Interpretable Machine Learning

Permutation Feature Importance (PFI)

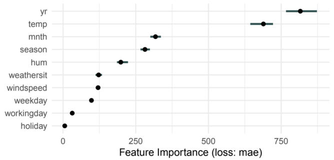


Figure: Bike Sharing Dataset

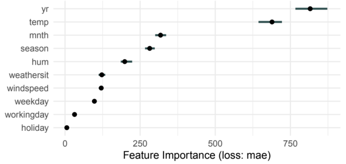
Learning goals

- Understand how PFI is computed
- Understanding strengths and weaknesses

Interpretable Machine Learning

Feature Importances 1

Permutation Feature Importance (PFI)



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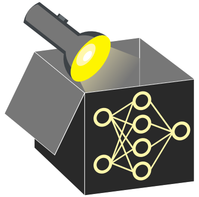
MOTIVATION FOR PFI



- **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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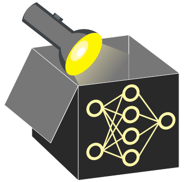

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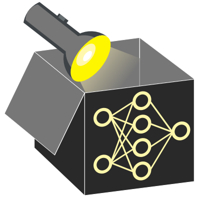

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- **Question:** Can we make X_S uninformative by removing it from the model?
  $\leadsto$ No, $\hat{f}$ was trained with X_S and retraining without X_S gives a different model

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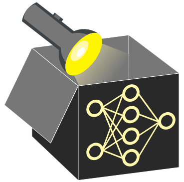

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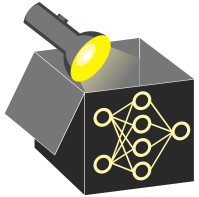

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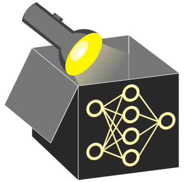
- **Question:** Can we make X_S uninformative by removing it from the model?
  $\rightsquigarrow$ No, $\hat{f}$ was trained with X_S and retraining without X_S gives a different model
- **Solution:** Simulate feature removal by replacing X_S with a perturbed version $\tilde{X}_S$ that is independent of (X_{-S}, Y) but preserves distribution $\mathbb{P}(X_S)$
  $\rightsquigarrow$ Compare baseline predictions $\hat{f}(X)$ with perturbed predictions $\hat{f}(\tilde{X}_S, X_{-S})$

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

- **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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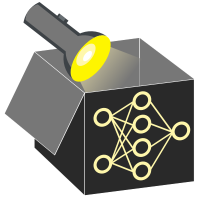
PERMUTATION FEATURE IMPORTANCE (PFI) ▸ Breiman (2001)

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:

$\mathcal{D}$

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

⇒

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

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

$\tilde{\mathcal{D}}^S_{(2)}$

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

$\tilde{\mathcal{D}}^S_{(3)}$

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

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

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

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

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

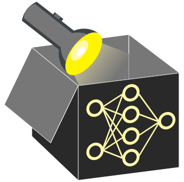
$\tilde{\mathcal{D}}^S_{(6)}$

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

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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⇒

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

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

$\tilde{\mathcal{D}}^S_{(2)}$

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

$\tilde{\mathcal{D}}^S_{(3)}$

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

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

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

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

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

$\tilde{\mathcal{D}}^S_{(6)}$

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

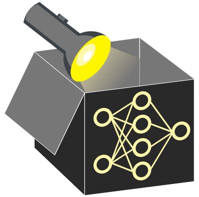
Note: S refers to a subset of features, here $|S| = 1$ to measure impact of permuting x_1 on performance

PERMUTATION FEATURE IMPORTANCE

$\tilde{\mathcal{D}}^{S}_{(k)}$ and $\mathcal{D}$

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



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 $\tilde{x}_S$

PERMUTATION FEATURE IMPORTANCE

$\mathcal{D}S_{(k)}$ and $\mathcal{D}$

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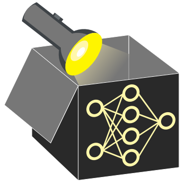

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PERMUTATION FEATURE IMPORTANCE

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i	$\mathbf{x}_S$	$\mathbf{x}_2$	$\mathbf{x}_3$
1	2	4	7
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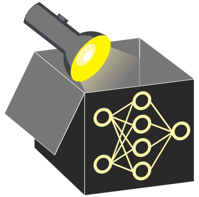
$\mathcal{D}$

$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$
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



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2. **Prediction:** Make predictions for both data, i.e., $\mathcal{D}$ and $\tilde{\mathcal{D}}^S$

PERMUTATION FEATURE IMPORTANCE

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

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0.6
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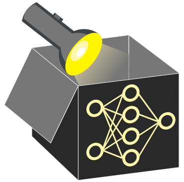

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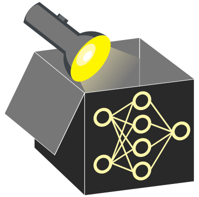


$\tilde{\mathcal{D}}^S_{(k)}$

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

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

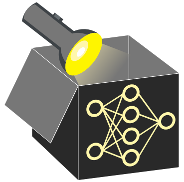
$\mathcal{D}$

$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$
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



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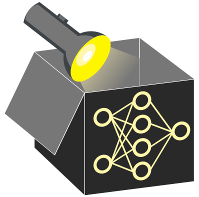
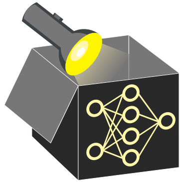


	$\tilde{\mathcal{D}}^S_{(k)}$			$\mathcal{D}$			
i	$\mathbf{x}_S$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\Delta \mathbf{L}$
1	2	4	7	1	4	7	0.65
⋮	1	5	8	2	5	8	0.15
n	3	6	9	3	6	9	0

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



	$\mathcal{D}S_{(k)}$			$\mathcal{D}$			
i	$\mathbf{x}_S$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\Delta \mathbf{L}$
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⋮	1	5	8	2	5	8	0.15
n	3	6	9	3	6	9	0

$L(\hat{f}, y)$		$L(\hat{f}, y)$
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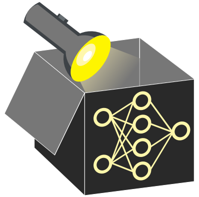
PERMUTATION FEATURE IMPORTANCE

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



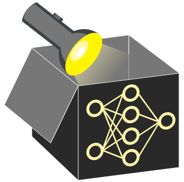
i	x_S	x_2	x_3	x_1	x_2	x_3	ΔL
1	2	4	7	1	4	7	0.65
⋮	1	5	8	2	5	8	0.15
n	3	6	9	3	6	9	0

= 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

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



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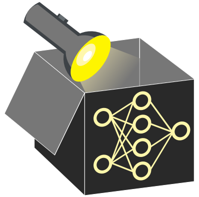
$\mathcal{R}_{\text{emp}}(\hat{f}, \tilde{\mathcal{D}}^S_{(k)}) - \mathcal{R}_{\text{emp}}(\hat{f}, \mathcal{D})$



	i	x_S	x_2	x_3	x_1	x_2	x_3	ΔL
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

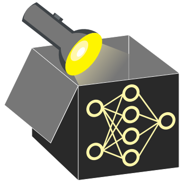
= 0.4

$\widehat{PFI}_S$ = ½ (0.267 + 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

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



	i	x_S	x_2	x_3	x_1	x_2	x_3	ΔL
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	⋮	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

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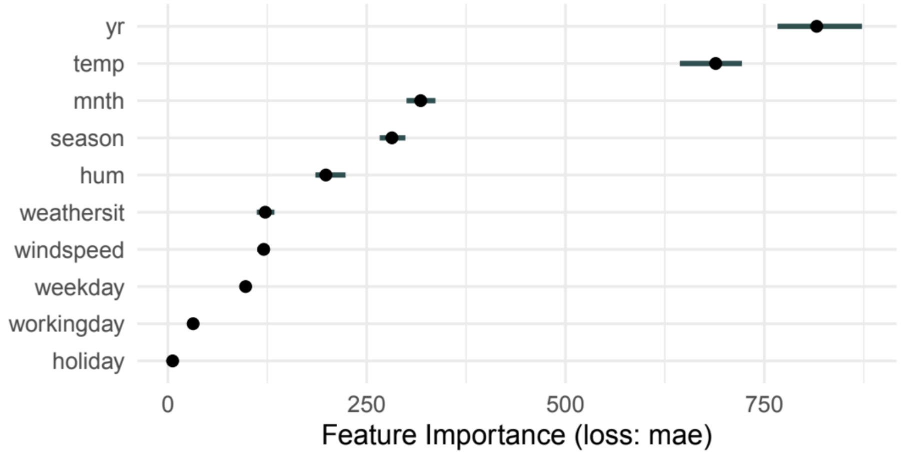
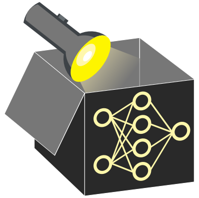
EXAMPLE: BIKE SHARING DATASET

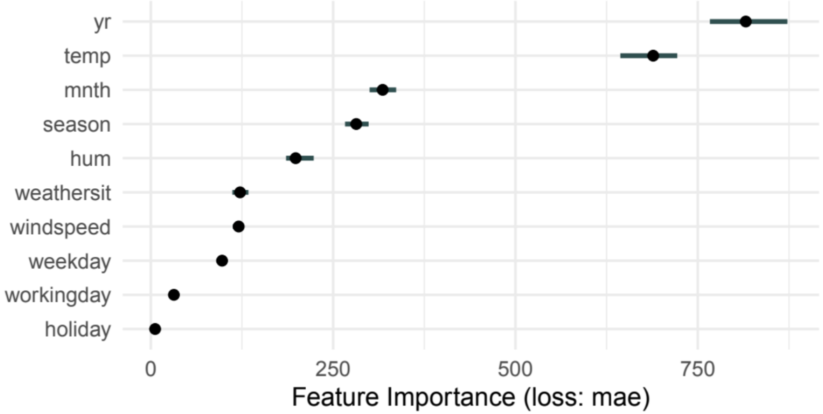


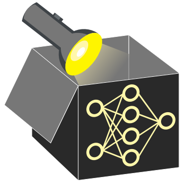


Interpretation:

- `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





Interpretation:

- `yr` and `temp` are most important feats using mean absolute error (MAE)
- Destroying info. about `yr` by permuting it increases MAE of model by 816
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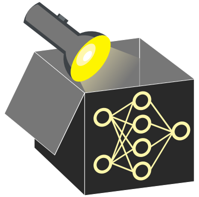

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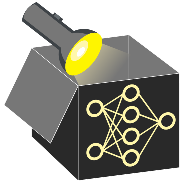

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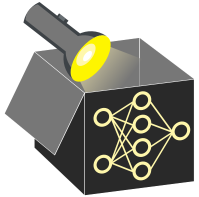

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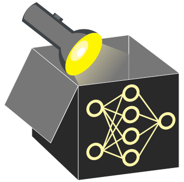

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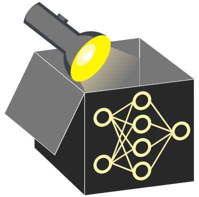

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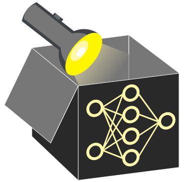

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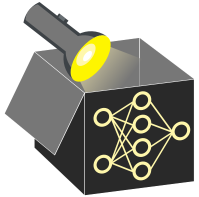

Example: Let $y = x_3 + \epsilon_y$, with $\epsilon_y \sim \mathcal{N}(0, 0.1)$.

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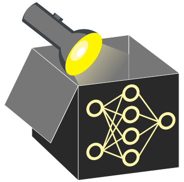

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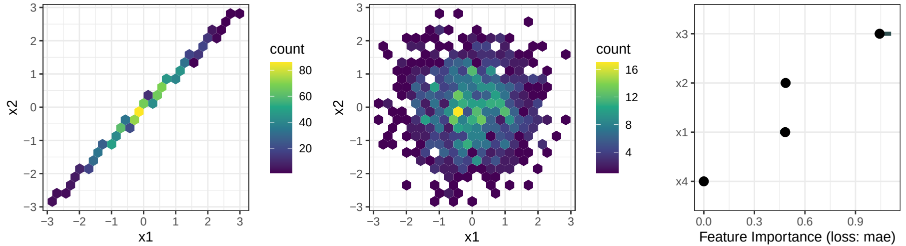

Hexbin plot of (x_1, x_2) before (left) and after (center) permuting x_1; PFI scores (right).

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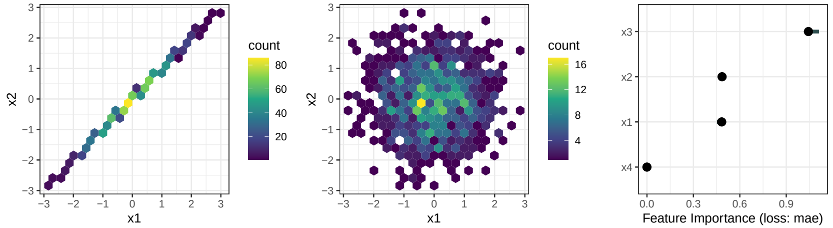

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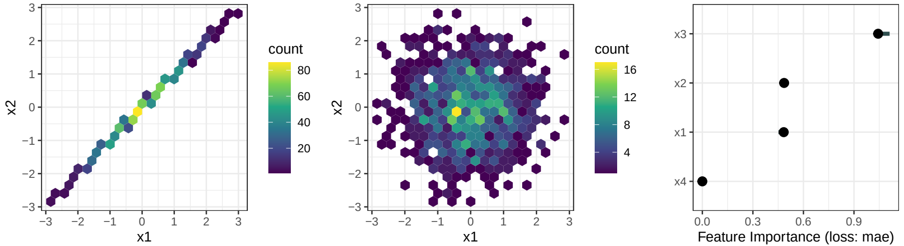

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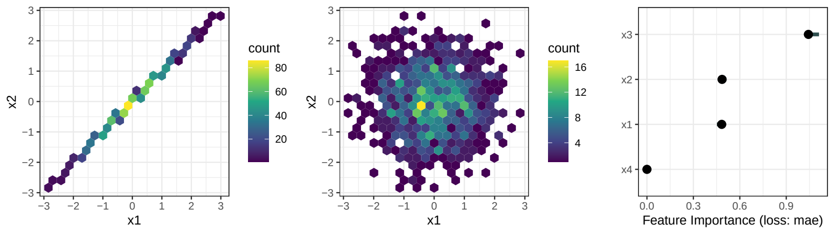

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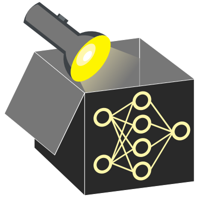

Example: Let $x_1, \dots, x_4$ be independently and uniformly sampled from $\{-1, 1\}$ and

$$y := x_1 x_2 + x_3 + \epsilon_Y \text{ with } \epsilon_Y \sim N(0, 1)$$

Fitting a LM yields $\hat{f}(x) \approx x_1 x_2 + x_3$.

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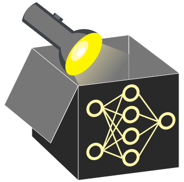

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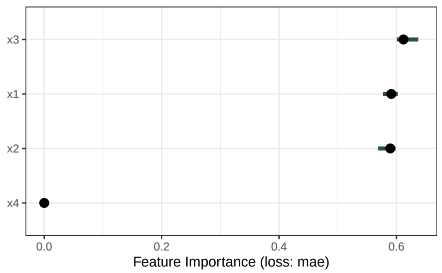

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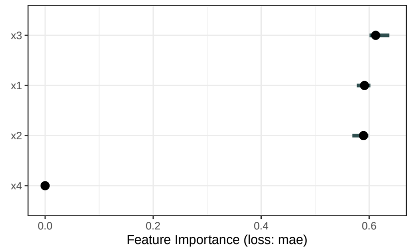

COMMENTS ON PFI - TRAIN VS. TEST DATA

Example:

- $x_1, \dots, x_{20}, y$ are independently sampled from $\mathcal{U}(-10, 10)$
- Train set: $n = 50$ (intentionally small) and large test set
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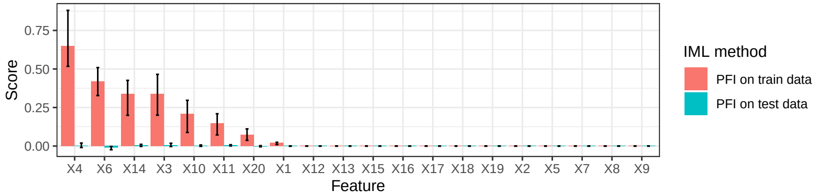

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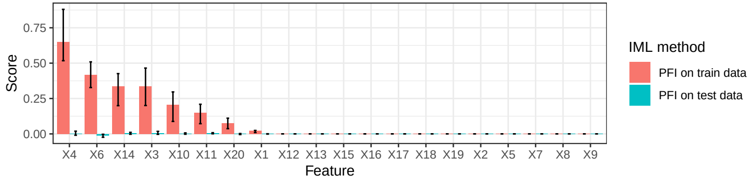

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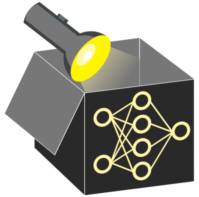

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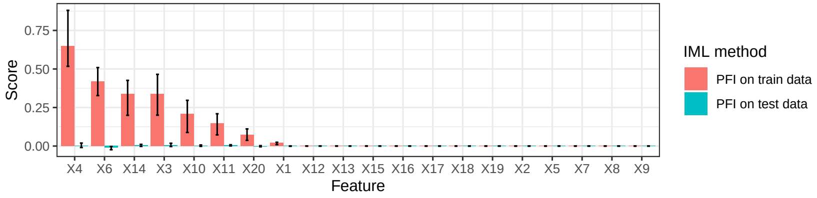

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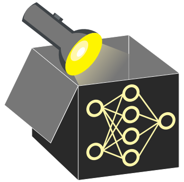

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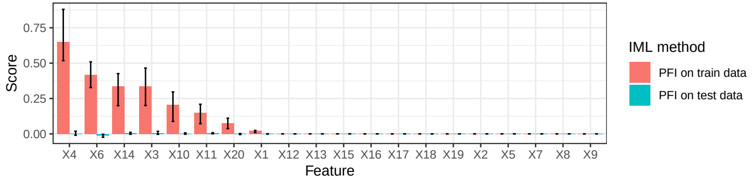

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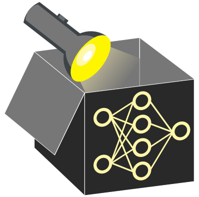

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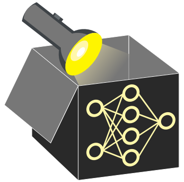

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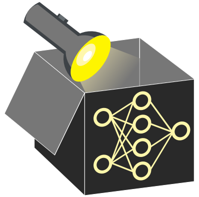

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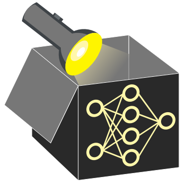

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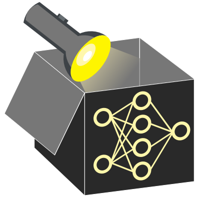

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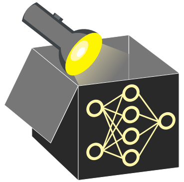

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