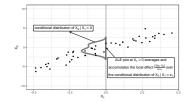
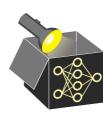
Interpretable Machine Learning

Accumulated Local Effect (ALE): Introduction



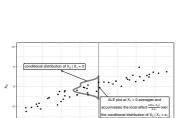
Learning goals

- PD plots and its extrapolation issue
- M plots and its omitted-variable bias
- Understand ALE plots



Interpretable Machine Learning



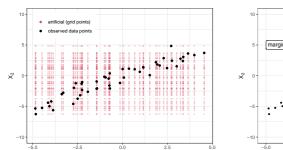


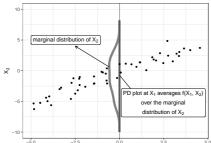
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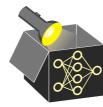


MOTIVATION - CORRELATED FEATURES

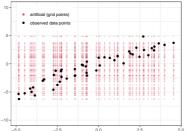


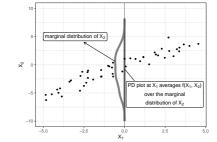


- PD plots average over predictions of artificial points that are out of distribution/ unlikely (red)
 - \Rightarrow Can lead to misleading / biased interpretations, especially if model also contains interactions
- Not wanted if interest is to interpret effects within data distribution



MOTIVATION - CORRELATED FEATURES





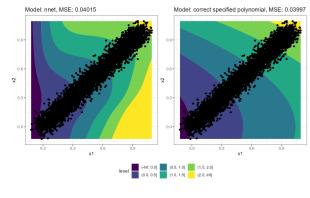


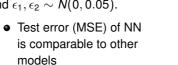
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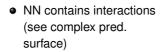
MOTIVATION - CORRELATED FEATURES

Example: Fit an NN to 5000 simulated data points with $x \sim \textit{Unif}(0, 1), \epsilon \sim \textit{N}(0, 0.2)$ and

$$y = x_1 + x_2^2 + \epsilon$$
, where $x_1 = x + \epsilon_1$, $x_2 = x + \epsilon_2$ and $\epsilon_1, \epsilon_2 \sim N(0, 0.05)$.





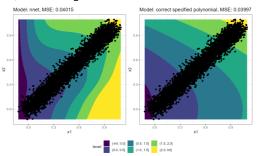




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- Test error (MSE) of NN is comparable to other models
- NN contains interactions (see complex pred. surface)

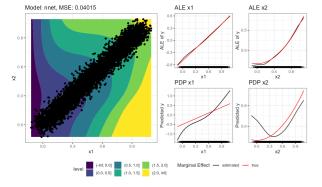


Interpretable Machine Learning - 2 / 6

MOTIVATION - CORRELATED FEATURES

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 ⇒ Due to interactions and averaging of points

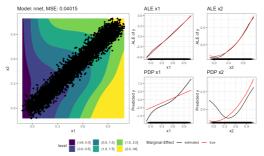
outside data distribution



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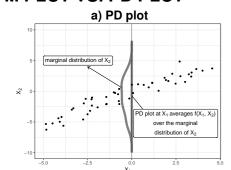


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Interpretable Machine Learning - 2 / 6

M PLOT VS. PD PLOT

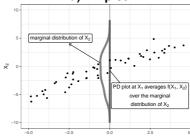


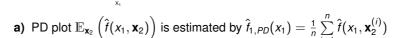
a) PD plot $\mathbb{E}_{\mathbf{x}_2}\left(\hat{f}(x_1,\mathbf{x}_2)\right)$ is estimated by $\hat{f}_{1,PD}(x_1)=\frac{1}{n}\sum_{i=1}^n\hat{f}(x_1,\mathbf{x}_2^{(i)})$



M PLOT VS. PD PLOT

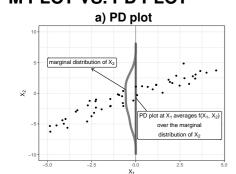


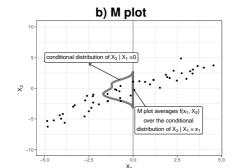






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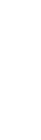


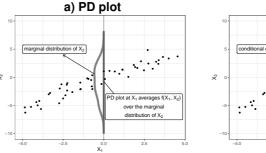


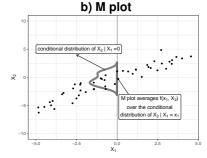


- a) PD plot $\mathbb{E}_{\mathbf{x}_2}\left(\hat{f}(x_1,\mathbf{x}_2)\right)$ is estimated by $\hat{f}_{1,PD}(x_1)=\frac{1}{n}\sum_{i=1}^n\hat{f}(x_1,\mathbf{x}_2^{(i)})$
- **b)** M plot $\mathbb{E}_{\mathbf{x}_2|\mathbf{x}_1}\left(\hat{f}(x_1,\mathbf{x}_2)\Big|\mathbf{x}_1\right)$ is estimated by $\hat{f}_{1,M}(x_1)=\frac{1}{|N(x_1)|}\sum_{i\in N(x_1)}\hat{f}(x_1,\mathbf{x}_2^{(i)}),$ where index set $N(x_1)=\{i:x_1^{(i)}\in[x_1-\epsilon,x_1+\epsilon]\}$ refers to observations with feature value close to x_1 .

M PLOT VS. PD PLOT



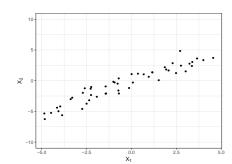


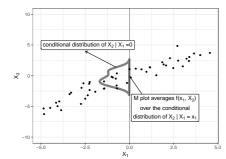




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M PLOT VS. PD PLOT

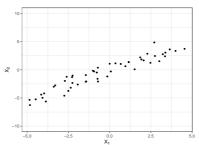


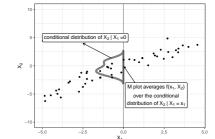


- M plots average predictions over conditional distribution (e.g., $\mathbb{P}(\mathbf{x}_2|x_1)$)
 - ⇒ Averaging predictions close to data distribution avoid extrapolation issues
- But: M plots suffer from omitted-variable bias (OVB)
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 - Useless in assessing a feature's marginal effect if feature dependencies are present



M PLOT VS. PD PLOT

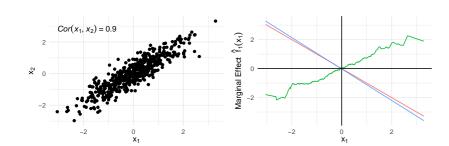






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M PLOT VS. PD PLOT - OVB EXAMPLE





Method — function f(x) = -x — M-plot — PD plot

Illustration: Fit LM on 500 i.i.d. observations with features $x_1, x_2 \sim N(0, 1)$, $Cor(x_1, x_2) = 0.9$ and

$$y = -x_1 + 2 \cdot x_2 + \epsilon, \ \epsilon \sim N(0, 1).$$

Results: M plot of x_1 also includes marginal effect of all other dependent features (here: x_2)

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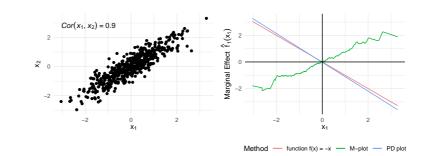




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Idea: To remove unwanted effects of other features, take partial derivatives (local effects) of prediction function w.r.t. feature of interest and integrate (accumulate) them w.r.t. the same feature

- \Rightarrow Computing the partial derivative of \hat{f} w.r.t. \mathbf{x}_{j} removes other main effects
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Example:

• Consider an additive prediction function:

$$\hat{f}(x_1, x_2) = 2x_1 + 2x_2 - 4x_1x_2$$



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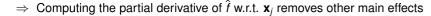
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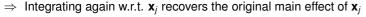
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Interpretable Machine Learning - 6 / 6

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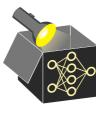


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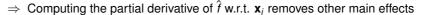
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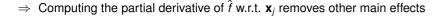
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Interpretable Machine Learning - 6 / 6

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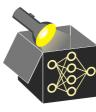
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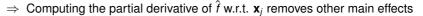
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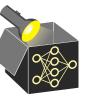
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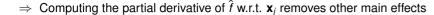
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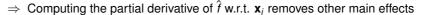
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