Interpretable Machine Learning

Conditional Feature Importance (CFI)

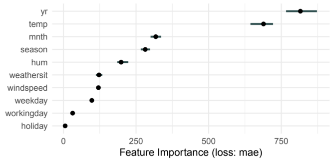


Figure: Bike Sharing Dataset

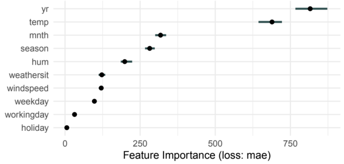
Learning goals

- 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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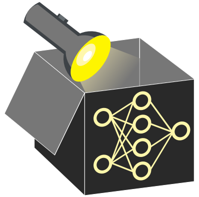
CFI MOTIVATION



- **PFI Idea:** Replace feature(s) X_S with perturbed $\tilde{X}_S$ to preserve marginal distibution $\mathbb{P}(X_S)$ so that $\tilde{X}_S \perp\!\!\!\perp Y$ (independent), e.g., by random permutations

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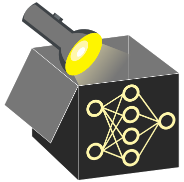

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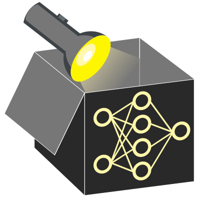

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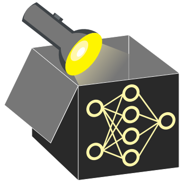

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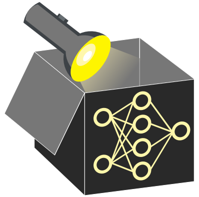

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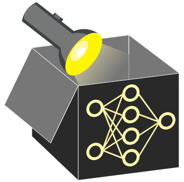

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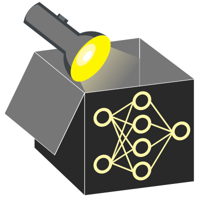

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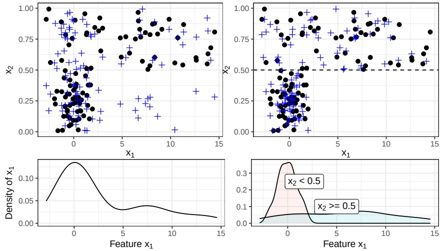
Example: Conditional permutation scheme
Black dots: $X_2 \sim \mathcal{U}(0,1)$ and $X_1 \sim \mathcal{N}(0,1)$ (if $X_2 < 0.5$) or $\mathcal{N}(4,4)$ (if $X_2 \geq 0.5$)



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)

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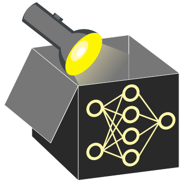

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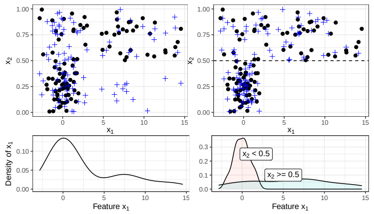

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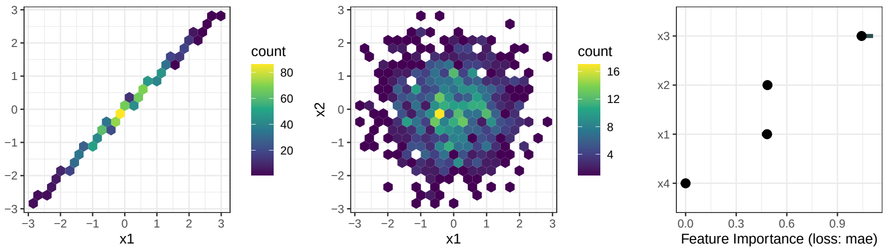
RECALL: EXTRAPOLATION IN PFI

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

$\Rightarrow$ But PFI evaluates model on unrealistic inputs (caused by permutation)

- $\rightsquigarrow$ *PFI* > 0 for x_1, x_2 due to extrapolation
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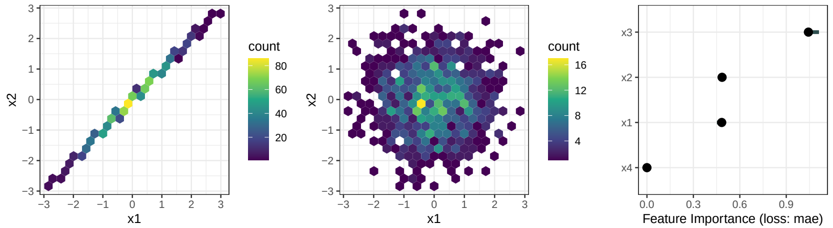

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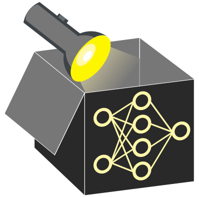
CFI ‣ Strobl et al. (2008) ‣ Hooker et al. (2021)



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
5	B	5.4
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Permuted Conditionally on X_{-S}

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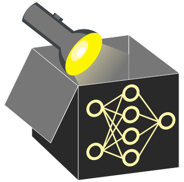

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IMPLICATIONS OF CFI ▸ König et al. (2020)

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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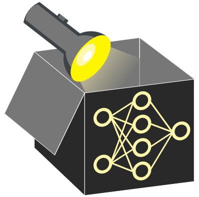

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- If feature x_S does not contribute unique information about y, i.e., $x_S \perp\!\!\!\perp y | x_{-S}$ $\Rightarrow$ CFI $= 0$
- Why? Under the conditional independence $\mathbb{P}(\tilde{X}_S, X_{-S}, Y) = \mathbb{P}(X_S, X_{-S}, Y)$ $\rightsquigarrow$ no prediction-relevant information is destroyed by permutation of x_S conditional on x_{-S}

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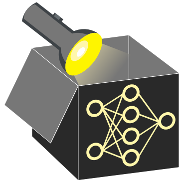

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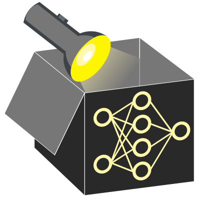

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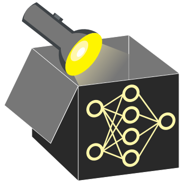

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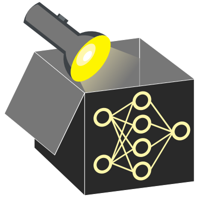

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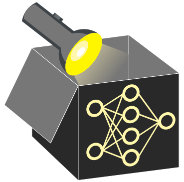

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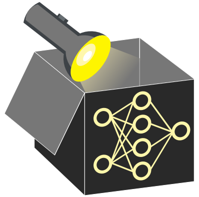

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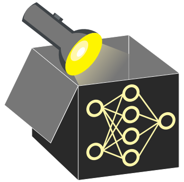

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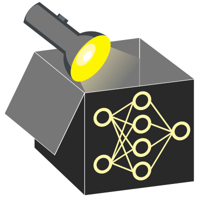

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   - $CFI_j \neq 0 \Rightarrow x_j$ contributes unique information (meaning $x_j \not\perp\!\!\!\perp y | x_{-j}$)
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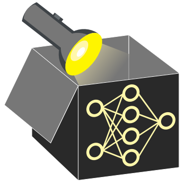

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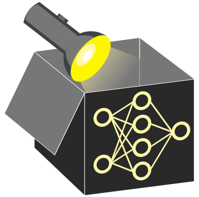
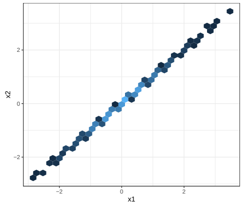
EXTRAPOLATION: COMPARE PFI AND CFI



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



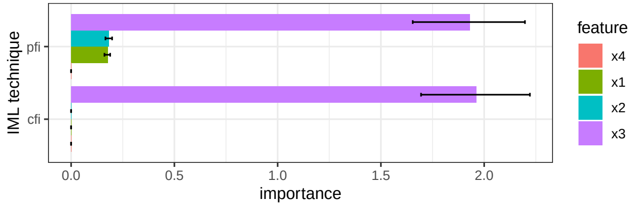
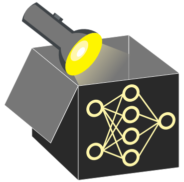


Figure: Density plot for x_1, x_2 before permuting x_1 (left). PFI and CFI (right).

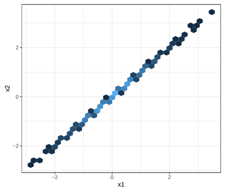
- x_1 and x_2 cancel in $\hat{f}(\mathbf{x})$ and should be irrelevant for the prediction
- PFI evaluates model on unrealistic obs. $\rightsquigarrow$ x_1, x_2 appear relevant (PFI > 0)
- CFI evaluates model on realistic obs. (due to conditional sampling) $\rightsquigarrow$ x_1, x_2 appear irrelevant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

EXTRAPOLATION: COMPARE PFI AND CFI



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

- $x_1 := \epsilon_1$, $x_2 := x_1 + \epsilon_2$; 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 $\epsilon_3, \epsilon_4 \sim \mathcal{N}(0, 1)$; all noise terms ϵ_j are indep.
- Fitting a linear model yields $\hat{f}(\mathbf{x}) \approx 0.3x_1 - 0.3x_2 + x_3$



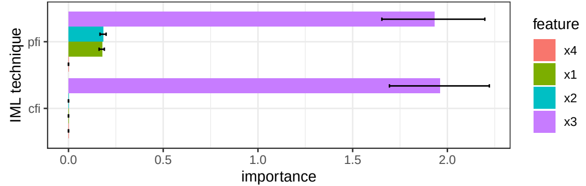


Figure: Density plot for x_1, x_2 before permuting x_1 (left). PFI and CFI (right).

- 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)
- CFI evaluates model on realistic obs. (due to conditional sampling) $\rightsquigarrow$ x_1, x_2 appear irrelevant (CFI $= 0$)