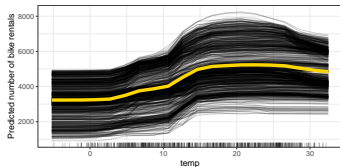
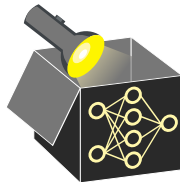


Interpretable Machine Learning

Feature Effects

Partial Dependence (PD) plot



Learning goals

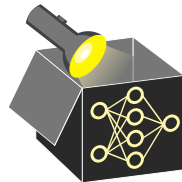
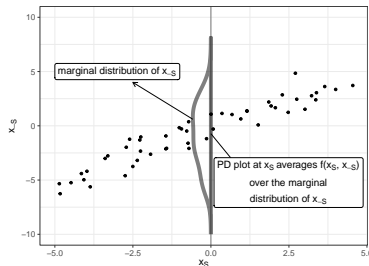
- PD plots and relation to ICE plots
- Interpretation of PDP

PARTIAL DEPENDENCE (PD)

► “Friedman” 2001

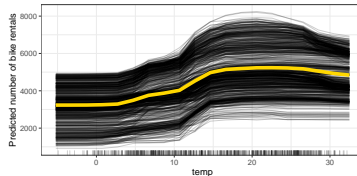
Definition: PD function is expectation of $\hat{f}(\mathbf{x}_S, \mathbf{x}_{-S})$ w.r.t. marginal distribution of features \mathbf{x}_{-S} :

$$\begin{aligned} f_{S,PD}(\mathbf{x}_S) &= \mathbb{E}_{\mathbf{x}_{-S}} \left(\hat{f}(\mathbf{x}_S, \mathbf{x}_{-S}) \right) \\ &= \int_{-\infty}^{\infty} \hat{f}(\mathbf{x}_S, \mathbf{x}_{-S}) d\mathbb{P}(\mathbf{x}_{-S}) \end{aligned}$$

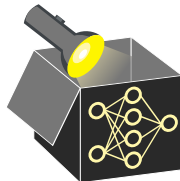


Estimation: For a grid value \mathbf{x}_S^* , average ICE curves point-wise at \mathbf{x}_S^* over all observed $\mathbf{x}_{-S}^{(i)}$:

$$\begin{aligned} \hat{f}_{S,PD}(\mathbf{x}_S^*) &= \frac{1}{n} \sum_{i=1}^n \hat{f}(\mathbf{x}_S^*, \mathbf{x}_{-S}^{(i)}) \\ &= \frac{1}{n} \sum_{i=1}^n \hat{f}_{S,ICE}^{(i)}(\mathbf{x}_S^*) \end{aligned}$$



PARTIAL DEPENDENCE



| i | \mathbf{x}_s | \mathbf{x}_2 | \mathbf{x}_3 | \hat{f} |
|-----|----------------|----------------|----------------|-----------|
| 1 | 1 | 4 | 7 | 0.4 |
| 2 | 1 | 5 | 8 | 0.6 |
| 3 | 1 | 6 | 9 | 0.1 |

| i | \mathbf{x}_s | \mathbf{x}_2 | \mathbf{x}_3 | \hat{f} |
|-----|----------------|----------------|----------------|-----------|
| 1 | 2 | 4 | 7 | 0.6 |
| 2 | 2 | 5 | 8 | 0.8 |
| 3 | 2 | 6 | 9 | 0.5 |

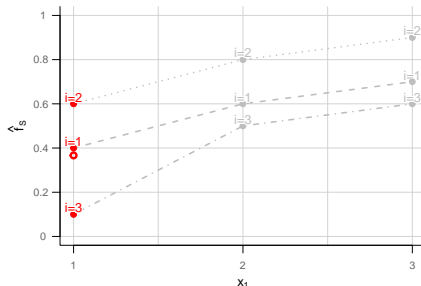
| i | \mathbf{x}_s | \mathbf{x}_2 | \mathbf{x}_3 | \hat{f} |
|-----|----------------|----------------|----------------|-----------|
| 1 | 3 | 4 | 7 | 0.7 |
| 2 | 3 | 5 | 8 | 0.9 |
| 3 | 3 | 6 | 9 | 0.6 |

$$\frac{1}{3} \sum_{i=1}^3 \hat{f}$$

$$\frac{1}{3} (0.4 + 0.6 + 0.1)$$

$$\frac{1}{3} (0.6 + 0.8 + 0.5)$$

$$\frac{1}{3} (0.7 + 0.9 + 0.6)$$

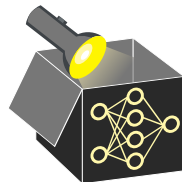


Estimate PD function by **point-wise** average of ICE curves at grid value

$$\mathbf{x}_s^* = x_1^* = 1 :$$

$$\hat{f}_{1,PD}(x_1^*) = \frac{1}{n} \sum_{i=1}^n \hat{f}(x_1^*, \mathbf{x}_{2,3}^{(i)})$$

PARTIAL DEPENDENCE



| i | \mathbf{x}_s | \mathbf{x}_2 | \mathbf{x}_3 | \hat{f} |
|-----|----------------|----------------|----------------|-----------|
| 1 | 1 | 4 | 7 | 0.4 |
| 2 | 1 | 5 | 8 | 0.6 |
| 3 | 1 | 6 | 9 | 0.1 |

| i | \mathbf{x}_s | \mathbf{x}_2 | \mathbf{x}_3 | \hat{f} |
|-----|----------------|----------------|----------------|-----------|
| 1 | 2 | 4 | 7 | 0.6 |
| 2 | 2 | 5 | 8 | 0.8 |
| 3 | 2 | 6 | 9 | 0.5 |

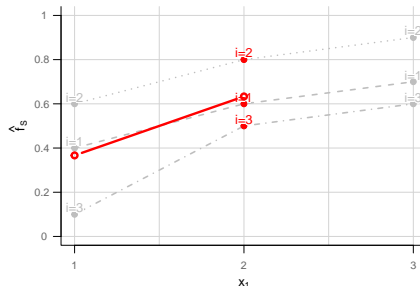
$$\frac{1}{3} \sum_{i=1}^3 \hat{f}$$

$$\frac{1}{3} (0.4 + 0.6 + 0.1)$$

$$\frac{1}{3} (0.6 + 0.8 + 0.5)$$

$$\frac{1}{3} (0.7 + 0.9 + 0.6)$$

| i | \mathbf{x}_s | \mathbf{x}_2 | \mathbf{x}_3 | \hat{f} |
|-----|----------------|----------------|----------------|-----------|
| 1 | 3 | 4 | 7 | 0.7 |
| 2 | 3 | 5 | 8 | 0.9 |
| 3 | 3 | 6 | 9 | 0.6 |

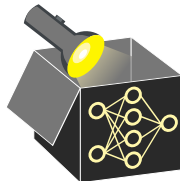


Estimate PD function by **point-wise** average of ICE curves at grid value

$$\mathbf{x}_s^* = x_1^* = 2 :$$

$$\hat{f}_{1,PD}(x_1^*) = \frac{1}{n} \sum_{i=1}^n \hat{f}(x_1^*, \mathbf{x}_{2,3}^{(i)})$$

PARTIAL DEPENDENCE



| i | \mathbf{x}_s | \mathbf{x}_2 | \mathbf{x}_3 | \hat{f} |
|-----|----------------|----------------|----------------|-----------|
| 1 | 1 | 4 | 7 | 0.4 |
| 2 | 1 | 5 | 8 | 0.6 |
| 3 | 1 | 6 | 9 | 0.1 |

| i | \mathbf{x}_s | \mathbf{x}_2 | \mathbf{x}_3 | \hat{f} |
|-----|----------------|----------------|----------------|-----------|
| 1 | 2 | 4 | 7 | 0.6 |
| 2 | 2 | 5 | 8 | 0.8 |
| 3 | 2 | 6 | 9 | 0.5 |

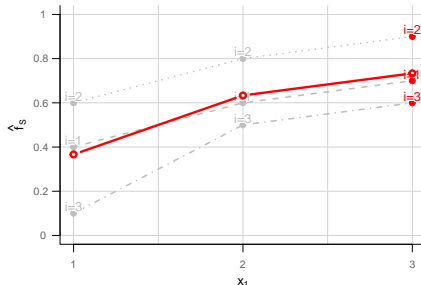
| i | \mathbf{x}_s | \mathbf{x}_2 | \mathbf{x}_3 | \hat{f} |
|-----|----------------|----------------|----------------|-----------|
| 1 | 3 | 4 | 7 | 0.7 |
| 2 | 3 | 5 | 8 | 0.9 |
| 3 | 3 | 6 | 9 | 0.6 |

$$\frac{1}{3} \sum_{i=1}^3 \hat{f}$$

$$\frac{1}{3} (0.4 + 0.6 + 0.1)$$

$$\frac{1}{3} (0.6 + 0.8 + 0.5)$$

$$\frac{1}{3} (0.7 + 0.9 + 0.6)$$



Estimate PD function by **point-wise** average of ICE curves at grid value

$$\mathbf{x}_s^* = x_1^* = 3 :$$

$$\hat{f}_{1,PD}(x_1^*) = \frac{1}{n} \sum_{i=1}^n \hat{f}(x_1^*, \mathbf{x}_{2,3}^{(i)})$$

EXAMPLE: PD FOR LINEAR MODEL

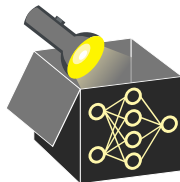
Assume a linear regression model with two features:

$$\hat{f}(\mathbf{x}) = \hat{f}(\mathbf{x}_1, \mathbf{x}_2) = \hat{\theta}_1 \mathbf{x}_1 + \hat{\theta}_2 \mathbf{x}_2 + \hat{\theta}_0$$

PD function for feature of interest $S = \{1\}$ (with $-S = \{2\}$) is:

$$\begin{aligned} f_{1,PD}(\mathbf{x}_1) &= \mathbb{E}_{\mathbf{x}_2} \left(\hat{f}(\mathbf{x}_1, \mathbf{x}_2) \right) = \int_{-\infty}^{\infty} \left(\hat{\theta}_1 \mathbf{x}_1 + \hat{\theta}_2 \mathbf{x}_2 + \hat{\theta}_0 \right) d\mathbb{P}(\mathbf{x}_2) \\ &= \hat{\theta}_1 \mathbf{x}_1 + \hat{\theta}_2 \cdot \int_{-\infty}^{\infty} \mathbf{x}_2 d\mathbb{P}(\mathbf{x}_2) + \hat{\theta}_0 \\ &= \hat{\theta}_1 \mathbf{x}_1 + \underbrace{\hat{\theta}_2 \cdot \mathbb{E}_{\mathbf{x}_2}(\mathbf{x}_2)}_{:=const} + \hat{\theta}_0 \end{aligned}$$

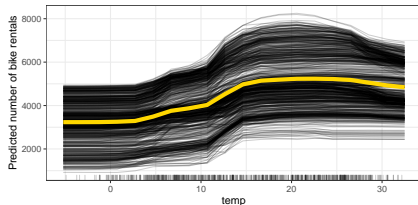
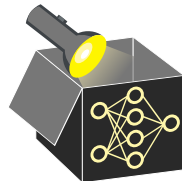
\Rightarrow PD plot visualizes function $f_{1,PD}(\mathbf{x}_1) = \hat{\theta}_1 \mathbf{x}_1 + const$ ($\hat{=}$ feature effect of \mathbf{x}_1).



INTERPRETATION: PD AND ICE

If feature varies:

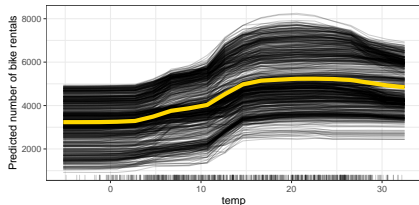
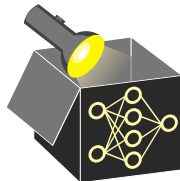
- **ICE:** How does **prediction of individual observation** change?
⇒ **local** interpretation
- **PD:** How does **average effect / expected prediction** change?
⇒ **global** interpretation



INTERPRETATION: PD AND ICE

If feature varies:

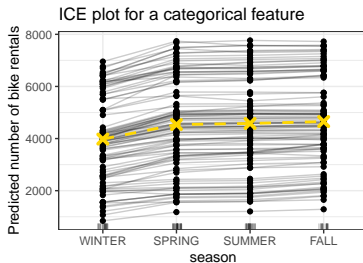
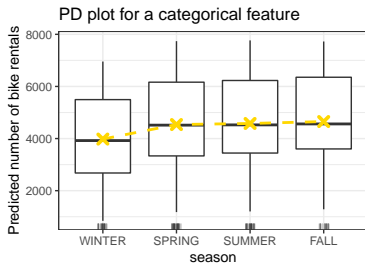
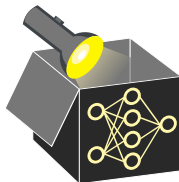
- **ICE:** How does **prediction of individual observation** change?
⇒ **local** interpretation
- **PD:** How does **average effect / expected prediction** change?
⇒ **global** interpretation



Insights from bike sharing data:

- Parallel ICE curves = homogeneous effect across obs.
- Warmer ⇒ more rented bikes
- Too hot ⇒ slightly less bikes
- Steepest increase in rentals occurs as temperature rises from 10°C to 15°C.

INTERPRETATION: CATEGORICAL FEATURES



- PDP with boxplots and ICE with parallel coordinates plots
- NB: Categories can be unordered, if so, rather compare pairwise