Interpretable Machine Learning

Conditional Feature Importance (CFI)

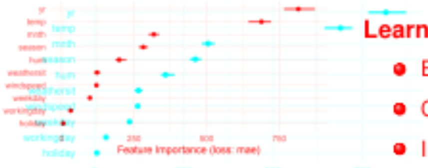


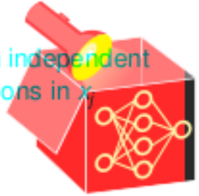
Figure: Bike Sharing Dataset

Learning goals

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

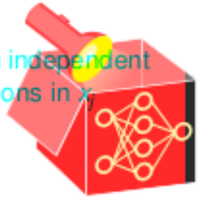
Learning goals
Extrapolation and Conditional Sampling
Conditional Feature Importance (CFI)
Interpretation of CFI and difference to PFI
Figure: Bike Sharing Dataset

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

CONDITIONAL FEATURE IMPORTANCE IDEA

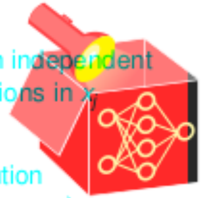


- **Permutation Feature Importance Idea:** Replace the feat. of interest x_j with an indep. sample from the marginal dist. $\mathbb{P}(x_j)$, e.g. by randomly perm. obs. in x_j
- **Problem:** Under dependent features, permutation leads to extrapolation

- **Permutation Feature Importance Idea:** Replace the feature of interest x_j with an independent sample from the marginal distribution $\mathbb{P}(x_j)$, e.g. by randomly permuting observations in x_j
- **Problem:** Under dependent features, permutation leads to extrapolation

Interpretable Machine Learning – 1 / 6

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
- **Problem:** Under dependent features, permutation leads to extrapolation
- **Conditional Feature Importance Idea:** Resample x_j from the cond. dist. $\mathbb{P}(x_j|x_{-j})$, s.t. the joint dist. is preserved, i.e., $\mathbb{P}(x_j|x_{-j})\mathbb{P}(x_{-j}) = \mathbb{P}(x_j, x_{-j})$

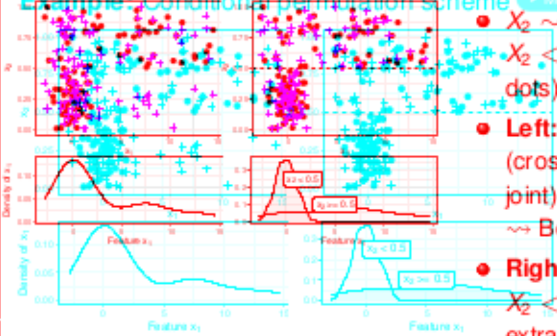
- **Permutation Feature Importance Idea:** Replace the feature of interest x_j with an independent sample from the marginal distribution $\mathbb{P}(x_j)$, e.g. by randomly permuting observations in x_j
- **Problem:** Under dependent features, permutation leads to extrapolation
- **Conditional Feature Importance Idea:** Resample x_j from the conditional distribution $\mathbb{P}(x_j|x_{-j})$, such that the joint distribution is preserved, i.e., $\mathbb{P}(x_j|x_{-j})\mathbb{P}(x_{-j}) = \mathbb{P}(x_j, x_{-j})$

Interpretable Machine Learning – 1 / 6

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
- **Problem:** Under dependent features, permutation leads to extrapolation
- **Conditional Feature Importance Idea:** Resample x_j from the cond. dist. $\mathbb{P}(x_j|x_{-j})$, s.t. the joint dist. is preserved, i.e., $\mathbb{P}(x_j|x_{-j})\mathbb{P}(x_{-j}) = \mathbb{P}(x_j, x_{-j})$

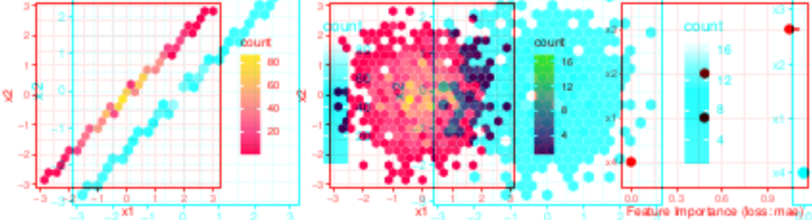
Example: Conditional permutation scheme ▸ Molnar et. al (2020)



- $X_2 \sim U(0,1)$ 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
  $\leadsto$ Bottom: Marginal density of X_1
- **Right:** Permuting X_1 within subgroups $X_2 < 0.5$ & $X_2 \geq 0.5$ reduces extrapolation
  $\leadsto$ 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}.

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}.

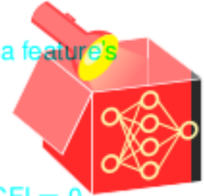
Interpretable Machine Learning – 3 / 6

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.

Interpretable Machine Learning – 4 / 6

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.

Entanglement with data:

- If feature x_S does not contribute unique information about y, i.e., $x_S \perp\!\!\!\perp y \mid x_{-S} \Rightarrow$ 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}

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.

Entanglement with data:

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

Entanglement with model:

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

IMPLICATIONS OF CFI

Can we gain insight into whether ...

1. the feature x_j is causal for the prediction?
   - $CFI_j \neq 0 \Rightarrow$ model relies on x_j (converse does not hold, see next slide)

Interpretable Machine Learning – 5 / 6

IMPLICATIONS OF CFI

Can we gain insight into whether ...

1. the feature x_j is causal for the prediction?
   - $CFI_j \neq 0 \Rightarrow$ model relies on x_j (converse does not hold, see next slide)
2. the variable x_j contains prediction-relevant information?
   - If $x_j \not\perp\!\!\!\perp y$ but $x_j \perp\!\!\!\perp y | x_{-j}$ (e.g., x_j and x_{-j} share information) $\Rightarrow CFI_j = 0$
   - x_j is not exploited by model (regardless of whether it is useful for y or not) $\Rightarrow CFI_j = 0$

Interpretable Machine Learning – 5 / 6

IMPLICATIONS OF CFI

Can we gain insight into whether ...

1. the feature x_j is causal for the prediction?
   - $CFI_j \neq 0 \Rightarrow$ model relies on x_j (converse does not hold, see next slide)
2. the variable x_j contains prediction-relevant information?
   - If $x_j \not\perp y$ but $x_j \perp y | x_{-j}$ (e.g., x_j and x_{-j} share information) $\Rightarrow CFI_j = 0$
   - x_j is not exploited by model (regardless of whether it is useful for y or not) $\Rightarrow CFI_j = 0$
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 $x_j \not\perp y | x_{-j}$)
   - 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 $\hat{f}(\mathbf{x}) \approx 0.3x_1 - 0.3x_2 + x_3$.

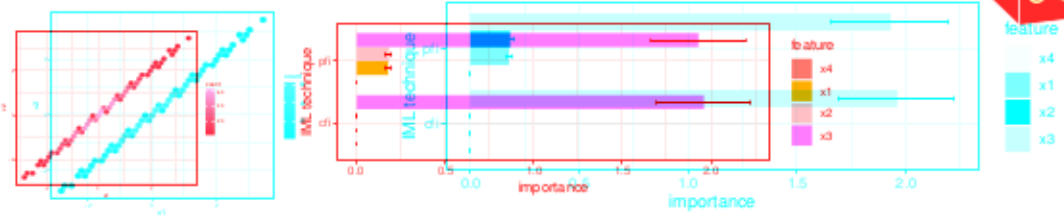


Figure: Density plot for x_1, x_2 before permuting x_1 (left). PFI and CFI (right).

$\Rightarrow$ 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