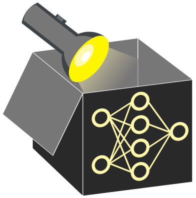
Interpretable Machine Learning

Conditional Feature Importance (CFI)



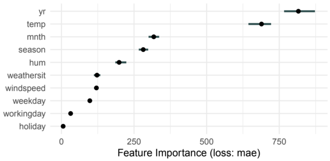
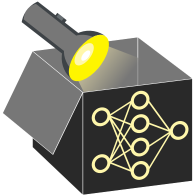


Figure: Bike Sharing Dataset

Learning goals

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

CONDITIONAL FEATURE IMPORTANCE IDEA



- **Permutation Feature Importance Idea:** Replace the feat. of interest x_j with an indep. sample from the marginal dist. $\mathbb{P}(x_j)$, e.g. by randomly perm. obs. in x_j

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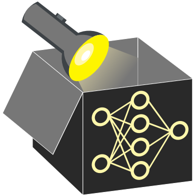

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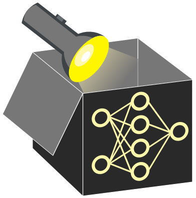

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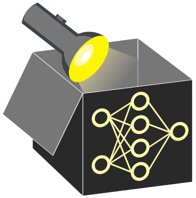

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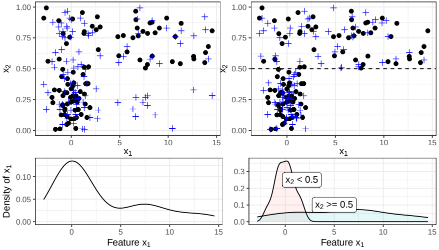
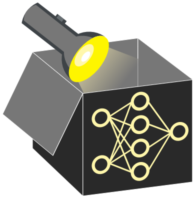
Example: Conditional permutation scheme ▸ Molnar et. al (2020)

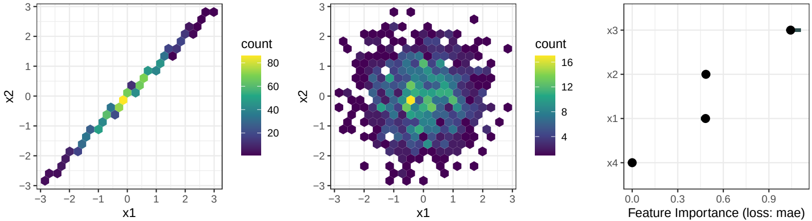


- $X_2 \sim U(0,1)$ and $X_1 \sim N(0,1)$ if $X_2 < 0.5$, else $X_1 \sim N(4,4)$ (black dots)
- **Left:** For $X_2 < 0.5$, permuting X_1 (crosses) preserves marginal (but not joint) distribution
  $\rightsquigarrow$ Bottom: Marginal density of X_1
- **Right:** Permuting X_1 within subgroups $X_2 < 0.5$ & $X_2 \geq 0.5$ reduces extrapolation
  $\rightsquigarrow$ Bottom: Density of X_1 conditional on groups

RECALL: EXTRAPOLATION IN PFI



Example: Let $y = x_3 + \epsilon_y$ with $\epsilon_y \sim N(0, 0.1)$ where $x_1 := \epsilon_1$, $x_2 := x_1 + \epsilon_2$ are highly correlated ($\epsilon_1 \sim N(0,1), \epsilon_2 \sim N(0, 0.01)$) and $x_3 := \epsilon_3$, $x_4 := \epsilon_4$, with $\epsilon_3, \epsilon_4 \sim N(0,1)$. All noise terms are independent. Fitting a LM yields $\hat{f}(\mathbf{x}) \approx 0.3x_1 - 0.3x_2 + x_3$.

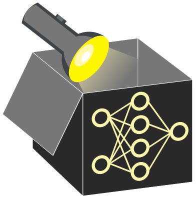


Hexbin plot of x_1, x_2 before permuting x_1 (left), after permuting x_1 (center), and PFI scores (right) $\Rightarrow$ x_1 and x_2 should be irrelevant for the prediction $\hat{f}(\mathbf{x})$ for

$\{\mathbf{x} : \mathbb{P}(\mathbf{x}) > 0\}$ as $0.3x_1 - 0.3x_2 \approx 0$
$\Rightarrow$ PFI evaluates model on unrealistic obs. outside $\mathbb{P}(\mathbf{x})$ $\rightsquigarrow$ x_1 and x_2 are considered relevant

CONDITIONAL FEATURE IMPORTANCE ▸ Strobl et al. (2008)

▸ Hooker et al. (2021)



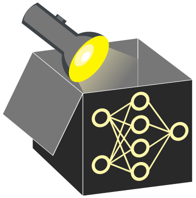
Conditional feature importance (CFI) for features x_S using test data $\mathcal{D}$:

- Measure the error **with unperturbed features**.
- Measure the error **with perturbed feature values** $\tilde{x}^{S|-S}$, where $\tilde{x}_S^{S|-S} \sim \mathbb{P}(x_S|x_{-S})$
- Repeat permuting the feature (e.g., m times) and average the 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 the dataset where features x_S where sampled conditional on the remaining features x_{-S}.

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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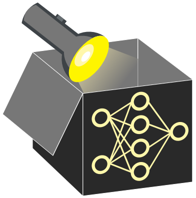

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- If feature x_S does not contribute unique information about y, i.e., $x_S \perp\!\!\!\perp y | x_{-S} \Rightarrow$ CFI $= 0$
- Why? Under the conditional independence $\mathbb{P}(\tilde{x}^{S|-S}, y) = \mathbb{P}(x, y)$ $\rightsquigarrow$ no prediction-relevant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

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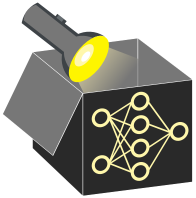

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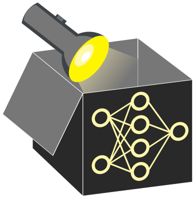
Entanglement with model:

- If the model does not use a feature $\Rightarrow$ CFI $= 0$
- Why? Then the prediction is not affected by any perturbation of the feature
  $\rightsquigarrow$ model performance does not change after conditional permutation

IMPLICATIONS OF CFI



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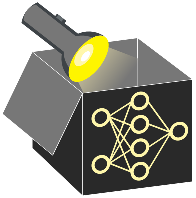

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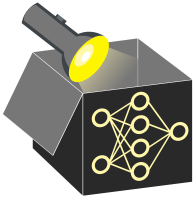

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3. Does the model require access to x_j to achieve its prediction performance?
   - $CFI_j \neq 0 \Rightarrow x_j$ contributes unique information (meaning $x_j \not\perp\!\!\!\perp y | x_{-j}$)
   - Only uncovers the relationships that were exploited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

COMPARISON: PFI AND CFI

Example: Let $y = x_3 + \epsilon_y$ with $\epsilon_Y \sim N(0, 0.1)$ where $x_1 := \epsilon_1$, $x_2 := x_1 + \epsilon_2$ are highly correlated ($\epsilon_1 \sim N(0, 1), \epsilon_2 \sim N(0, 0.01)$) and $x_3 := \epsilon_3$, $x_4 := \epsilon_4$, with $\epsilon_3, \epsilon_4 \sim N(0, 1)$. All noise terms are independent. Fitting a LM yields $\hat{f}(\mathbf{x}) \approx 0.3x_1 - 0.3x_2 + x_3$.

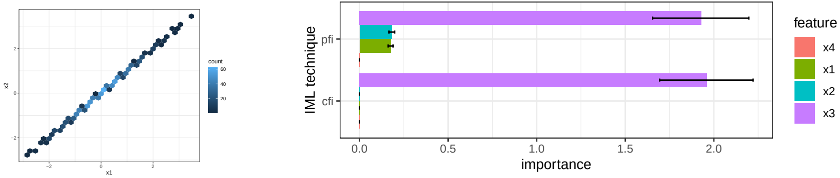

Figure: Density plot for x_1, x_2 before permuting x_1 (left). PFI and CFI (right).

$\Rightarrow$ x_1 and x_2 are irrelevant for the prediction $\hat{f}(\mathbf{x})$ for $\{\mathbf{x} : \mathbb{P}(\mathbf{x}) > 0\}$ as $0.3x_1 - 0.3x_2 \approx 0$

$\Rightarrow$ PFI evaluates model on unrealistic obs. outside $\mathbb{P}(\mathbf{x}) \rightsquigarrow x_1, x_2$ are considered relevant (PFI > 0)

$\Rightarrow$ Since x_1 can be reconstructed from x_2 and vice versa, CFI considers x_1 and x_2 to be irrelevant