Interpretable Machine Learning

Introduction to Loss-based Feature Importance

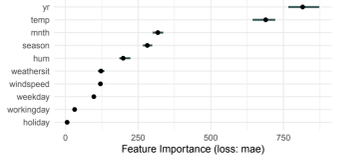

Figure: Bike Sharing Dataset

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- Develop an intuition for possible use-cases
- Know characteristics of feature importance methods

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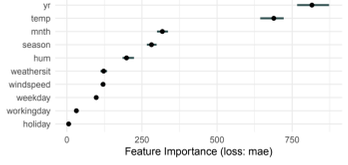
Feature Importances 1
Intro to Loss-based Feature Importance



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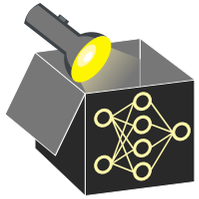

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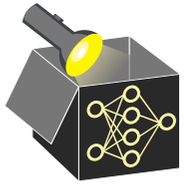

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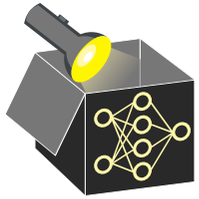

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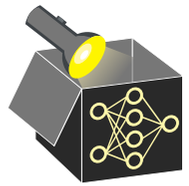

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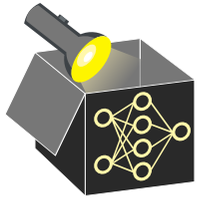

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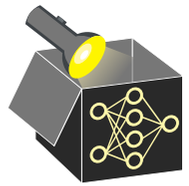

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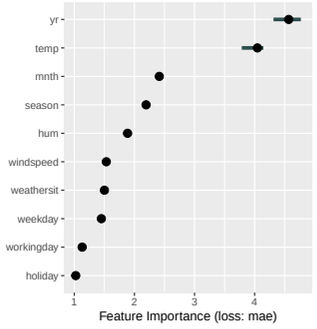
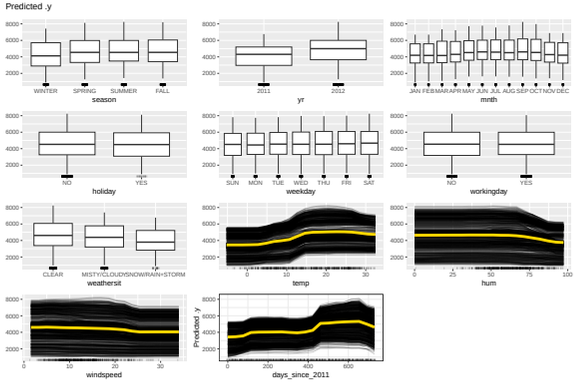
Feature importance offers condensed summary of feat. relevance w.r.t. performance

- Fit random forest on bike sharing data
- Left: Feature importance ranking by permutation feature importance (PFI)
- Right: Feature effects for all features





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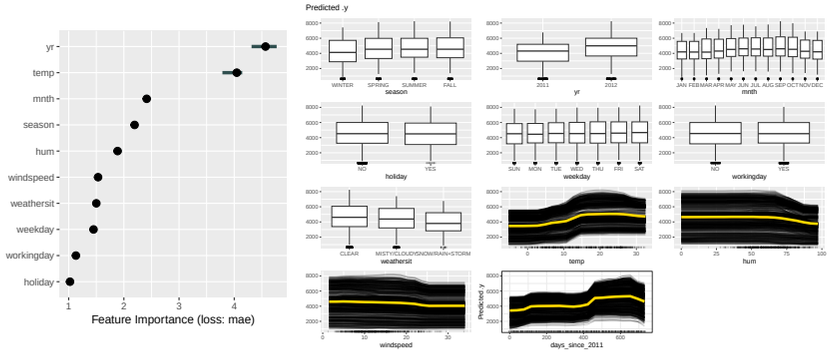
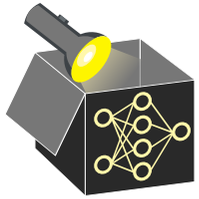


FEATURE IMPORTANCE - DIFFERENCES

Ewald et al. 2024



Many loss-based feature importance methods exist, which mainly differ in

(1) How they "remove" or "perturb" the feature of interest (FOI) X_j

- **Remove** X_j **and refit:** Drop the X_j and retrain model without it
- **Perturb** X_j**:** Replace X_j by $\tilde{X}_j$ sampled from *marginal* or *conditional* distribution
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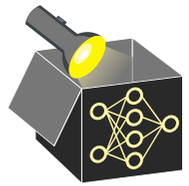
EWALD_2024



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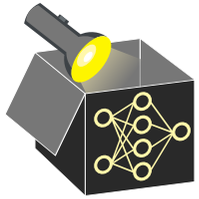

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- **Compare "reduced model" without FOI vs. full model**:
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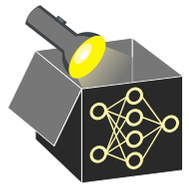

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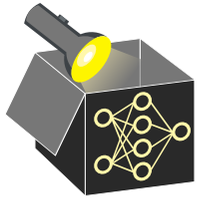

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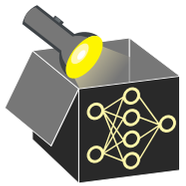

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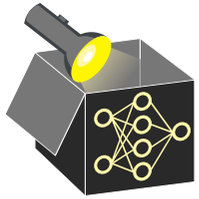

Feature importance methods provide condensed insights, but only into specific aspects of model and data. Interpretation goals often differ and typically address non-overlapping questions (except for special cases).

For example, one may be interested in getting insight into whether the ...

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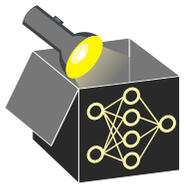

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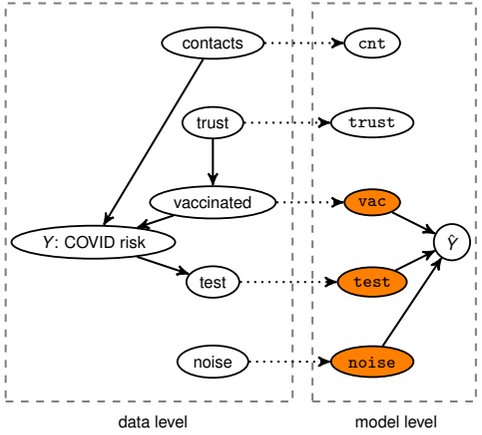

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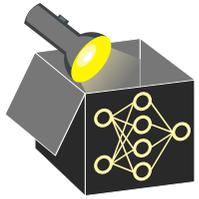

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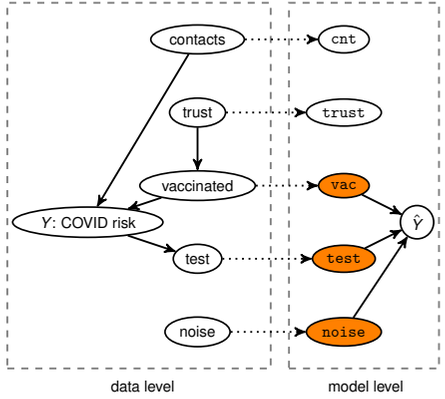

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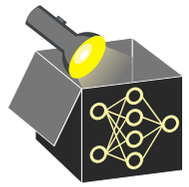

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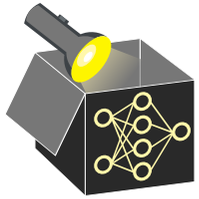

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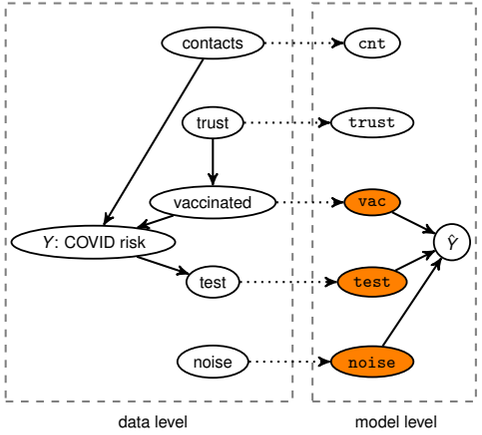

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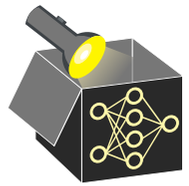

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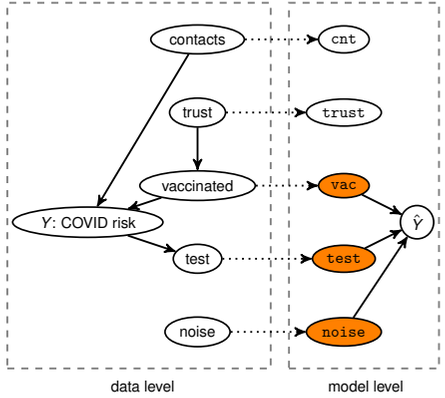

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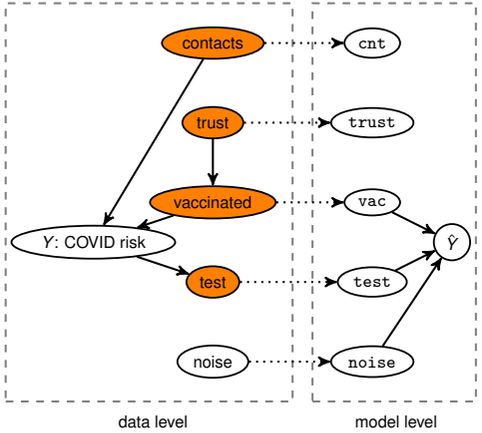

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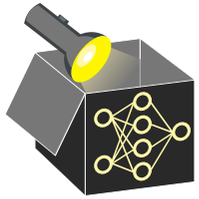

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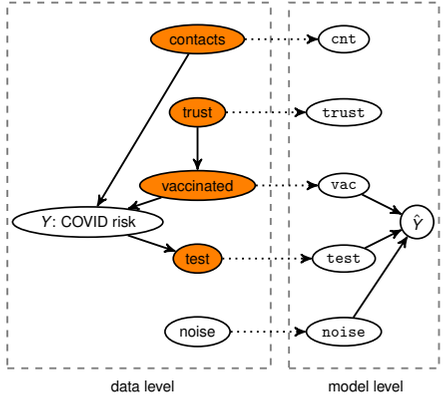

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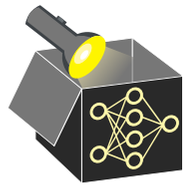

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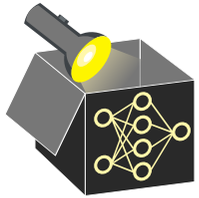

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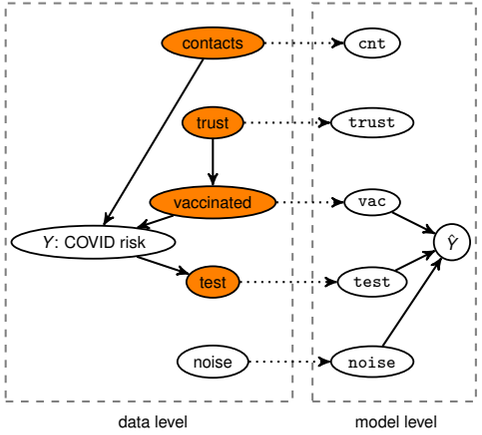
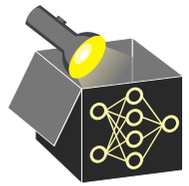


Example: underfitting, model multiplicity

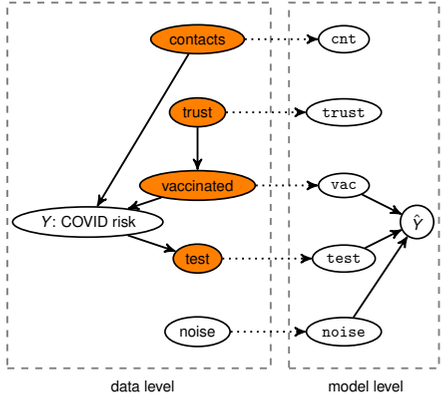
- All prediction-relevant features for y are of interest
- Example: All features that are directly or indirectly (i.e., via another feature) connected to y

$\Rightarrow$ Underfitted models may ignore prediction-relevant features such as `contacts` here

EXAMPLE: PREDICTION-RELEVANT INFORMATION (2)



A feature may contain prediction-relevant information (2) without causing the prediction (1)



Example: underfitting, model multiplicity

- All prediction-relevant features for y are of interest
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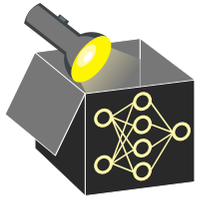
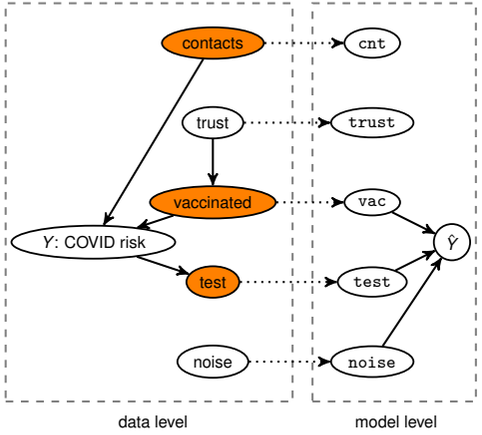
EXAMPLE: REQUIRES ACCESS TO FEATURE (3)



A feature may contain prediction-relevant information (2), without the model requiring access to the feature for (optimal) prediction performance (3)



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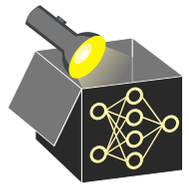

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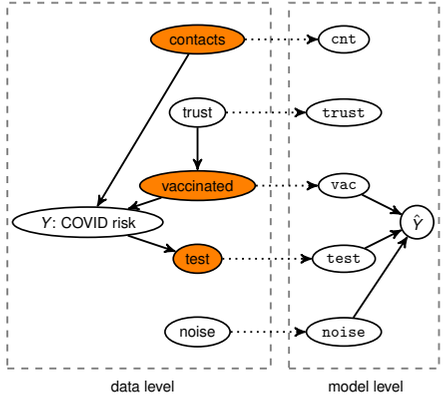

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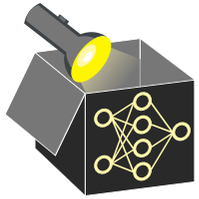

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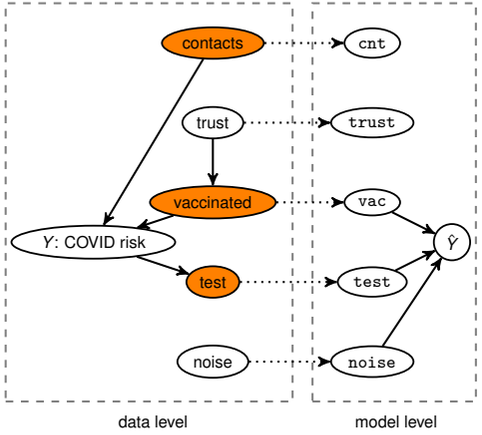

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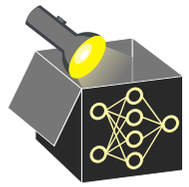

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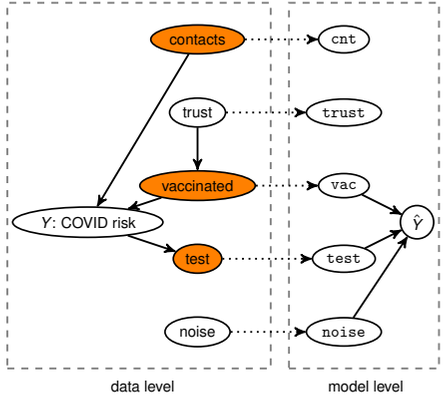

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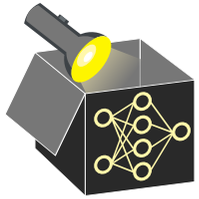
POTENTIAL INTERPRETATION GOALS



For example, one may be interested in getting insight into whether the ...

(1) feature x_j is causal for the prediction?

- A symptom may help predict a disease ($\rightsquigarrow$ causal for $\hat{y}$)
- Intervening on symptom may not affect disease ($\rightsquigarrow$ not causal for y)

(2) feature x_j contains prediction-relevant information about y?

- x_j helps predict y (e.g., conditional expectation) w.r.t. performance
- If $x_j \perp\!\!\!\perp y$, then $\mathbb{E}[y|x_j] = \mathbb{E}[y]$ and x_j and y have zero mutual information
  $\rightsquigarrow$ x_j carries no prediction-relevant information

(3) model requires access to x_j to achieve it's prediction performance?

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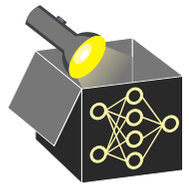

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Interpretable Machine Learning

Permutation Feature Importance (PFI)

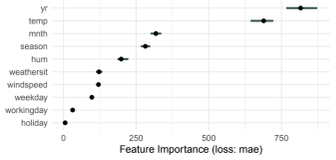

Figure: Bike Sharing Dataset

Learning goals

- Understand how PFI is computed
- Understanding strengths and weaknesses

Interpretable Machine Learning

Feature Importances 1
Permutation Feature Importance (PFI)

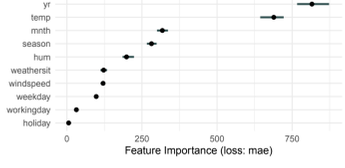

Figure: Bike Sharing Dataset

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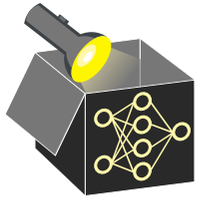
- Understand how PFI is computed
- Understanding strengths and weaknesses

MOTIVATION FOR PFI

- **Goal:** Assess how important feature(s) X_S are for predictive performance of a **fixed trained model** $\hat{f}$ on a given dataset $\mathcal{D}$
- **Idea:** Estimate change in model performance when X_S is "made uninformative"



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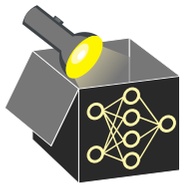

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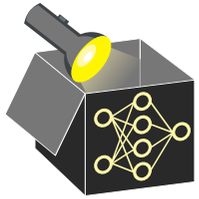

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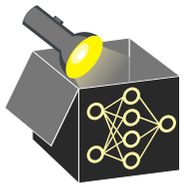

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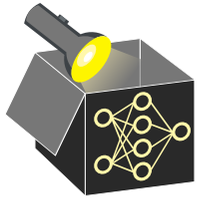

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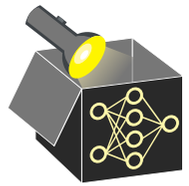
$$\text{PFI}_S := \underbrace{\mathbb{E}\Big[L\big(\hat{f}(\tilde{X}_S, X_{-S}), Y\big)\Big]}_{\text{risk after "destroying" } X_S} - \underbrace{\mathbb{E}\Big[L\big(\hat{f}(X), Y\big)\Big]}_{\text{baseline risk}},$$

- **How to perturb X_S?**
  - Add random noise: distorts $\mathbb{P}(X_S)$ (not used)
  - Permutation: preserves marginal $\mathbb{P}(X_S)$, breaks dependence with Y (used)

MOTIVATION FOR PFI



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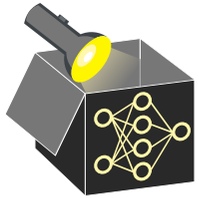
PERMUTATION FEATURE IMPORTANCE (PFI)

Breiman (2001)



Sample estimator (using independent test set $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^{n}$)

- Measure the error **with feat. values** x_S and **with permuted feat. values** $\tilde{x}_S$
- Repeat permutation (e.g., m times) and average difference of both errors:

$$\widehat{PFI}_S = \frac{1}{m} \sum_{k=1}^{m} \left[\mathcal{R}_{\text{emp}}(\hat{f}, \tilde{\mathcal{D}}^S_{(k)}) - \mathcal{R}_{\text{emp}}(\hat{f}, \mathcal{D}) \right]$$

- $\mathcal{D}^{(k)}_S$: dataset where column(s) x_S are **permuted** once (in repetition k)
- $\mathcal{R}_{\text{emp}}(\hat{f}, \mathcal{D}) = \frac{1}{n} \sum_{(x,y) \in \mathcal{D}} L(\hat{f}(x), y)$: Measures performance of $\hat{f}$ using $\mathcal{D}$
- Average over m permutations to reduce Monte-Carlo variance

Example of permuting feature x_S with $S = \{1\}$ and $m = 6$ permutations:

$\mathcal{D}$

$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$
1	4	7
2	5	8
3	6	9

$\Rightarrow$

$\tilde{\mathcal{D}}^S_{(1)}$

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$\tilde{\mathcal{D}}^S_{(4)}$

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1	4	7
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$\tilde{\mathcal{D}}^S_{(5)}$

$\mathbf{x}_S$	$\mathbf{x}_2$	$\mathbf{x}_3$
3	4	7
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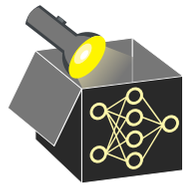
Note: S refers to a subset of features, here $|S| = 1$ to measure impact of permuting x_1 on performance

PERMUTATION FEATURE IMPORTANCE (PFI)

BREIMAN_2001



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PERMUTATION FEATURE IMPORTANCE

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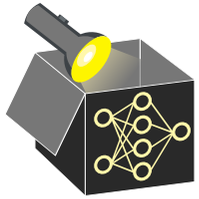

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PERMUTATION FEATURE IMPORTANCE

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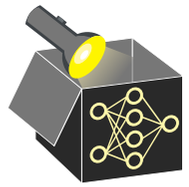

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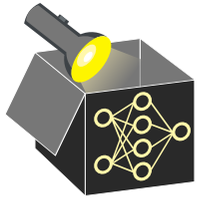
PERMUTATION FEATURE IMPORTANCE



$\tilde{\mathcal{D}}^S_{(k)}$

i	$\mathbf{x}_S$	$\mathbf{x}_2$	$\mathbf{x}_3$
1	2	4	7
⋮	1	5	8
n	3	6	9

$\mathcal{D}$

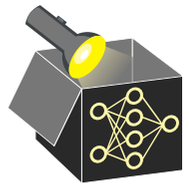
$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$
1	4	7
2	5	8
3	6	9

$\hat{f}$
0.6
0.6
0.6

$\hat{f}$
0.4
0.8
0.6

1. **Perturbation:** Sample feature values from the distribution of x_S ($P(X_S)$).
   $\Rightarrow$ Randomly permute feature x_S
   $\Rightarrow$ Replace x_S with permuted feature $\tilde{x}_S$ and create data $\tilde{\mathcal{D}}^S$ containing $\tilde{x}_S$
2. **Prediction:** Make predictions for both data, i.e., $\mathcal{D}$ and $\tilde{\mathcal{D}}^S$

PERMUTATION FEATURE IMPORTANCE



$\mathcal{DS}_{(k)}$

i	$\mathbf{x}_S$	$\mathbf{x}_2$	$\mathbf{x}_3$
1	2	4	7
⋮	1	5	8
n	3	6	9

$\mathcal{D}$

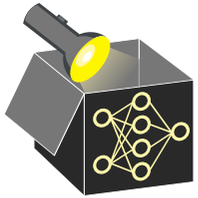
$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$
1	4	7
2	5	8
3	6	9

$\hat{f}$
0.6
0.6
0.6

$\hat{f}$
0.4
0.8
0.6

1. **Perturbation:** Sample feature values from the distribution of x_S ($P(X_S)$).
   $\Rightarrow$ Randomly permute feature x_S
   $\Rightarrow$ Replace x_S with permuted feat. x_S and create data $\mathcal{DS}$ containing x_S
2. **Prediction:** Make predictions for both data, i.e., $\mathcal{D}$ and $\mathcal{DS}$

PERMUTATION FEATURE IMPORTANCE



$\tilde{\mathcal{D}}^S_{(k)}$

i	x_S	x_2	x_3
1	2	4	7
⋮	1	5	8
n	3	6	9

$L(\hat{f}, y)$
0.9
0.5
0.1

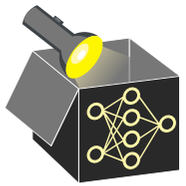
$\mathcal{D}$

x_1	x_2	x_3
1	4	7
2	5	8
3	6	9

$L(\hat{f}, y)$
0.25
0.35
0.1

3. **Aggregation:**
   - Compute the loss for each observation in both data sets

PERMUTATION FEATURE IMPORTANCE



$\mathcal{DS}_{(k)}$

i	x_S	x_2	x_3
1	2	4	7
⋮	1	5	8
n	3	6	9

$L(\hat{f}, y)$
0.9
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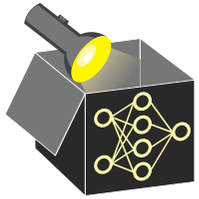


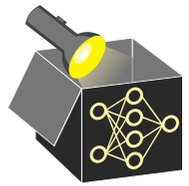
$\tilde{\mathcal{D}}^S_{(k)}$ $\mathcal{D}$

i	x_S	x_2	x_3	x_1	x_2	x_3	ΔL
1	2	4	7	1	4	7	0.65
⋮	1	5	8	2	5	8	0.15
n	3	6	9	3	6	9	0

$L(\hat{f}, y)$		$L(\hat{f}, y)$
0.9	-	0.25
0.5		0.35
0.1		0.1

3. **Aggregation:**
   - Compute the loss for each observation in both data sets
   - Take the difference of both losses ΔL for each observation

PERMUTATION FEATURE IMPORTANCE



$\mathcal{DS}_{(k)}$ $\mathcal{D}$

i	x_S	x_2	x_3	x_1	x_2	x_3	ΔL
1	2	4	7	1	4	7	0.65
⋮	1	5	8	2	5	8	0.15
n	3	6	9	3	6	9	0

$L(\hat{f}, y)$		$L(\hat{f}, y)$
0.9	-	0.25
0.5		0.35
0.1		0.1

3. **Aggregation:**
   - Compute the loss for each observation in both data sets
   - Take the difference of both losses ΔL for each observation

PERMUTATION FEATURE IMPORTANCE

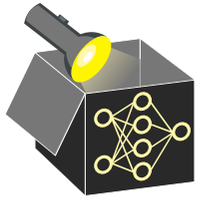
$$\mathcal{R}_{\text{emp}}(\hat{f}, \tilde{\mathcal{D}}^{S}_{(k)}) - \mathcal{R}_{\text{emp}}(\hat{f}, \mathcal{D})$$

i	$\mathbf{x}_S$	$\mathbf{x}_2$	$\mathbf{x}_3$
1	2	4	7
⋮	1	5	8
n	3	6	9

$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$
1	4	7
2	5	8
3	6	9

$\Delta\mathbf{L}$
0.65
0.15
0

= 0.267



3. **Aggregation:**
   - Compute the loss for each observation in both data sets
   - Take the difference of both losses ΔL for each observation
   - Average this change in loss across all observations
     Note: Same as computing $\mathcal{R}_{\text{emp}}$ on both data sets and taking difference

PERMUTATION FEATURE IMPORTANCE

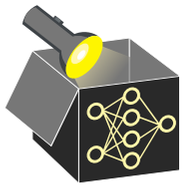
$$\mathcal{R}_{\text{emp}}(\hat{f}, \mathcal{DS}_{(k)}) - \mathcal{R}_{\text{emp}}(\hat{f}, \mathcal{D})$$

i	$\mathbf{x}_S$	$\mathbf{x}_2$	$\mathbf{x}_3$
1	2	4	7
⋮	1	5	8
n	3	6	9

$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$
1	4	7
2	5	8
3	6	9

$\Delta\mathbf{L}$
0.65
0.15
0

= 0.267



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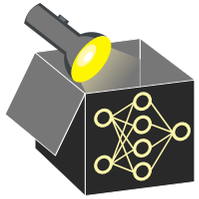
   - Compute the loss for each observation in both data sets
   - Take the difference of both losses ΔL for each observation
   - Average this change in loss across all observations
     Note: Same as computing $\mathcal{R}_{\text{emp}}$ on both data sets and taking difference

PERMUTATION FEATURE IMPORTANCE



$$\mathcal{R}_{\text{emp}}(\hat{f}, \tilde{\mathcal{D}}^{S}_{(k)}) - \mathcal{R}_{\text{emp}}(\hat{f}, \mathcal{D})$$

	i	$\mathbf{x}_S$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\Delta\mathbf{L}$
1	1	2	4	7	1	4	7	0.65
	⋮	1	5	8	2	5	8	0.15
	n	3	6	9	3	6	9	0
⋮								
m	1	3	4	7	1	4	7	0.85
	⋮	2	5	8	2	5	8	0
	n	1	6	9	3	6	9	0.35

= 0.267

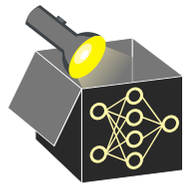
$\widehat{PFI}_S$ = ½ (0.267 + 0.4)

= 0.4

3. Aggregation:

- Compute the loss for each observation in both data sets
- Take the difference of both losses ΔL for each observation
- Average this change in loss across all observations
- Repeat perturbation and average over multiple repetitions

PERMUTATION FEATURE IMPORTANCE



$$\mathcal{R}_{\text{emp}}(\hat{f}, \mathcal{DS}_{(k)}) - \mathcal{R}_{\text{emp}}(\hat{f}, \mathcal{D})$$

	i	$\mathbf{x}_S$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\Delta\mathbf{L}$
1	1	2	4	7	1	4	7	0.65
	⋮	1	5	8	2	5	8	0.15
	n	3	6	9	3	6	9	0
⋮								
m	1	3	4	7	1	4	7	0.85
	⋮	2	5	8	2	5	8	0
	n	1	6	9	3	6	9	0.35

= 0.267

$\widehat{PFI}_S$ = ½ (0.267 + 0.4)

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3. Aggregation:

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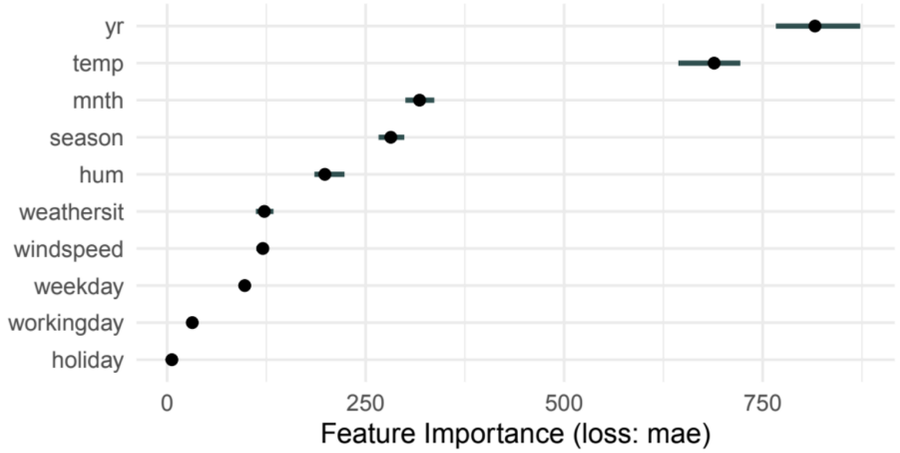
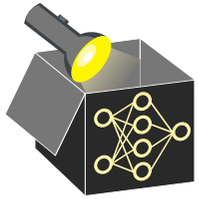
EXAMPLE: BIKE SHARING DATASET

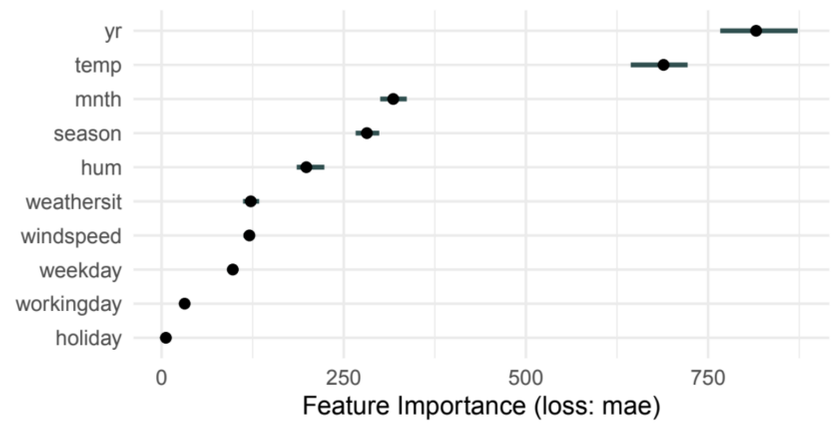


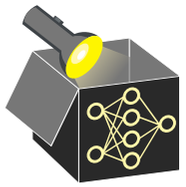


Interpretation:

- `yr` and `temp` are most important features using mean absolute error (MAE)
- Destroying information about `yr` by permuting it increases MAE of model by 816
- Error bars show 5% and 95% quantiles over multiple permutations

EXAMPLE: BIKE SHARING DATASET





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- `yr` and `temp` are most important feats using mean absolute error (MAE)
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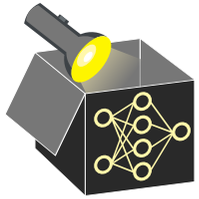
COMMENTS ON PFI

- Interpretation: Increase in error when feature's information is destroyed



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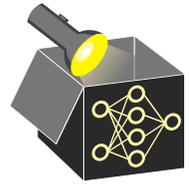
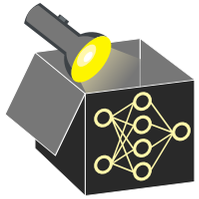


COMMENTS ON PFI

- Interpretation: Increase in error when feature's information is destroyed
- Results can be unreliable due to random permutations
  $\Rightarrow$ Solution: Average results over multiple repetitions



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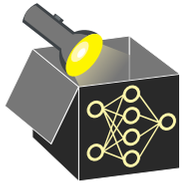

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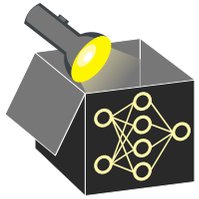

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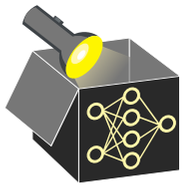

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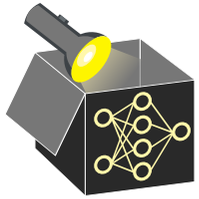

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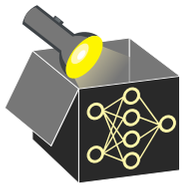
- PFI automatically includes importance of interaction effects with other features
  $\Rightarrow$ Permuting x_j also destroys interactions with permuted feature
  $\Rightarrow$ PFI score contains importance of all interactions with permuted feature

COMMENTS ON PFI



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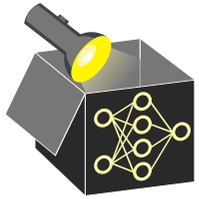

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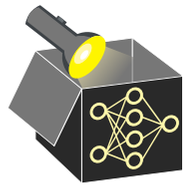
- Interpretation of PFI depends on whether training or test data is used

COMMENTS ON PFI



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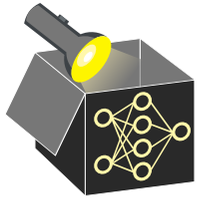
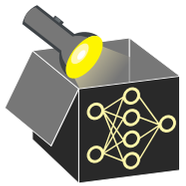
COMMENTS ON PFI - EXTRAPOLATION



Example: Let $y = x_3 + \epsilon_y$, with $\epsilon_y \sim \mathcal{N}(0, 0.1)$.

- $x_1 := \epsilon_1$, $x_2 := x_1 + \epsilon_2$ are highly correlated ($\epsilon_1 \sim \mathcal{N}(0, 1)$, $\epsilon_2 \sim \mathcal{N}(0, 0.01)$)
- $x_3 := \epsilon_3$, $x_4 := \epsilon_4$, with $\epsilon_3, \epsilon_4 \sim \mathcal{N}(0, 1)$ and all noise terms ϵ_j are independent
- Fitting a linear model yields $\hat{f}(\mathbf{x}) \approx 0.3x_1 - 0.3x_2 + x_3$

COMMENTS ON PFI - EXTRAPOLATION



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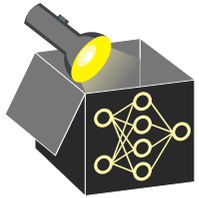

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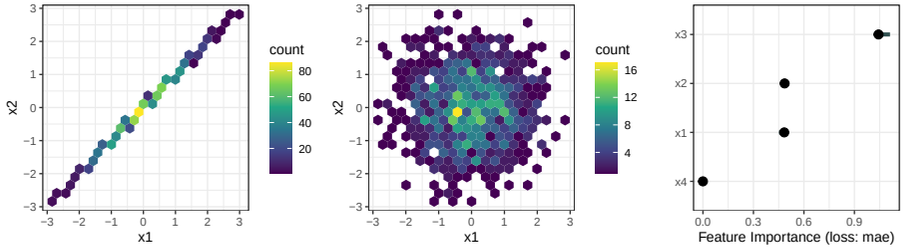

Hexbin plot of (x_1, x_2) before (left) and after (center) permuting x_1; PFI scores (right).

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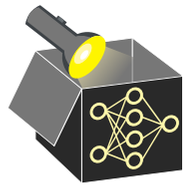

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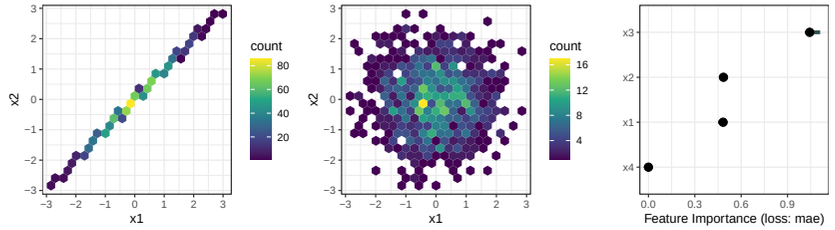

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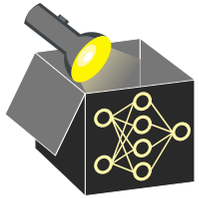

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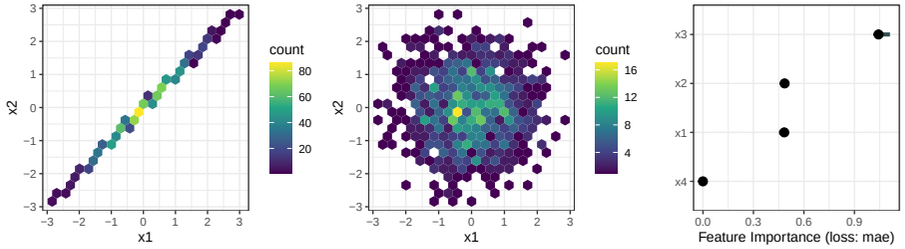

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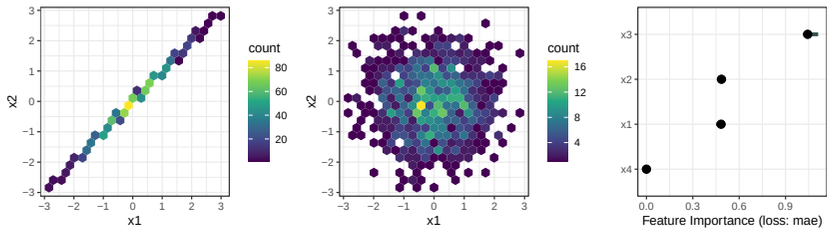

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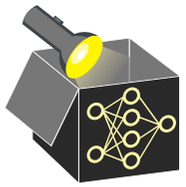
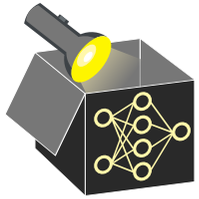


COMMENTS ON PFI - INTERACTIONS



Example: Let $x_1, \ldots, x_4$ be independently and uniformly sampled from $\{-1, 1\}$ and

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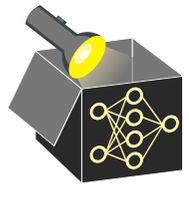

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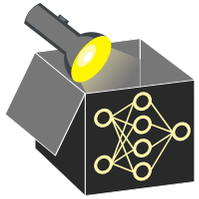

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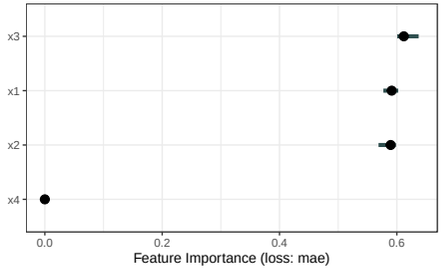

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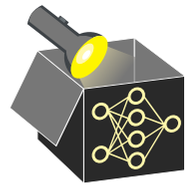

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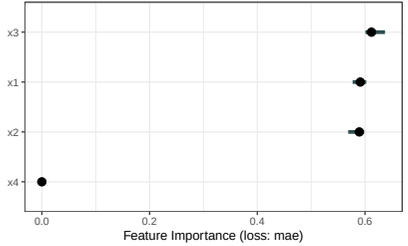

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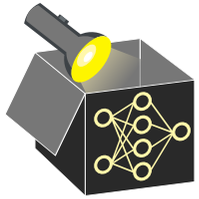

Example:

- $x_1, \ldots, x_{20}, y$ are independently sampled from $\mathcal{U}(-10, 10)$
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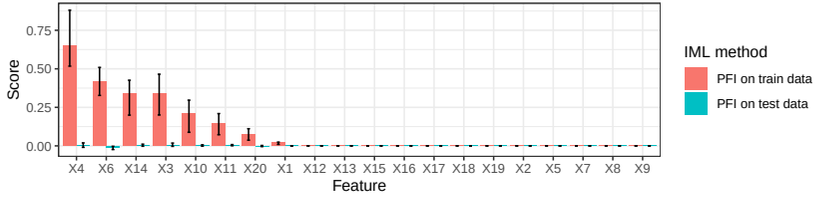

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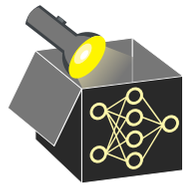

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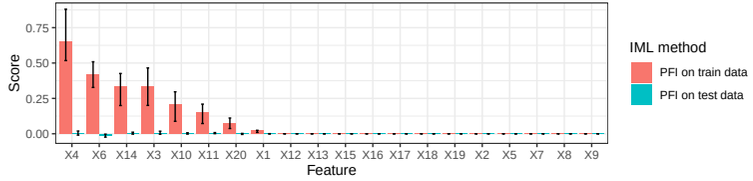

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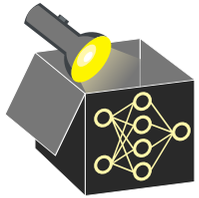

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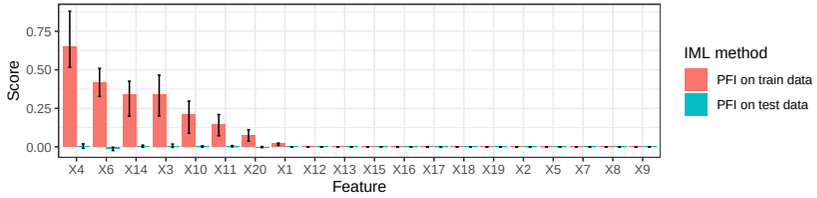

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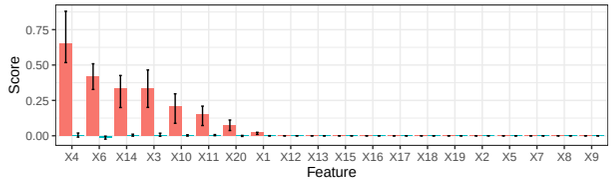

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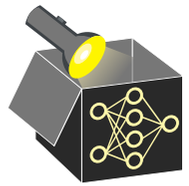

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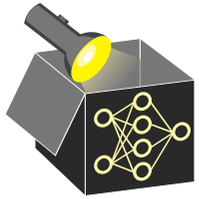

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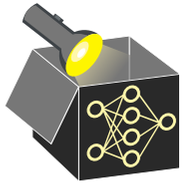

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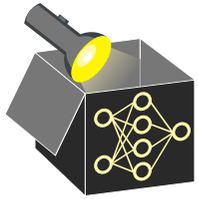

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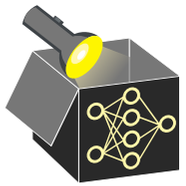

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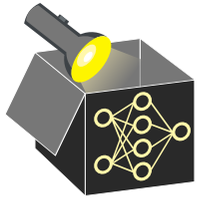

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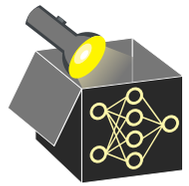

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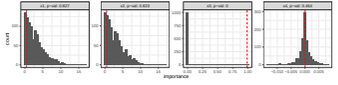
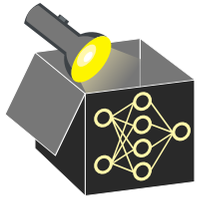
Interpretable Machine Learning

Permutation IMPortance (PIMP)



Learning goals

- Understand PIMP and its motivation
- Address multiple testing in feature importance



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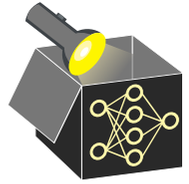

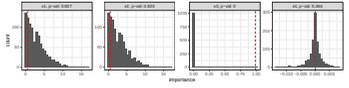

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TESTING IMPORTANCE (PIMP) ▸ Altmann et al. (2010)

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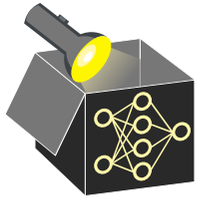

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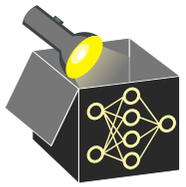

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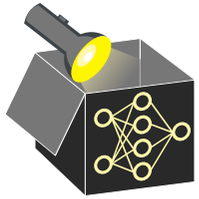

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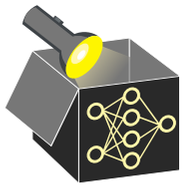

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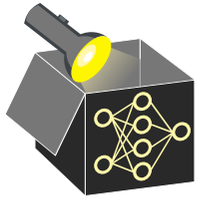

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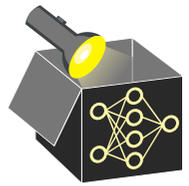

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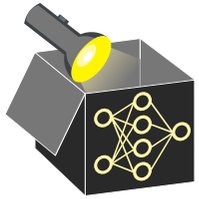

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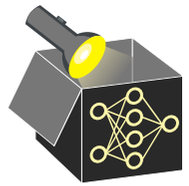

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Interpretable Machine Learning – 1 / 4

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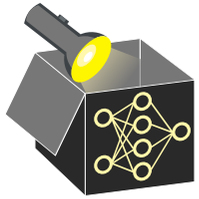

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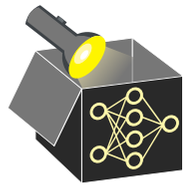

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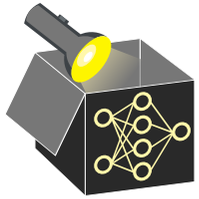

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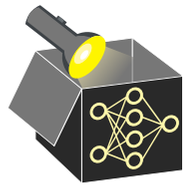

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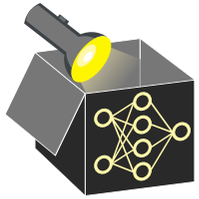

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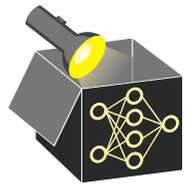

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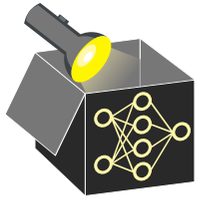

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   - Compute p-value: Probability that null importance exceeds observed:
     - parametric by taking tail probability of assumed distribution

$$\mathbb{P}(\widehat{\text{PFI}}_j^{(m)} \geq \widehat{\text{PFI}}_j^{\text{obs}})$$

     - non-parametric by computing empirical tail probability:

$$p_j := \frac{1}{B} \sum_{b=1}^{B} \mathbb{I}[\widehat{\text{PFI}}_j^{(b)} \geq \widehat{\text{PFI}}_j^{\text{obs}}]$$

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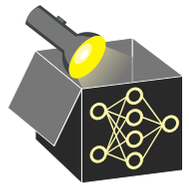

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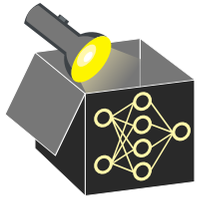
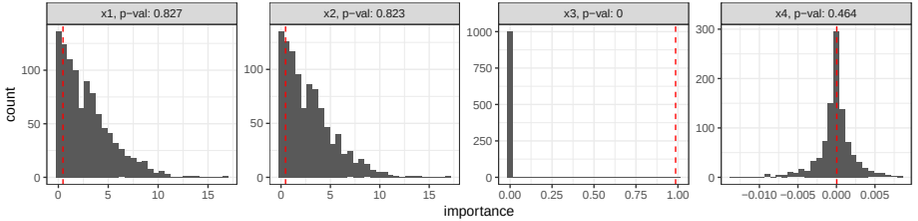
PIMP FOR EXTRAPOLATION EXAMPLE



Recall: Let $y = x_3 + \epsilon_y$, with $\epsilon_y \sim \mathcal{N}(0, 0.1)$.

- $x_1 := \epsilon_1$, $x_2 := x_1 + \epsilon_2$ are highly correlated ($\epsilon_1 \sim \mathcal{N}(0, 1)$, $\epsilon_2 \sim \mathcal{N}(0, 0.01)$)
- $x_3 := \epsilon_3$, $x_4 := \epsilon_4$, with $\epsilon_3, \epsilon_4 \sim \mathcal{N}(0, 1)$ and all noise terms ϵ_j are independent
- Fitting a linear model yields $\hat{f}(\mathbf{x}) \approx 0.3x_1 - 0.3x_2 + x_3$



- Histograms: H_0 distribution of PFI scores after permuting y (1000 repetitions)
- Red: Observed PFI score (under H_1) $\rightsquigarrow$ compare against H_0 distribution
- Recall: PFI for x_1, x_2, x_3 is nonzero suggesting they are important (red lines)
- PIMP considers x_1, x_2 not significantly relevant (p-value > 0.05)

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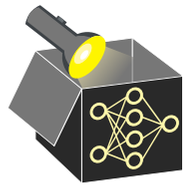

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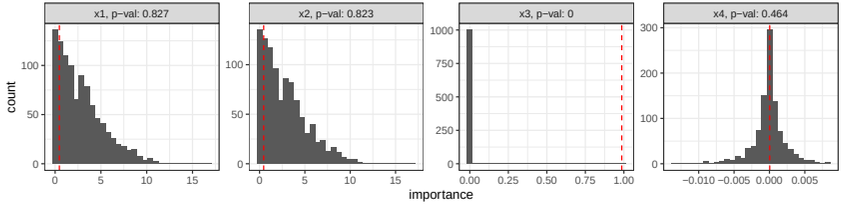

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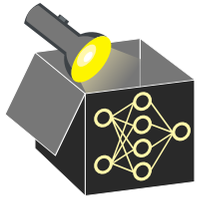
DIGRESSION: MULTIPLE TESTING

Romano et al. (2010)



- When should we reject H_0 for a given feature?
- PIMP conducts one hypothesis test per feature $\Rightarrow$ **multiple testing problem**
- With many tests, rejections of true H_0 just by chance (type-I errors) accumulate
- To account for this, control a suitable error rate, e.g., the **family-wise error rate**
  FWE: probability of making at least one type-I error across all tests
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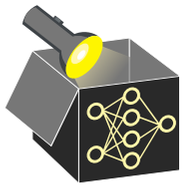

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Interpretable Machine Learning

Conditional Feature Importance (CFI)

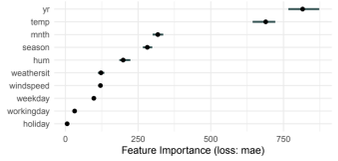


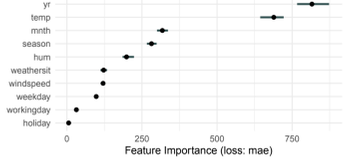
Figure: Bike Sharing Dataset

Learning goals

- Extrapolation and Conditional Sampling
- Conditional Feature Importance (CFI)
- Interpretation of CFI and difference to PFI

Interpretable Machine Learning

Feature Importances 1
Conditional Feature Importance (CFI)



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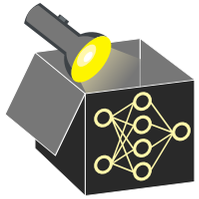

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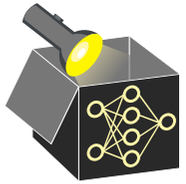

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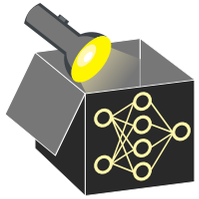

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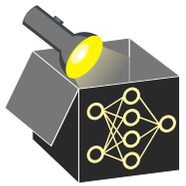

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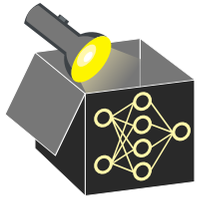

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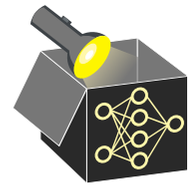

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Interpretable Machine Learning – 1 / 6

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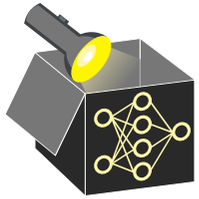

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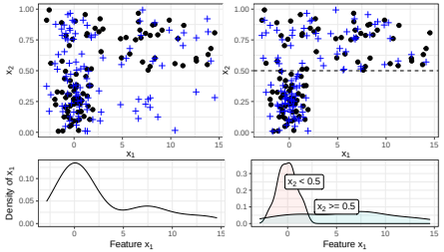
Example: Conditional permutation scheme
Black dots: $X_2 \sim \mathcal{U}(0,1)$ and $X_1 \sim \mathcal{N}(0,1)$ (if $X_2 < 0.5$) or $\mathcal{N}(4,4)$ (if $X_2 \geq 0.5$)

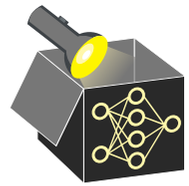


Left: For $X_2 < 0.5$, permuting X_1 (crosses) preserves marginal (but not joint) distribution
$\rightsquigarrow$ Bottom: Marginal density of X_1

Right: Permuting X_1 within subgroups $X_2 < 0.5$ & $X_2 \geq 0.5$ reduces extrapolation
$\rightsquigarrow$ Bottom: X_1-density conditional on groups

▸ Molnar et. al (2020)

CFI MOTIVATION



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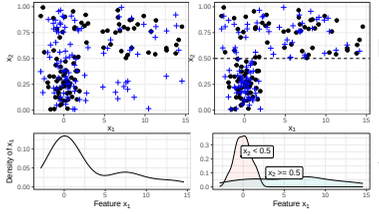

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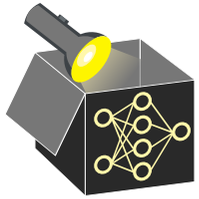
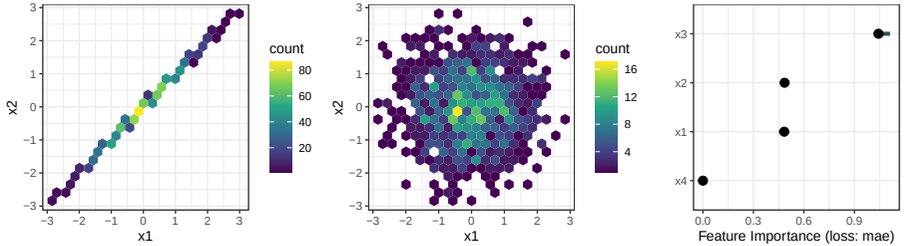
▸ Molnar 2020

RECALL: EXTRAPOLATION IN PFI



Recall: Let $y = x_3 + \epsilon_y$, with $\epsilon_y \sim \mathcal{N}(0, 0.1)$.

- $x_1 := \epsilon_1$, $x_2 := x_1 + \epsilon_2$ are highly correlated ($\epsilon_1 \sim \mathcal{N}(0,1)$, $\epsilon_2 \sim \mathcal{N}(0, 0.01)$)
- $x_3 := \epsilon_3$, $x_4 := \epsilon_4$, with $\epsilon_3, \epsilon_4 \sim \mathcal{N}(0,1)$ and all noise terms ϵ_j are independent
- Fitting a linear model yields $\hat{f}(\mathbf{x}) \approx 0.3x_1 - 0.3x_2 + x_3$



Hexbin plot of (x_1, x_2) before (left) and after (center) permuting x_1; PFI scores (right).

$\Rightarrow$ x_1, x_2 cancel in $\hat{f}$ and should be irrelevant

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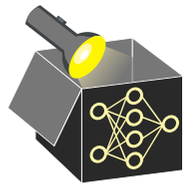

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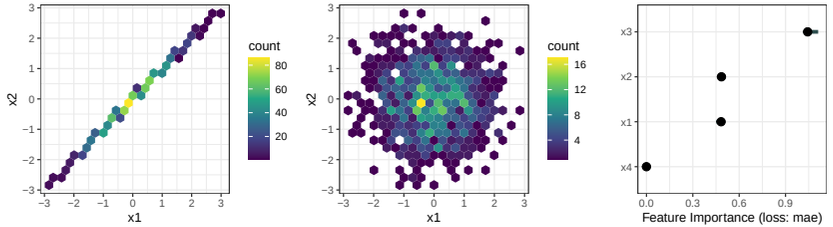

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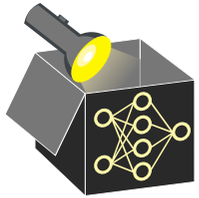
CFI

Strobl et al. (2008) | Hooker et al. (2021)



CFI for X_S using test data $\mathcal{D}$:

- Measure the error **with unperturbed features** x_S.
- Measure the error **with perturbed feature values** $\tilde{x}_S \sim \mathbb{P}(X_S|X_{-S})$
- Repeat perturbing X_S (e.g., m times) and average difference of both errors:

$$\widehat{CFI}_S = \frac{1}{m} \sum_{k=1}^{m} \mathcal{R}_{\text{emp}}(\hat{f}, \tilde{\mathcal{D}}_{(k)}^{S|-S}) - \mathcal{R}_{\text{emp}}(\hat{f}, \mathcal{D})$$

Here, $\tilde{\mathcal{D}}^{S|-S}$ denotes data, where x_S values are conditionally resampled given x_{-S}.

Illustrative example: Conditional permutation when X_{-S} is categorical:

Original Data

ID	X_{-S}	X_S
1	A	3.1
2	A	2.7
3	A	3.4
4	B	6.0
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CFI

STROBL_2008 | HOOKER_2021

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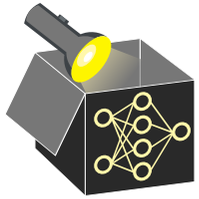
IMPLICATIONS OF CFI ▸ König et al. (2020)

Interpretation: Due to the conditional sampling w.r.t. all other features, CFI quantifies a feature's unique contribution to the model performance.



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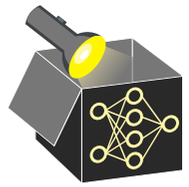

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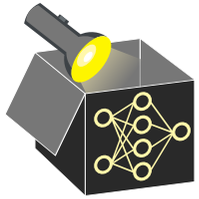

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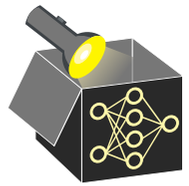

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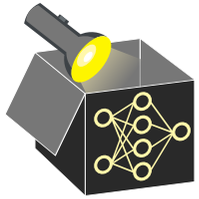

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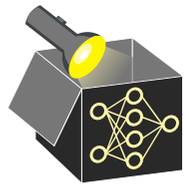
IMPLICATIONS OF CFI K_NIG_ET_2020



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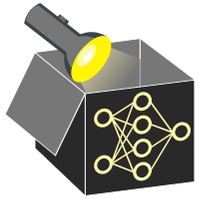

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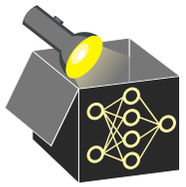

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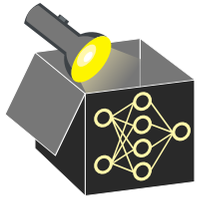

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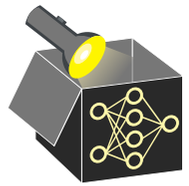

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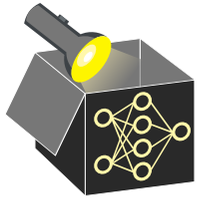

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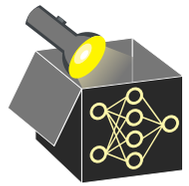
3. Does the model require access to x_j to achieve its prediction performance?
   - $CFI_j \neq 0 \Rightarrow x_j$ contributes unique information (meaning $x_j \not\perp\!\!\!\perp y|x_{-j}$)
   - Only uncovers the relationships that were exploited by the model

IMPLICATIONS OF CFI



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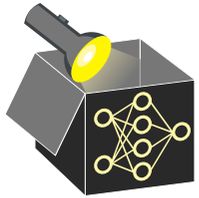
   - $CFI_j \neq 0 \Rightarrow x_j$ contributes unique information (meaning $x_j \not\perp\!\!\!\perp y|x_{-j}$)
   - Only uncovers the relationships that were exploited by the model

EXTRAPOLATION: COMPARE PFI AND CFI



Recall: Let $y = x_3 + \epsilon_y$, with $\epsilon_y \sim \mathcal{N}(0, 0.1)$.

- $x_1 := \epsilon_1$, $x_2 := x_1 + \epsilon_2$ are highly correlated ($\epsilon_1 \sim \mathcal{N}(0, 1)$, $\epsilon_2 \sim \mathcal{N}(0, 0.01)$)
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- Fitting a linear model yields $\hat{f}(\mathbf{x}) \approx 0.3x_1 - 0.3x_2 + x_3$

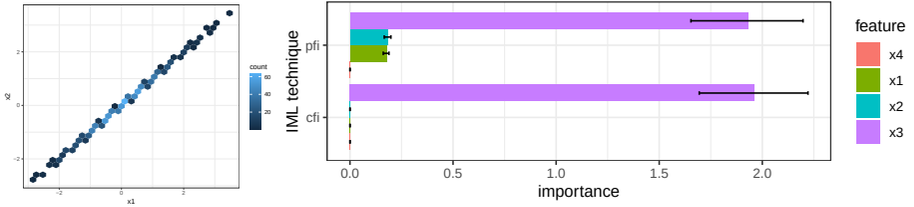

Figure: Density plot for x_1, x_2 before permuting x_1 (left). PFI and CFI (right).

- x_1 and x_2 cancel in $\hat{f}(\mathbf{x})$ and should be irrelevant for the prediction
- PFI evaluates model on unrealistic obs. $\rightsquigarrow$ x_1, x_2 appear relevant (PFI > 0)
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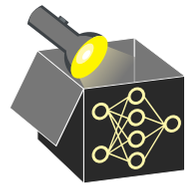

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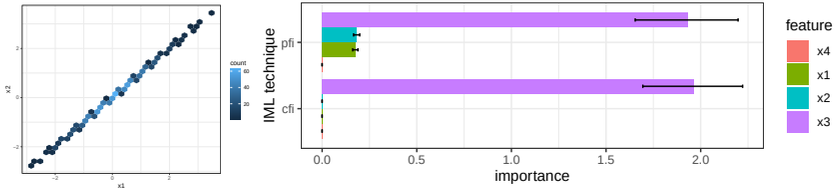

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Interpretable Machine Learning

Shapley Additive Global Importance (SAGE)

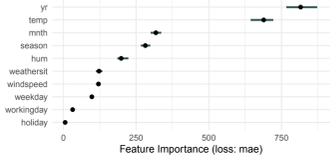

Figure: Bike Sharing Dataset

Learning goals

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

Interpretable Machine Learning

Feature Importances 1
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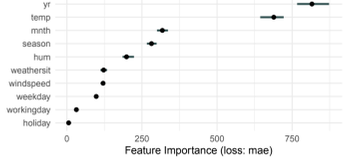

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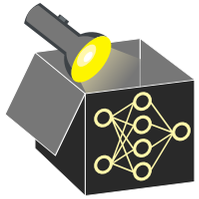
CHALLENGE: FAIR ATTRIBUTION OF IMPORTANCE



Recap:

- Data: $x_1, \ldots, x_4$ uniformly sampled from $[-1, 1]$
- DGP: $y := x_1 x_2 + x_3 + \epsilon_Y$ with $\epsilon_Y \sim N(0, 1)$
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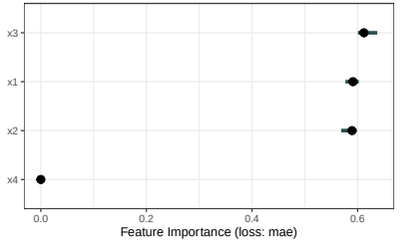

Although x_3 alone contributes as much to the prediction as x_1 and x_2 jointly, all three are considered equally relevant by PFI.

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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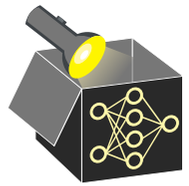

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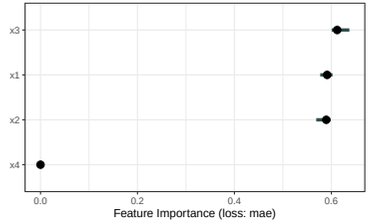

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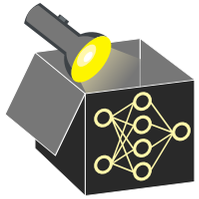
Interpretable Machine Learning – 1 / 12

SAGE IDEA

Covert et al. (2020)

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



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  $\rightsquigarrow$ features jointly contribute to achieve a certain model performance
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- 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)
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COVERT_2020

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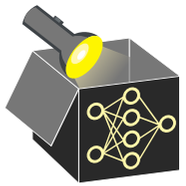

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Removal Idea: To deprive information of the non-coalition features $-S$ from the model, marginalize the prediction function over the features $-S$ to be "dropped".

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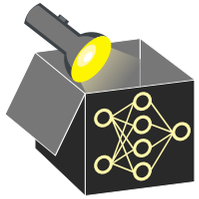

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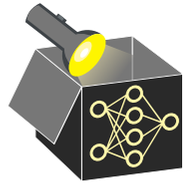

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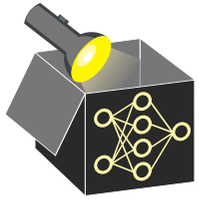

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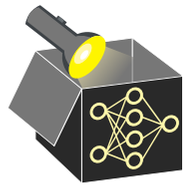

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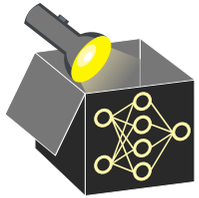

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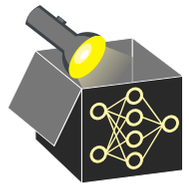

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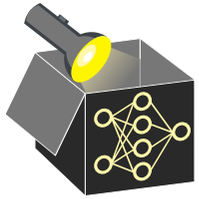

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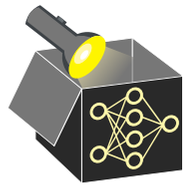

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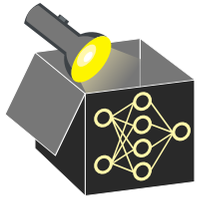

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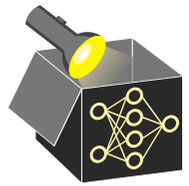

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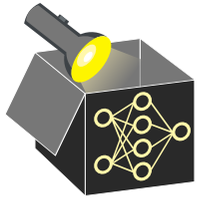

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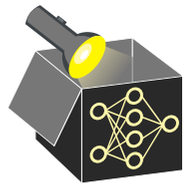

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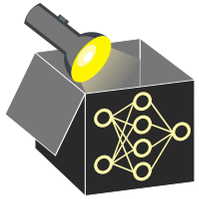

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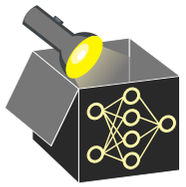

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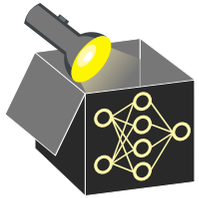

Example:

- $y = x_3 + \epsilon_y$
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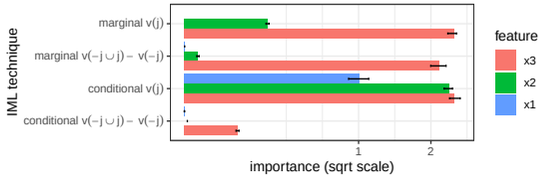

- Marginal $v(j)$ are only nonzero for features that are used by $\hat{f}$
- Conditional $v(j)$ are also nonzero for features that are not used by $\hat{f}$ (e.g., due to correlation)
- For conditional value function v, the difference $v(-j \cup j) - v(-j)$ quantifies the unique contribution of x_j over 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 $j = 3$)

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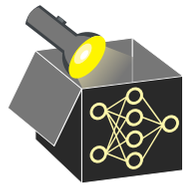

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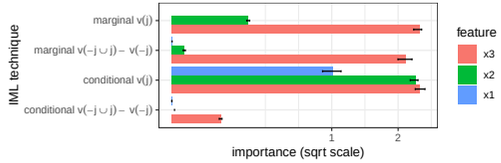

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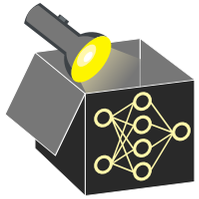
SAGE value function $v(S)$: measure contribution of a specific feature set over the empty coalition



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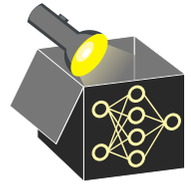

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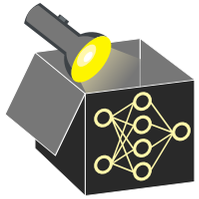

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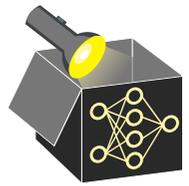

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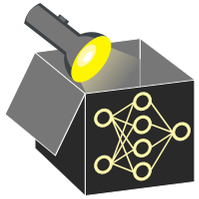

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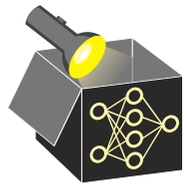

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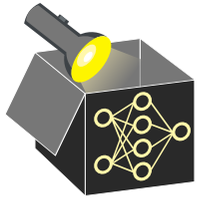

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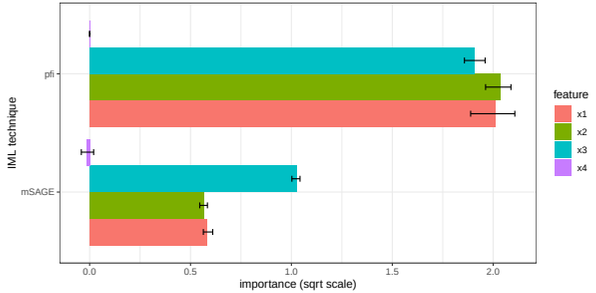

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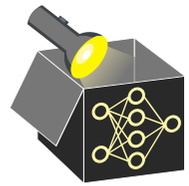

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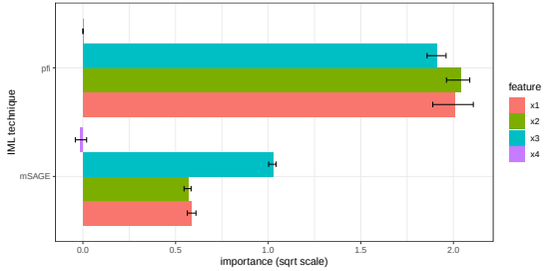

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SAGE LOSS FUNCTIONS

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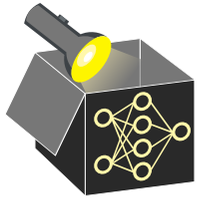

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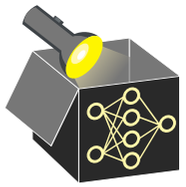

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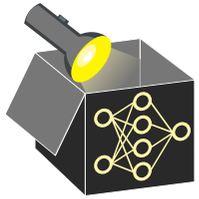

For cross-entropy loss:

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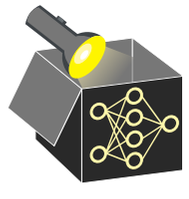

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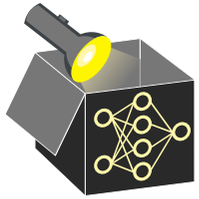

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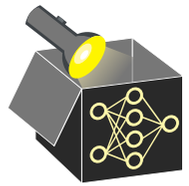

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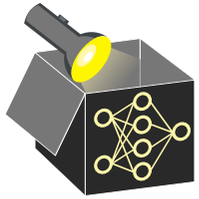

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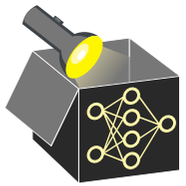

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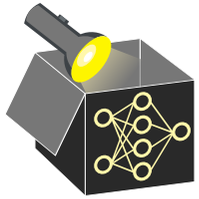

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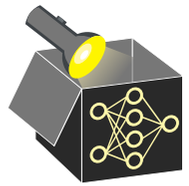

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Interpretable Machine Learning – 9 / 12

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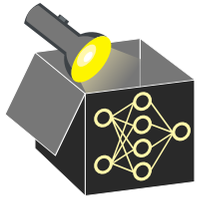

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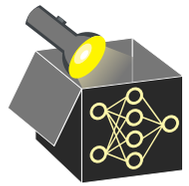

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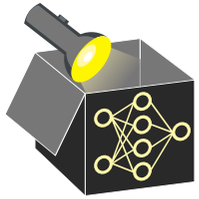

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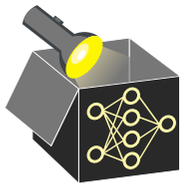

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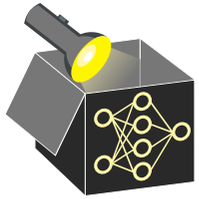

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IMPLICATIONS CONDITIONAL SAGE VALUES

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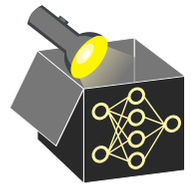

2. feature $\mathbf{x}_j$ contains prediction-relevant information about y?
   - e.g. for cross-entropy optimal $\hat{f}$, $v(j)$ measures mutual info. $I(y; x_j)$
     $\rightsquigarrow$ prediction-relevance implies nonzero ϕ_j
   - $x_j \perp\!\!\!\perp y$ does not imply $x_j \perp\!\!\!\perp y|x_S$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

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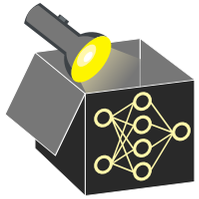

3. model requires access to x_j to achieve it's prediction performance?
   - e.g. for cross-entropy optimal $\hat{f}$, the surplus contribution $v(j \cup -j) - v(-j)$ captures the conditional mutual information $I(y; x_j | x_{-j})$
     $\rightsquigarrow \phi_j$ is nonzero for features with unique contribution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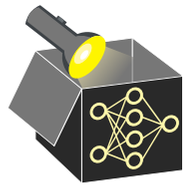

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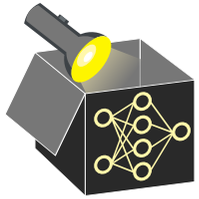
DEEP DIVE: SHAPLEY AXIOMS FOR SAGE



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	$\sum_{i=1}^{p} \phi_j(v) = \mathcal{R}(\hat{f}_\emptyset) - \mathcal{R}(\hat{f})$
symmetry	$x_j = x_i \implies \phi_i = \phi_j$
linearity	ϕ_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 $\forall S : \hat{f}(x) \perp\!\!\!\perp x_j \vert x_S \Rightarrow \phi_j = 0$

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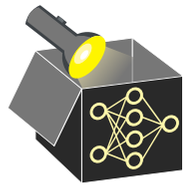

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Interpretable Machine Learning – 11 / 12

DEEP DIVE: SHAPLEY AXIOMS FOR SAGE

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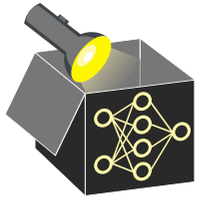

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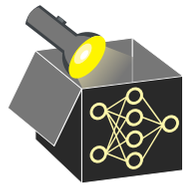


Interpretable Machine Learning – 12 / 12

Interpretable Machine Learning

Leave One Covariate Out (LOCO)

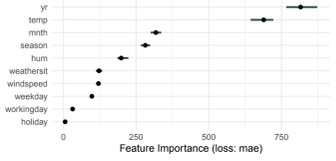
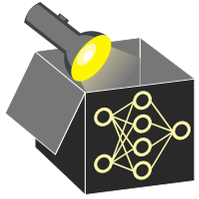


Figure: Bike Sharing Dataset

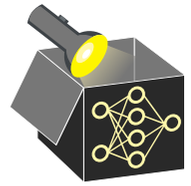
Learning goals

- Definition of LOCO
- Interpretation of LOCO



Interpretable Machine Learning

Feature Importances 1
Leave One Covariate Out (LOCO)



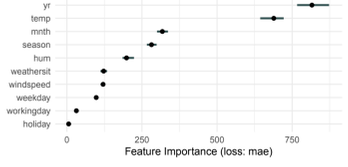


Figure: Bike Sharing Dataset

Learning goals

- Definition of LOCO
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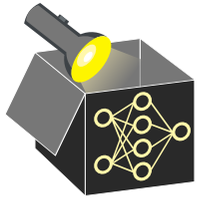
LOCO

Lei et al. (2018) Tibshirani (2018)

LOCO idea: Remove the feature from data, refit model on reduced data, and measure the loss in performance compared to model fitted on complete data.



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LEI_2018 TIBSHIRANI_2018

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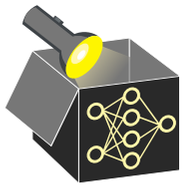

LOCO

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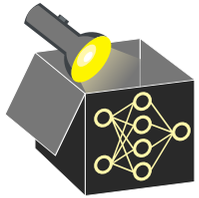

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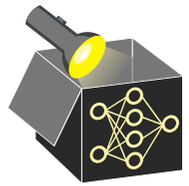
LOCO

LEI_2018 TIBSHIRANI_2018



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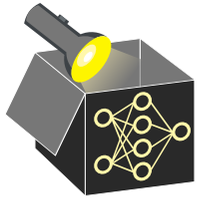

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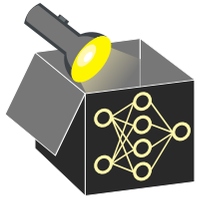

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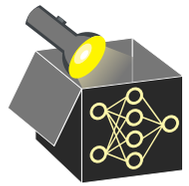

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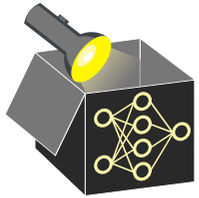

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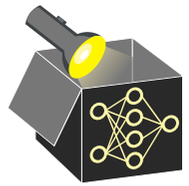

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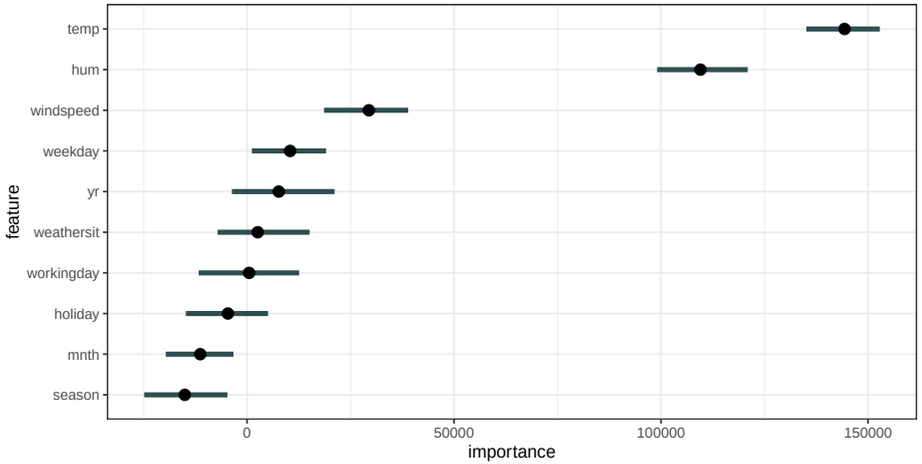
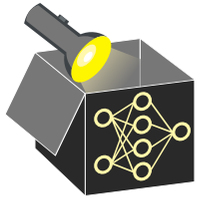
BIKE SHARING EXAMPLE





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- `temp` was most important: removing it increased MSE by approx. 140.000

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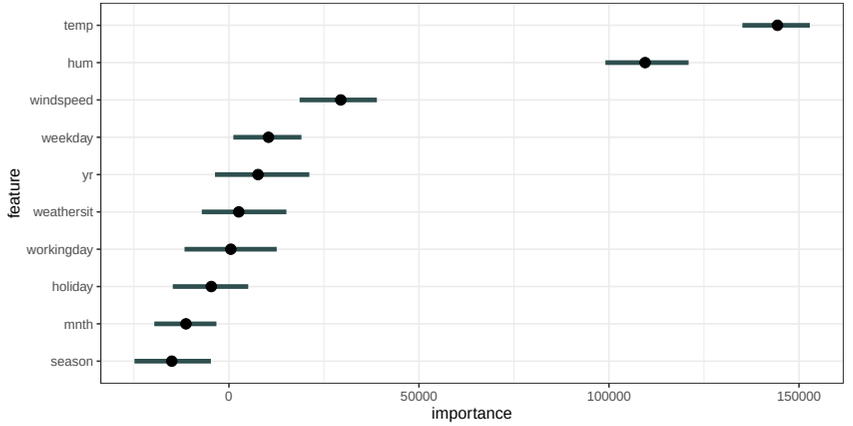

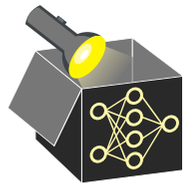

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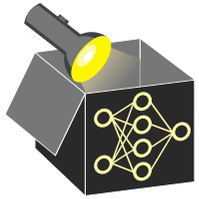
INTERPRETATION OF LOCO

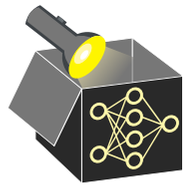


Interpretation: LOCO estimates the generalization error of the learner on a reduced dataset $\mathcal{D}_{-j}$.

Can we get insight into whether the ...

1. feature x_j is causal for the prediction $\hat{y}$?
   - In general, no also because we refit the model (counterexample next slide)
2. feature x_j contains prediction-relevant information?
   - In general, no (counterexample on the next slide)
3. model requires access to x_j to achieve its prediction performance?
   - Approximately, it provides insight into whether the *learner* requires access to x_j

INTERPRETATION OF LOCO



Interpretation: LOCO estimates the generalization error of the learner on a reduced dataset $\mathcal{D}_{-j}$.

Can we get insight into whether the ...

1. feature x_j is causal for the prediction $\hat{y}$?
   - In general, no, also because we refit the model (counterexample on the next slide)
2. feature x_j contains prediction-relevant information?
   - In general, no (counterexample on the next slide)
3. model requires access to x_j to achieve its prediction performance?
   - Approximately, it provides insight into whether the *learner* requires access to x_j

INTERPRETATION OF LOCO

Example: Sample 1000 observations with

- $x_1, x_3 \sim N(0, 5)$, $x_2 = x_1 + \epsilon_2$ with $\epsilon_2 \sim N(0, 0.1)$
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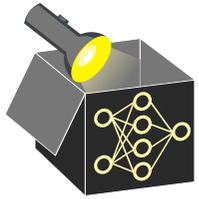

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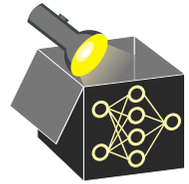

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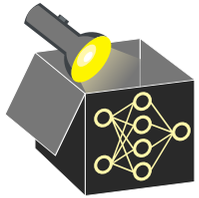

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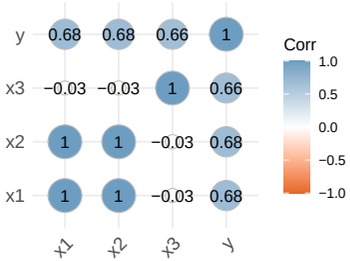

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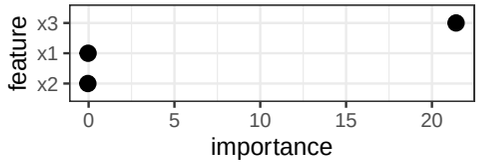

LOCO importance from LM trained on 70% of data, evaluated on remaining 30%

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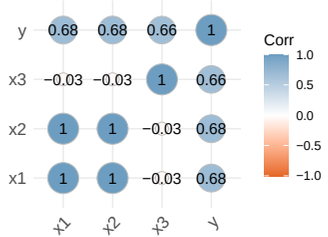

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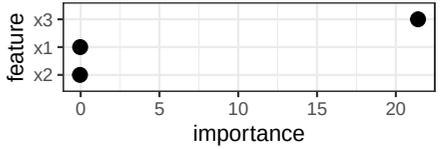

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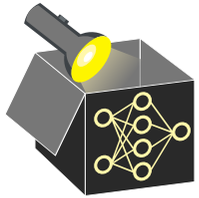

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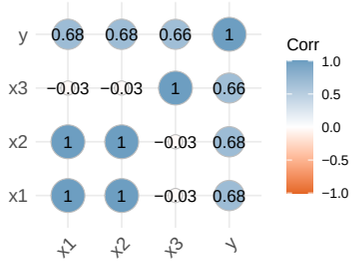

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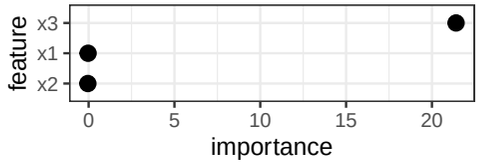

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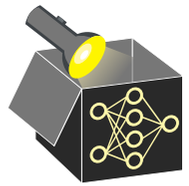

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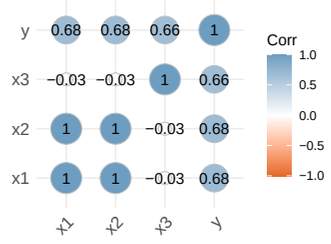

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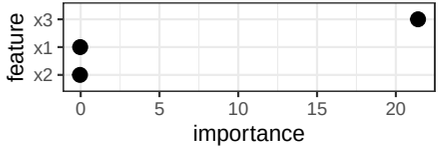

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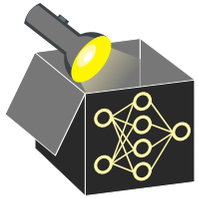

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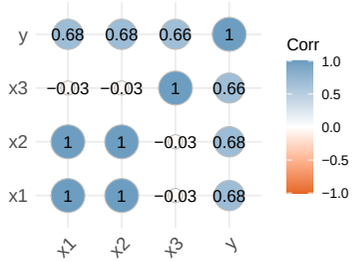

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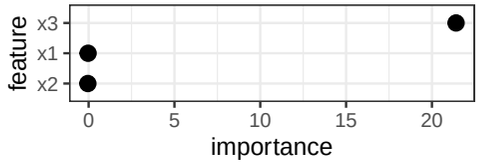

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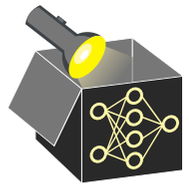

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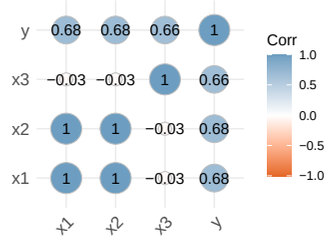

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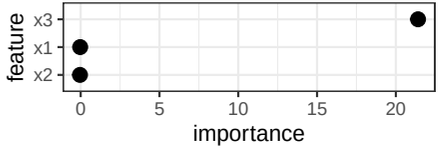

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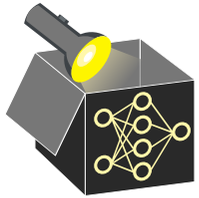

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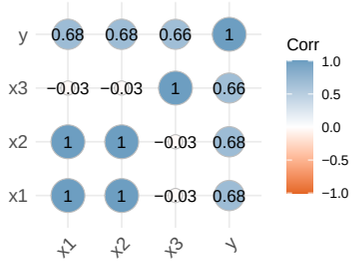

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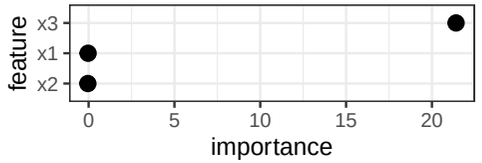

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$\rightsquigarrow$ x_2 and x_1 take each others place if one of them is left out (not the case for x_3)

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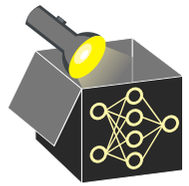

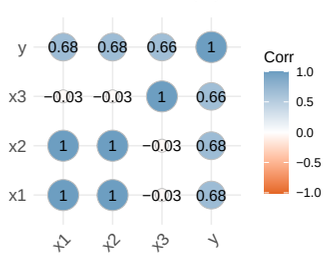

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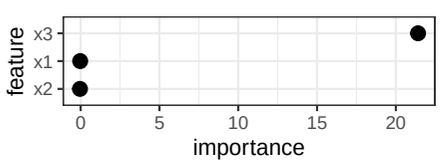

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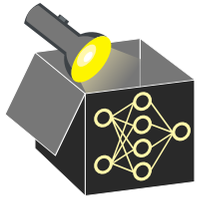
PROS AND CONS



Pros:

- Requires (only?) one refitting step per feature for evaluation
- Easy to implement
- Testing framework available in ▸ Lei et al. (2018)

Cons:

- Provides insight into a learner on specific data, not a specific model
  + for algorithm-level insight
  − for model-specific insights
- Model training is a random process and LOCO estimates can be noisy
  ⇝ Limits inference about on model and data, or multiple refittings necessary?
- Requires re-fitting the learner for each feature
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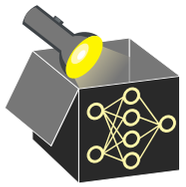

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