mathcal{R}(\hat{f}_{\emptyset}) - \mathcal{R}(\hat{f})$
symmetry	no intelligible implication
linearity	$\phi_j$ expectation of per-instance marginal SHAP applied to model loss
monotonicity	given models $f, f'$ , if $\forall S$ : $v_f(S \cup j) - v_f(S) \geq v_{f'}(S \cup j) - v_{f'}(S)$ then $\phi_j(v_f) \geq \phi_j(v_{f'})$
dummy	model invariant to $x_j \Rightarrow \phi_j = 0$