

Interpretable Machine Learning

Shapley Additive Global Importance (SAGE)

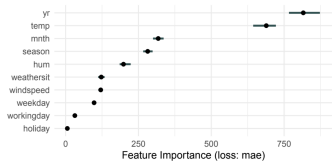


Figure: Bike Sharing Dataset

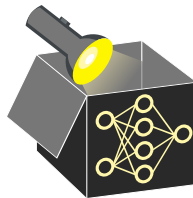
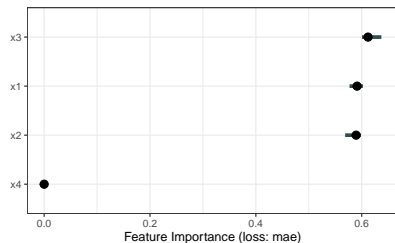
Learning goals

- 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:

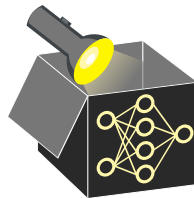
- Data: x_1, \dots, x_4 uniformly sampled from $[-1, 1]$
- DGP: $y := x_1 x_2 + x_3 + \epsilon_Y$ with $\epsilon_Y \sim N(0, 1)$
- Model: $\hat{f}(x) \approx x_1 x_2 + x_3$



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

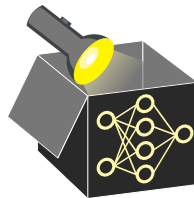
Note:

- Similar 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”.

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



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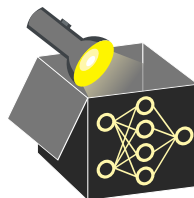
$$\hat{f}_S(x_S) = \mathbb{E}[\hat{f}(x)|X_S = x_S]$$

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

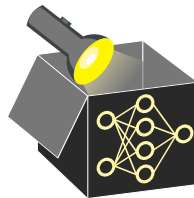
~> Risk of predictor $\hat{f}_S(x_S)$ is compared to the risk of the mean prediction \hat{f}_{\emptyset}



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↪ 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 :

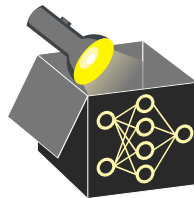
$$v_{\hat{f}}(S \cup \{j\}) - v_{\hat{f}}(S) = \mathcal{R}(\hat{f}_S) - \mathcal{R}(\hat{f}_{S \cup \{j\}})$$

↪ 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



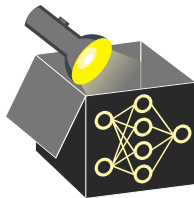
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Interpretation marginal sampling: $v(S)$ quantifies the reliance of the model on features x_S

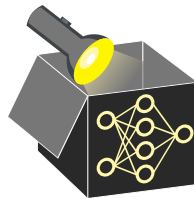
- features x_S not being causal for the prediction $\Rightarrow v(S) = 0$



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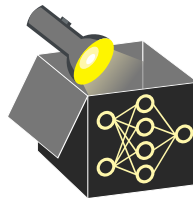
Interpretation conditional sampling: $v(S)$ quantifies whether variables x_S contain prediction-relevant information (e.g. $y \not\perp x_S$) that is (directly or indirectly) exploited by the model

- 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 ϵ_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

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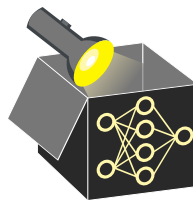
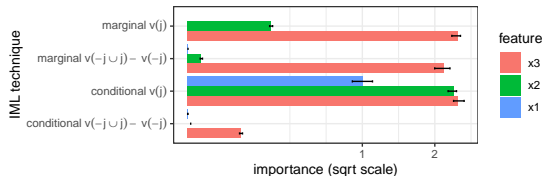
- Causal DAG:

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

- 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



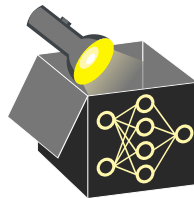
SAGE VALUE FUNCTIONS VERSUS SAGE VALUES

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

SAGE values ϕ_j : fair attribution of importance

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

Note: S_j^τ is the set of features preceding j in permutation τ



SAGE VALUE FUNCTIONS VERSUS SAGE VALUES

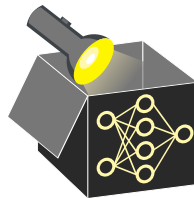
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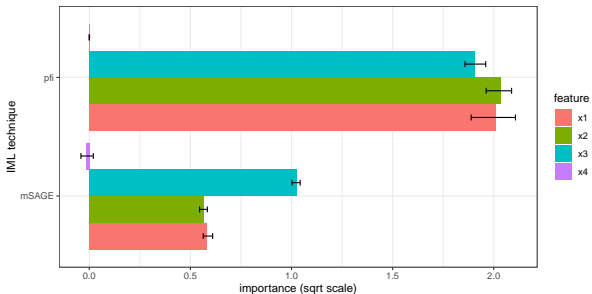
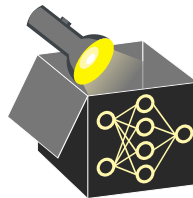
SAGE value approximation: Average over the contributions for M randomly sampled permutations

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



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.

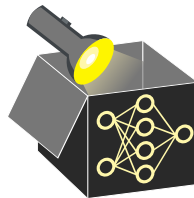


SAGE LOSS FUNCTIONS

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:
$$v_{f^*}(S \cup \{j\}) - v_{f^*}(S) = I(y, x_j | x_S)$$



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For MSE loss:

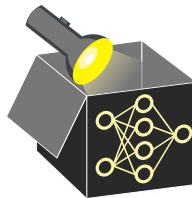
- value function is the expected reduction in variance given knowledge of the features x_S : $v_{f^*}(S) = \text{Var}(y) - \mathbb{E}[\text{Var}(y|x_S)]$
- surplus contribution is the respective reduction over x_S :
$$v_{f^*}(S \cup \{j\}) - v_{f^*}(S) = \mathbb{E}[\text{Var}(y|x_S)] - \mathbb{E}[\text{Var}(y|x_{S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

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

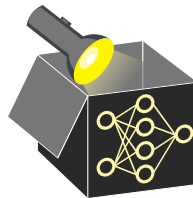
Can we gain insight into whether the ...



- 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

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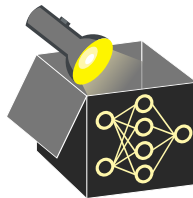
- ③ model requires access to x_j to achieve it's prediction performance?
 - like PFI, in general marginal value functions do not allow insight into unique contribution \rightsquigarrow no insight from ϕ_j

IMPLICATIONS CONDITIONAL SAGE VALUES

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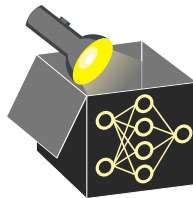
❶ feature \mathbf{x}_j is causal for the prediction?

- value functions may be nonzero although feature is not directly used by \hat{f}
 \rightsquigarrow nonzero ϕ_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 ϕ_j does not imply $\mathbf{x}_j \not\rightarrow \hat{y}$



IMPLICATIONS CONDITIONAL SAGE VALUES

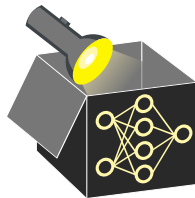
Can we gain insight into whether the ...



- 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 ϕ_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	$\sum_{i=1}^p \phi_j(v) = \mathcal{R}(\hat{f}_\emptyset) - \mathcal{R}(\hat{f})$
symmetry	$x_j = x_i \implies \phi_i = \phi_j$
linearity	ϕ_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

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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	ϕ_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 $x_j \Rightarrow \phi_j = 0$