# Interpretable Machine Learning

# Shapley Additive Global Importance (SAGE)

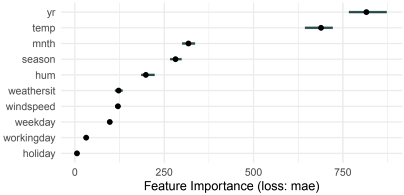



**Figure:** Bike Sharing Dataset

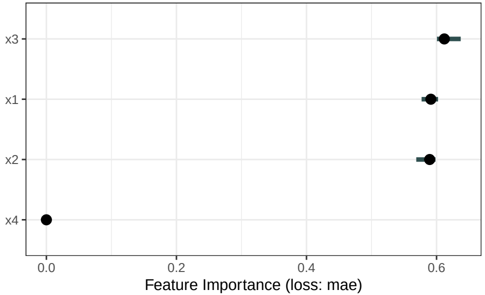
## Learning goals

- 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: $x_1, \ldots, x_4$ 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 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
  $\rightsquigarrow$ 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:**

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

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

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

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

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

$\rightsquigarrow$ 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 $x_S$ contains 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 $\not\Rightarrow v(S) = 0$
  - 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

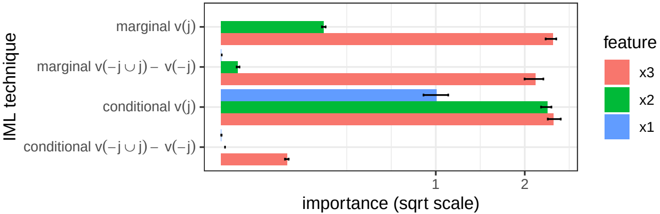
**Example:**

- $y = x_3 + \epsilon_y$
  $x_1 = \epsilon_1$
  $x_2 = x_1 + \epsilon_2$
  $x_3 = x_2 + \epsilon_3$ (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: $x_1 \to x_2 \to x_3 \to y$
- 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 $y \perp x_1, x_2 | x_3$, 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

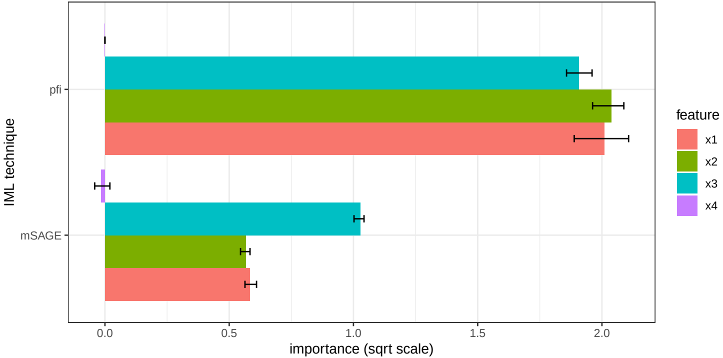
- can be computed by averaging the contribution of $x_j$ over all feature orderings
- for feature permutation $\tau$, the contribution of $j$ in the set $S_j^\tau$ is given as $v(S_j^\tau \cup \{j\}) - v(S_j^\tau)$
  Note: $S_j^\tau$ is the set of features preceding $j$ in permutation $\tau$

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

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

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

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

**For MSE loss:**

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

# IMPLICATIONS MARGINAL SAGE VALUES

Can we gain insight into whether the ...

1. 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 $x_j \perp y | x_S$ (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 ...

1. feature $\mathbf{x}_j$ is causal for the prediction?
   - value functions may be nonzero although feature is not directly used by the model $\rightsquigarrow$ 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 $\phi_j$
   - $x_j \perp y$ does not imply $x_j \perp y | x_S$ and consequently does not imply $v(j \cup S) - v(S) = 0$
     $\rightsquigarrow$ $\phi_j$ may be nonzero although $\mathbf{x}_j \perp y$

# 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
   - $x_j \perp y | x_{-j}$ does not imply conditional independence w.r.t. to arbitrary coalitions $x_j \perp y | x_S$
     $\rightsquigarrow \phi_j$ 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 | $\phi_j$ 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 $\phi_j(v_f) \geq \phi_j(v_{f'})$ |
| dummy | if $\forall S$ : $\hat{f}(x) \perp x_j \vert x_S \Rightarrow \phi_j = 0$ |

# 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 $\Longrightarrow$ | 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 | $\phi_j$ expecation 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 $x_j \Rightarrow \phi_j = 0$ |