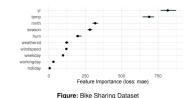
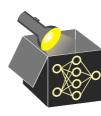
## **Interpretable Machine Learning**

## **Shapley Additive Global Importance (SAGE)**



#### Learning goals

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



## **Interpretable Machine Learning**



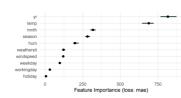


Figure: Bike Sharing Dataset

#### Learning goals

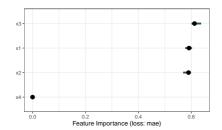
- How SAGE fairly distributes importance
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## CHALLENGE: FAIR ATTRIBUTION OF IMPORTANCE

#### Recap:

- Data:  $x_1, \ldots, x_4$  uniformly sampled from [-1, 1]
- DGP:  $y := x_1x_2 + x_3 + \epsilon_Y$  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.

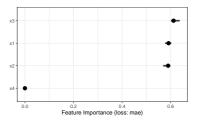
**Reason:** PFI assesses importance given that all remaining features are preserved. If we first permute  $x_1$  and then  $x_2$ , permutation of  $x_2$  would have no effect on the performance (and vice versa).



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## SAGE IDEA Covert et al. (2020)

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

#### Idea:

- Feature importance attribution can be regarded as cooperative game 

  → 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:

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

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## **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".

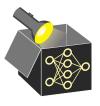
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#### SAGE value function:

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

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

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

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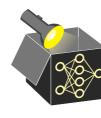
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When computing the marginalized prediction  $\hat{f}_S(x_S)$ , the "dropped" features can be sampled from

- the marginal distribution  $\mathbb{P}(x_{-S}) \Rightarrow$  marginal SAGE
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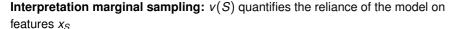
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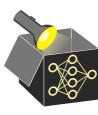
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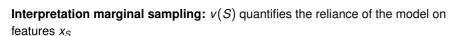
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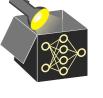
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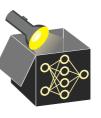
## Example:

- $y = x_3 + \epsilon_y$   $x_1 = \epsilon_1$   $x_2 = x_1 + \epsilon_2$  $x_3 = x_2 + \epsilon_3$  (all  $\epsilon_i$  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 COND. SAMPLING

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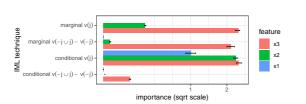
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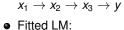
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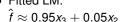


## Example:









- Marginal v(i) are only nonzero for features that are used by  $\hat{f}$
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#### SAGE - MARGINAL AND COND. SAMPLING

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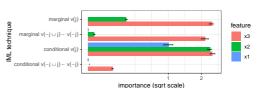
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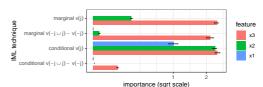
 $x_1 \rightarrow x_2 \rightarrow x_3 \rightarrow y$ 

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



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#### **SAGE values** $\phi_i$ : fair attribution of importance

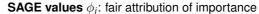
- $\bullet$  can be computed by averaging the contribution of  $x_i$  over all feature orderings
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Note:  $S_i^{\tau}$  is the set of features preceding j in permutation  $\tau$ 

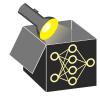


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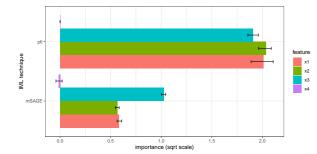
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#### INTERACTION EXAMPLE REVISITED

**Recap:** Data:  $x_1, \ldots, x_4$  uniformly sampled from  $\{-1, 1\}$  and  $y := x_1x_2 + x_3 + \epsilon_Y$  with  $\epsilon_Y \sim N(0, 1)$ . Model:  $\hat{f}(x) \approx x_1x_2 + x_3$ .

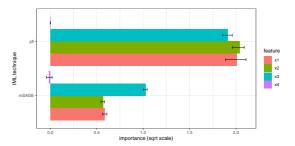


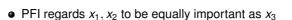
- PFI regards  $x_1, x_2$  to be equally important as  $x_3$
- Marginal SAGE fairly divides the contribution of the interaction  $x_1$  and  $x_2$



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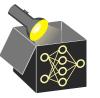
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When the loss-optimal model  $f^*$  is inspected using *conditional-sampling* based SAGE value functions, interesting links exist.



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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:  $v_{f^*}(S) = I(y; x_S)$
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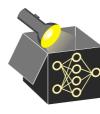
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#### IMPLICATIONS MARGINAL SAGE VALUES

Can we gain insight into whether the  $\dots$ 

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  - $\rightsquigarrow \phi_i$  is only nonzero if  $x_i$  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)  $\rightsquigarrow \phi_i$  may be zero although the feature is causal for the prediction



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  - $\rightsquigarrow \phi_i$  is only nonzero if  $x_i$  is causal for the prediction
  - $v(j \cup S) v(S)$  may be zero due to indep.  $x_j \perp \!\!\! \perp y | x_S$  (as for PFI)  $\rightsquigarrow \phi_i$  may be zero although the feature is causal for the prediction



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## IMPLICATIONS MARGINAL SAGE VALUES

Can we gain insight into whether the ...



- $\bullet$  feature  $x_i$  contains prediction-relevant information about y?
  - value functions may be nonzero despite independence due to extrapolation (as for PFI)
  - $\rightsquigarrow \phi_i$  may be nonzero without  $x_i$  being dependent with y
  - value functions may be zero despite  $x_j$  containing prediction-relevant information due to underfitting (as for PFI)
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#### IMPLICATIONS CONDITIONAL SAGE VALUES

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- feature  $\mathbf{x}_i$  is causal for the prediction?
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### IMPLICATIONS CONDITIONAL SAGE VALUES

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- 2 feature  $\mathbf{x}_i$  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  $\phi_i$
  - $x_j \perp \!\!\! \perp y$  does not imply  $x_j \perp \!\!\! \perp y | x_S$  and consequently does not imply  $v(j \cup S) v(S) = 0 \leadsto \phi_i$  may be nonzero although  $\mathbf{x}_i \perp \!\!\! \perp y$

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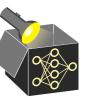
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#### IMPLICATIONS CONDITIONAL SAGE VALUES

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- model requires access to x<sub>j</sub> to achieve it's prediction performance?
   e.g. for cross-entropy optimal f̂, the surplus contribution v(j ∪ −j) − v(−j)
  - captures the conditional mutual information  $I(y; x_j|x_{-j})$
  - $\rightsquigarrow \phi_j$  is nonzero for features with unique contribution  $x_i \perp \!\!\! \perp y | x_{-j}$  does not imply  $x_i \perp \!\!\! \perp y | x_S$  (cond. w.r.t. to arbitrary coalitions S)
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## **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.

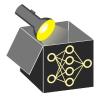
Shapley property $\implies$	conditional SAGE property
efficiency	$\sum_{i=1}^{p} \phi_j(\mathbf{v}) = \mathcal{R}(\hat{\mathbf{f}}_{\emptyset}) - \mathcal{R}(\hat{\mathbf{f}})$
symmetry	$x_j = x_i \implies \phi_i = \phi_j$
linearity	$\phi_j$ expecation of per-instance
	conditional SHAP applied to model 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 $\phi_j(v_f) \geq \phi_j(v_{f'})$
dummv	if $\forall S : \hat{f}(x) \perp x_i   x_S \Rightarrow \phi_i = 0$



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linearity	$\phi_i$ expectation of per-instance
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	$v_f(S \cup j) - v_f(S) \geq v_{f'}(S \cup j) - v_{f'}(S)$
	then $\phi_i(v_f) \geq \phi_i(v_{f'})$
dummy	if $\forall S : \hat{f}(x) \perp x_j   x_S \Rightarrow \phi_j = 0$



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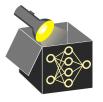
Shapley property $\Longrightarrow$	marginal SAGE property
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