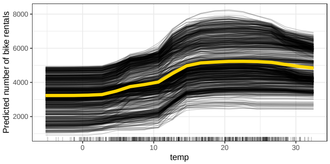
Interpretable Machine Learning

PDP - Comments and Extensions

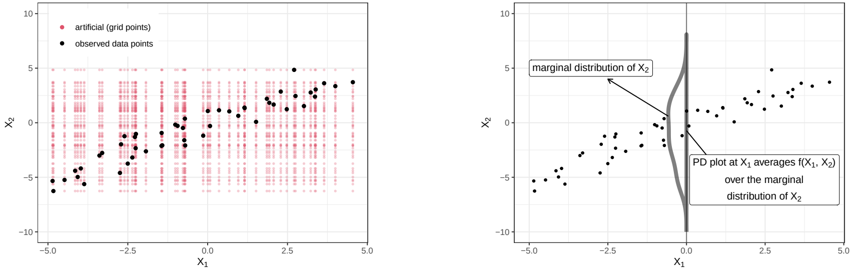


Learning goals

- PD plots and relation to ICE plots
- Interpretation of PDP
- Extrapolation and Interactions in PDPs
- Centered ICE and PDP

COMMENTS ON EXTRAPOLATION

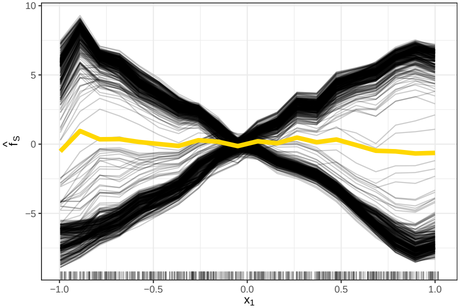
Extrapolation can cause issues in regions with few observations or if features are correlated



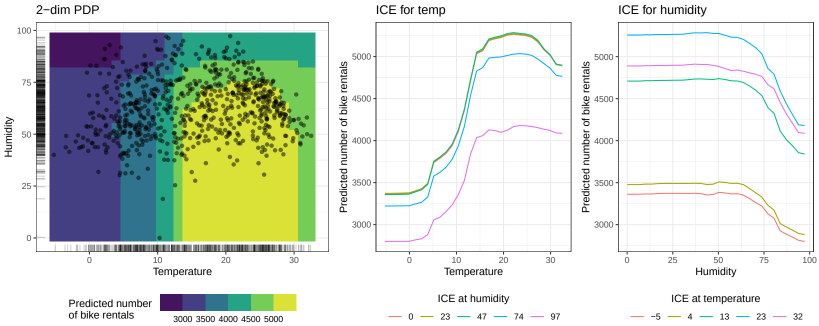
- **Example:** Features x_1 and x_2 are strongly correlated
- **Black points:** Observed points of the original data
- **Red:** Grid points used to calculate the ICE and PD curves (several unrealistic values)
  $\Rightarrow$ PD plot at $x_1 = 0$ averages predictions over the whole marginal distribution of feature x_2
  $\Rightarrow$ May be problematic if model behaves strange outside training distribution

COMMENTS ON INTERACTIONS

- PD plots: averaging of ICE curves might **obfuscate** heterogeneous effects and interactions
  ⇒ Ideally plot ICE curves and PD plots together to uncover this fact
  ⇒ Different shapes of ICE curves suggest interaction (but do not tell with which feature)



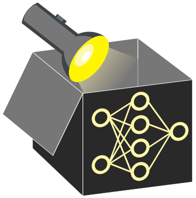
COMMENTS ON INTERACTIONS - 2D PARTIAL DEPENDENCE



- Humidity and temperature interact with each other at high values (see shape difference)
  $\rightsquigarrow$ Shape of ICE curves at different horizontal and vertical slices varies (for high values)
- Low to medium humidity and high temperature $\Rightarrow$ many rented bikes

CENTERED ICE PLOT (C-ICE)

Goldstein et al. (2015)



Issue: Difficult to identify heterogenous ICE curves if curves have different intercepts (are stacked)
Solution: Center ICE curves at fixed reference value $x' \sim \mathbb{P}(\mathbf{x}_S)$, often $x' = \min(\mathbf{x}_S)$
$\Rightarrow$ Easier to identify heterogenous shapes with c-ICE curves

$$\begin{aligned} \hat{f}^{(i)}_{S,cICE}(\mathbf{x}_S) &= \hat{f}(\mathbf{x}_S, \mathbf{x}^{(i)}_{-S}) - \hat{f}(x', \mathbf{x}^{(i)}_{-S}) \\ &= \hat{f}^{(i)}_S(\mathbf{x}_S) - \hat{f}^{(i)}_S(x') \end{aligned}$$

$\Rightarrow$ Visualize $\hat{f}^{(i)}_{S,cICE}(\mathbf{x}^*_S)$ vs. $\mathbf{x}^*_S$

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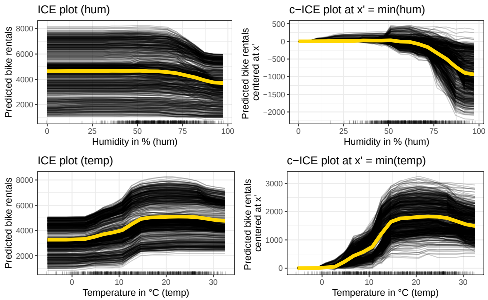
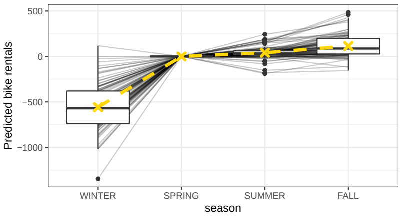


Interpretation

(yellow curve: analog to PDP the average of c-ICE curves):
On average, the number of bike rentals at $\sim$ 97 % humidity decreased by 1000 bikes compared to a humidity of 0 %

CENTERED ICE PLOT (C-ICE)

For categorical features, c-ICE plots can be interpreted as in LMs due to reference value



Interpretation:

- The reference category is $x' =$ SPRING
- Golden crosses: Average number of bike rentals if we jump from SPRING to any other season
  $\Rightarrow$ Number of bike rentals drops by $\sim$ 560 in WINTER and is slightly higher in SUMMER and FALL compared to SPRING