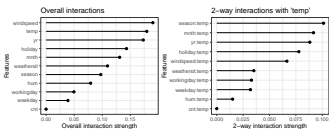
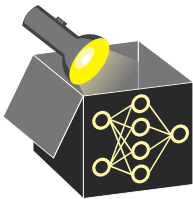


# Interpretable Machine Learning

## Friedman's H-Statistic



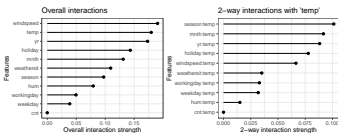
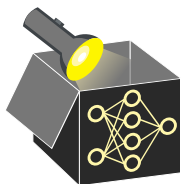
### Learning goals

- Friedman's H-statistic with two purposes:
- Measure general  $k$ -way interactions between arbitrary features
- Measure a single feature's overall interaction strength

# Interpretable Machine Learning

## Functional Decompositions

## Friedman's H-Statistic



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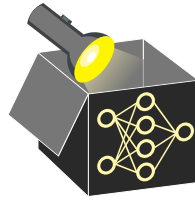
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# IDEA

► Friedman and Popescu (2008)

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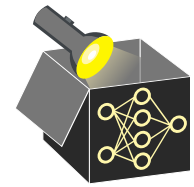


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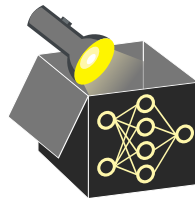
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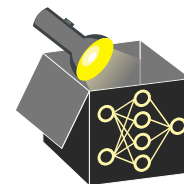
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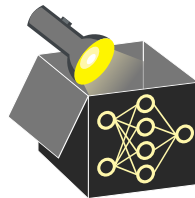
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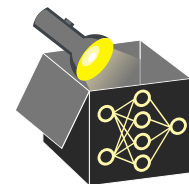
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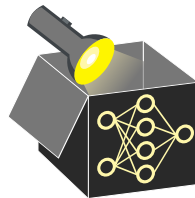
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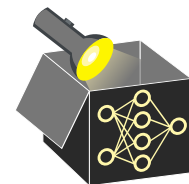
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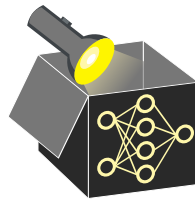
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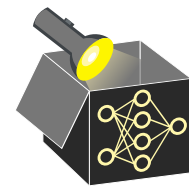
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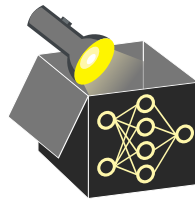
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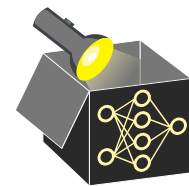
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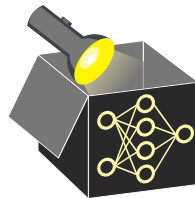
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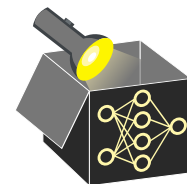
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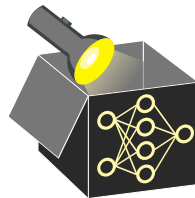
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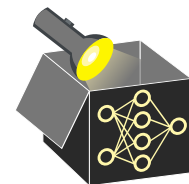
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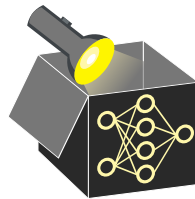
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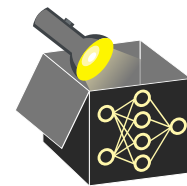
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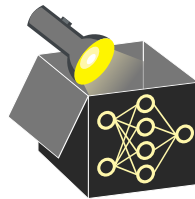
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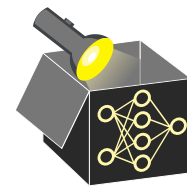
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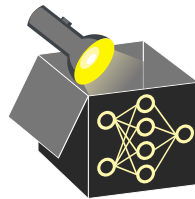
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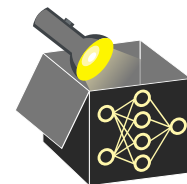
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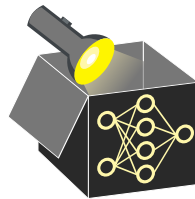
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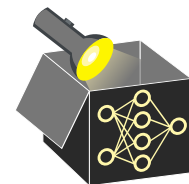
$$\hat{f}_{S,PD}(x_{i_1}, x_{i_2}, \dots, x_{i_k}) = \sum_{\substack{V \subseteq S \\ V \neq S}} g_V(\mathbf{x}_V) = \sum_{\substack{V \subseteq S \\ |V| < k}} g_V(\mathbf{x}_V)$$

**Overall interaction:**

- Question: Does feature  $j$  interact with any other feature at all?
- ⇒ H-statistic analogous to 2-way interactions, but for feature sets  $S = \{j\}$  and  $-S = \{1, \dots, p\} \setminus \{j\}$  instead of two single features:

$$\hat{f}(\mathbf{x}) - g_\emptyset = \hat{f}_{\{1, \dots, p\}, PD}^c(\mathbf{x}) = \hat{f}_{j, PD}^c(x_j) + \hat{f}_{-j, PD}^c(\mathbf{x}_{-j}) = \sum_{\substack{S: j \in S \\ |S| \geq 2}} g_S(\mathbf{x}_S)$$

- $-j$  denotes  $-S = \{1, \dots, p\} \setminus \{j\}$ , i.e. all other features
- $\hat{f}_{-j, PD}(\mathbf{x}_{-j})$ :  $(p-1)$ -dim PD function of all  $p$  features except feature  $j$

 **$k$ -way interaction:**

- **Analogous** for  $k$ -way interactions between feat  $S = \{i_1, i_2, \dots, i_k\}$ : No  $k$ -way interaction, if

$$\hat{f}_{S,PD}(x_{i_1}, x_{i_2}, \dots, x_{i_k}) = \sum_{\substack{V \subseteq S \\ V \neq S}} g_V(\mathbf{x}_V) = \sum_{\substack{V \subseteq S \\ |V| < k}} g_V(\mathbf{x}_V)$$

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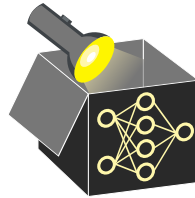
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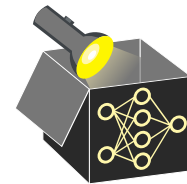
## 2-WAY INTERACTION STRENGTH

- **Question:** How to measure interaction strength without computing functional decomposition components  $g_S$ ?



## 2-WAY INTERACTION STRENGTH

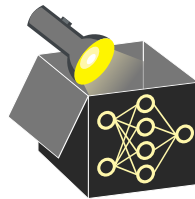
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## 2-WAY INTERACTION STRENGTH

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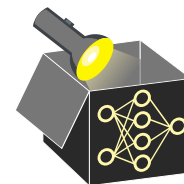
$$\hat{f}_{\{jk\},PD}^c(x_j, x_k) = \hat{f}_{j,PD}^c(x_j) + \hat{f}_{k,PD}^c(x_k) ?$$



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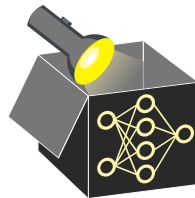
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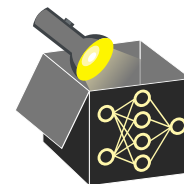
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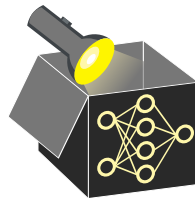
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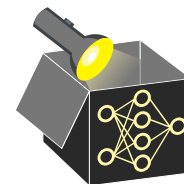
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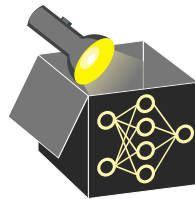
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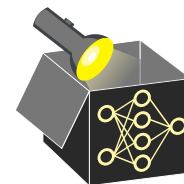
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# H-STATISTIC: EXAMPLES

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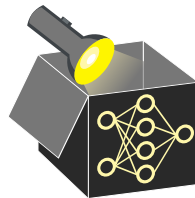
## Example

$$\hat{f}(x_1, x_2) = 4 - 2x_1 + 0.3e^{x_2} + |x_1|x_2 \quad (x_1, x_2) \in [0, 1]^2$$

$$\hat{f}_{1,PD}^c(x_1) = -2x_1 + 0.5|x_1| + 0.75$$

$$\hat{f}_{2,PD}^c(x_2) = 0.3e^{x_2} + 0.5x_2 - 0.3e + 0.05$$

$$\hat{f}_{1,2;PD}^c(x_1, x_2) = 1.05 - 2x_1 + 0.3e^{x_2} + |x_1|x_2 - 0.3e$$



# H-STATISTIC: EXAMPLES

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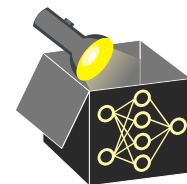
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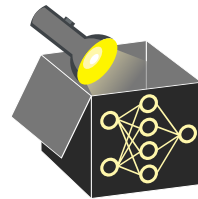
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# H-STATISTIC: EXAMPLES

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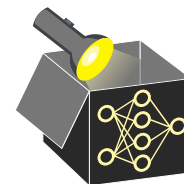
$$\hat{f}_{1,2;PD}^c(x_1, x_2) = 1.05 - 2x_1 + 0.3e^{x_2} + |x_1|x_2 - 0.3e$$

$$\begin{aligned} \Rightarrow H_{12}^2 &= \frac{\text{Var} \left[ \hat{f}_{jk,PD}^c(X_j, X_k) - \hat{f}_{j,PD}^c(X_j) - \hat{f}_{k,PD}^c(X_k) \right]}{\text{Var} \left[ \hat{f}_{jk,PD}^c(X_j, X_k) \right]} \\ &= \frac{\mathbb{E} \left[ (|x_1|x_2 - 0.5|x_1| - 0.5x_2 + 0.25)^2 \right]}{\mathbb{E} \left[ (1.05 - 2x_1 + 0.3e^{x_2} + |x_1|x_2 - 0.3e)^2 \right]} > 0 \end{aligned}$$

# H-STATISTIC: EXAMPLES

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## Example



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# 3-WAY INTERACTION STRENGTH

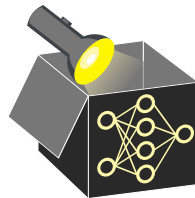
- Same idea as for 2-way, but different formula (see before):

$$\hat{f}_{\{ijk\},PD}^c(x_i, x_j, x_k) = \hat{f}_{\{ij\},PD}^c(x_i, x_j) + \hat{f}_{\{ik\},PD}^c(x_i, x_k) + \hat{f}_{\{jk\},PD}^c(x_j, x_k) - \hat{f}_{i,PD}^c(x_i) - \hat{f}_{j,PD}^c(x_j) - \hat{f}_{k,PD}^c(x_k)$$

⇒ H-statistic for a 3-way interaction between features  $i, j$  and  $k$ :

$$H_{ijk}^2 = \frac{\text{Var} \left[ \hat{f}_{ijk,PD}^c(x_i, x_j, x_k) - \hat{f}_{ij,PD}^c(x_i, x_j) - \hat{f}_{ik,PD}^c(x_i, x_k) - \hat{f}_{jk,PD}^c(x_j, x_k) + \hat{f}_{i,PD}^c(x_i) + \hat{f}_{j,PD}^c(x_j) + \hat{f}_{k,PD}^c(x_k) \right]}{\text{Var} \left[ \hat{f}_{ijk,PD}^c(x_i, x_j, x_k) \right]}$$

- Analogous for higher order interactions, but more complicated



# 3-WAY INTERACTION STRENGTH

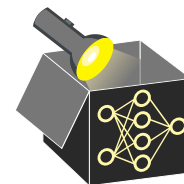
- Same idea as for 2-way, but different formula (see before):

$$\hat{f}_{\{ijk\},PD}^c(x_i, x_j, x_k) = \hat{f}_{\{ij\},PD}^c(x_i, x_j) + \hat{f}_{\{ik\},PD}^c(x_i, x_k) + \hat{f}_{\{jk\},PD}^c(x_j, x_k) - \hat{f}_{i,PD}^c(x_i) - \hat{f}_{j,PD}^c(x_j) - \hat{f}_{k,PD}^c(x_k)$$

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- Analogous for higher order interactions, but more complicated

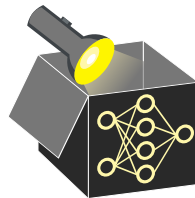


# OVERALL INTERACTION STRENGTH

- Measure overall strength of interactions between feature  $j$  and all other features

⇒ **H-statistic** analogous to 2-way interaction:

$$H_j^2 = \frac{\text{Var} \left[ \hat{f}^c(\mathbf{X}) - \hat{f}_{j,PD}^c(X_j) - \hat{f}_{-j,PD}^c(\mathbf{X}_{-j}) \right]}{\text{Var} \left[ \hat{f}^c(\mathbf{X}) \right]}$$
$$= \frac{\sum_{i=1}^n \left( \hat{f}^c(\mathbf{x}^{(i)}) - \hat{f}_{j,PD}^c(x_j^{(i)}) - \hat{f}_{-j,PD}^c(\mathbf{x}_{-j}^{(i)}) \right)^2}{\sum_{i=1}^n \left( \hat{f}^c(\mathbf{x}^{(i)}) \right)^2}$$

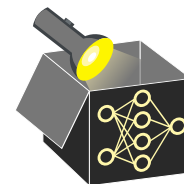


# OVERALL INTERACTION STRENGTH

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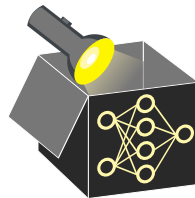
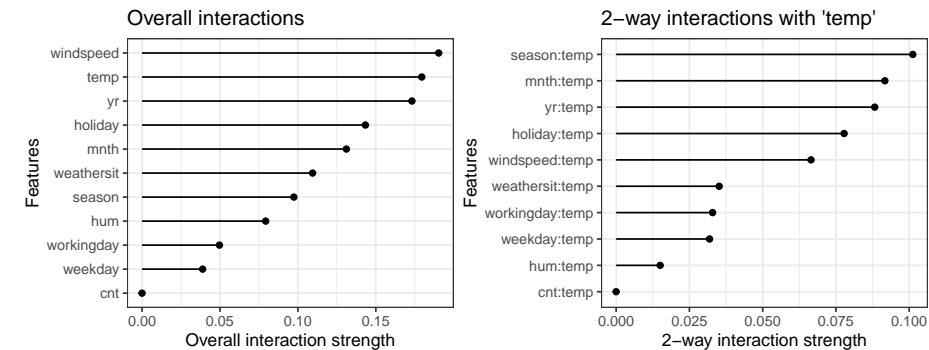
⇒ **H-statistic** analogous to 2-way interaction:

$$H_j^2 = \frac{\text{Var} \left[ \hat{f}^c() - \hat{f}_{j,PD}^c(X_j) - \hat{f}_{-j,PD}^c(-j) \right]}{\text{Var} \left[ \hat{f}^c() \right]}$$
$$= \frac{\sum_{i=1}^n \left( \hat{f}^c(\mathbf{x}^{(i)}) - \hat{f}_{j,PD}^c(x_j^{(i)}) - \hat{f}_{-j,PD}^c(\mathbf{x}_{-j}^{(i)}) \right)^2}{\sum_{i=1}^n \left( \hat{f}^c(\mathbf{x}^{(i)}) \right)^2}$$



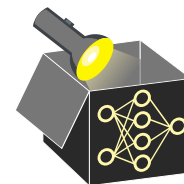
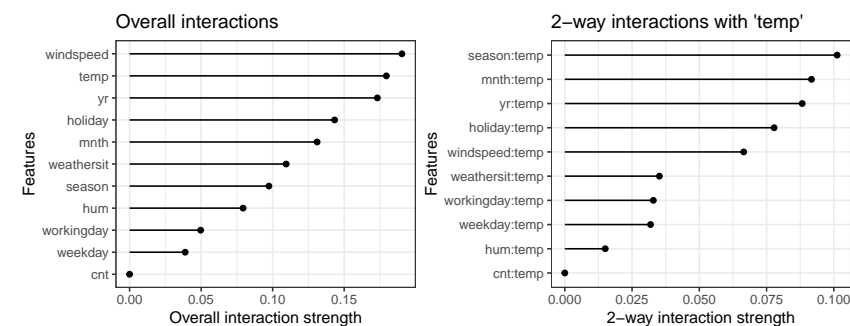
# H-STATISTIC: EXAMPLE

Measure interactions of a random forest for the bike data set



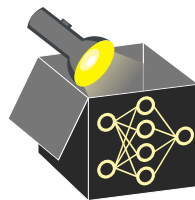
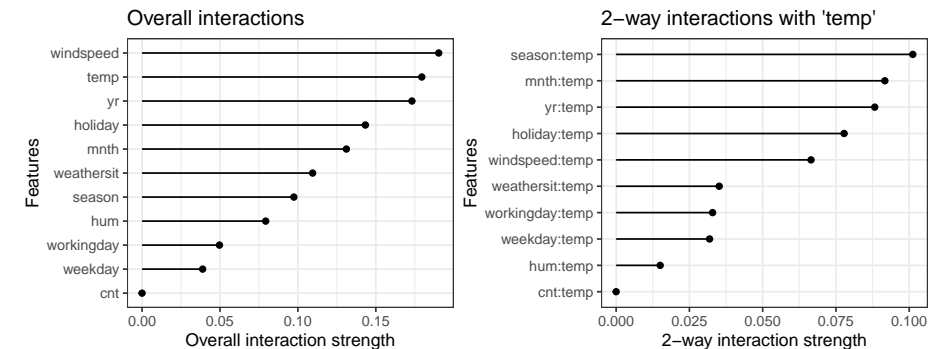
# H-STATISTIC: EXAMPLE

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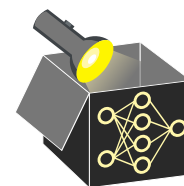
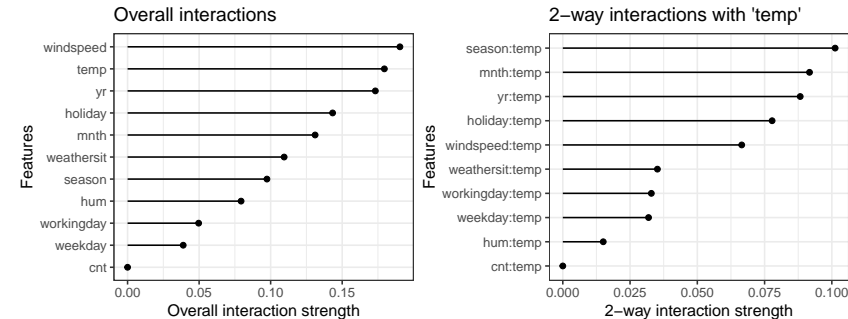


## Remarks and Conclusion:

- H-statistic provides **general definition of interactions** + an **algorithm for computation**  
Also adjustable to categorical / discrete features and / or function values
- For interaction order  $k$  still needs  $\approx 2^k$  PD-functions
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