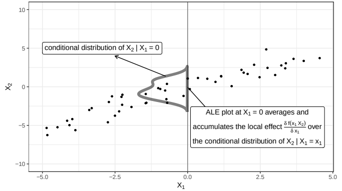
Interpretable Machine Learning

Accumulated Local Effect (ALE) plot



Learning goals

- Understand ALE plots
- Difference between ALE and PD plots

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Feature Effects

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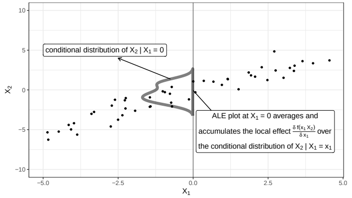

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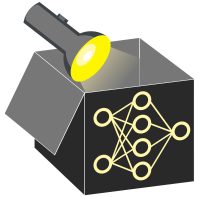
ACCUMULATED LOCAL EFFECTS (ALE) ▸ Apley, Zhu (2020)



ALE plots estimate the marginal effect of a feature by accumulating its local effects (integrating partial derivatives), evaluated in regions supported by the data.

Computation Steps:

1. **Estimate local effects** $\frac{\partial \hat{f}(x_S, \mathbf{x}_{-S})}{\partial x_S}$ (via finite differences)
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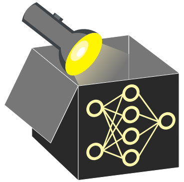
ACCUMULATED LOCAL EFFECTS (ALE) ▸ ZHU_2020



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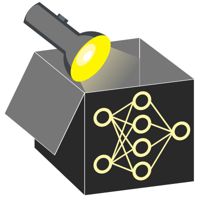

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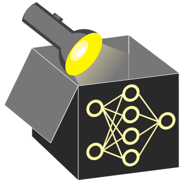

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FIRST ORDER ALE FUNCTION

Uncentered ALE Function evaluated at $x \in \mathcal{X}_S$ (domain of feature x_S):

$$\tilde{f}_{S,\text{ALE}}(x) = \underbrace{\int_{z_0}^{x}}_{(3)} \underbrace{\mathbb{E}_{\mathbf{x}_{-S}|x_S=z_S}}_{\text{(2) average locally}} \left(\underbrace{\frac{\partial \hat{f}(z_S, \mathbf{x}_{-S})}{\partial z_S}}_{\text{(1) local effect}} \right) dz_S = \int_{z_0}^{x} \int \frac{\partial \hat{f}(z_S, \mathbf{x}_{-S})}{\partial z_S} d\mathbb{P}(\mathbf{x}_{-S} \mid z_S) dz_S$$

- x_S is feature of interest, with minimum value $z_0 = \min(x_S)$
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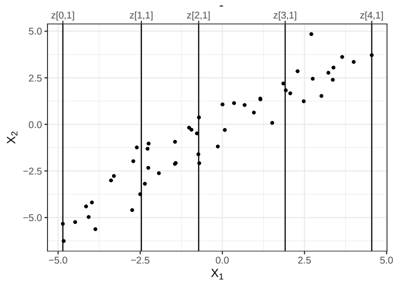

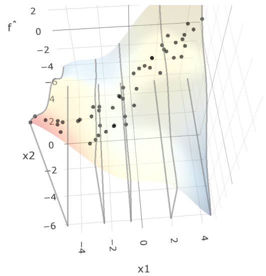

- **Motivation:** Partial derivatives are not well-defined for all models (e.g., tree-based methods). ⇒ Use finite differences within intervals instead.
- Partition the feature range of x_S into K intervals (vertical lines)
  - Define intervals:

$$x_S \in [\min(x_S), \max(x_S)] \Rightarrow x_S \in [z_0, z_{1,S}] \cup [z_{1,S}, z_{2,S}] \cup \cdots \cup [z_{K-1,S}, z_{K,S}]$$

  - *Equidistant*: preserves resolution
  - *Quantile-based*: balances sample size per interval

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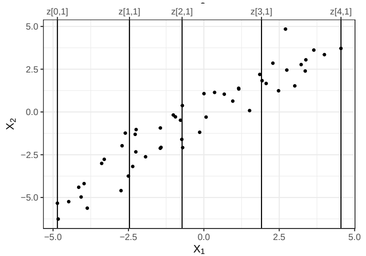

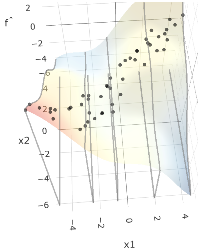

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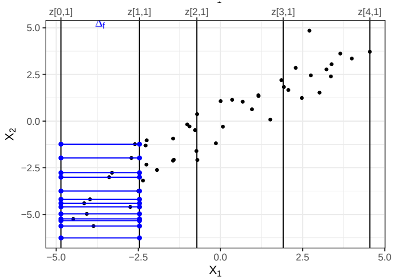

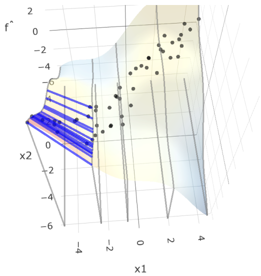

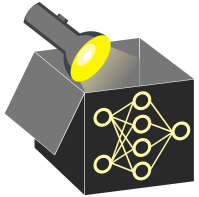

- For each observation in k-th interval, i.e., $\{i : x_S^{(i)} \in \; [z_{k-1,S}, z_{k,S}]\}$:
  - Replace $x_S^{(i)}$ with upper/lower interval bounds, keeping $\mathbf{x}_{-S}^{(i)}$ fixed
  - Compute observation-wise finite difference of i-th obs. in k-th interval
    $\rightsquigarrow \hat{f}(z_{k,S}, \mathbf{x}_{-S}^{(i)}) - \hat{f}(z_{k-1,S}, \mathbf{x}_{-S}^{(i)})$ (approximates local effect)

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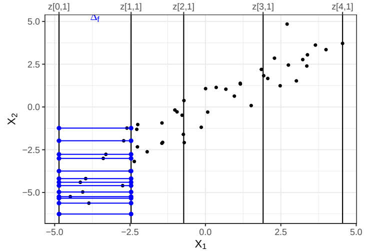

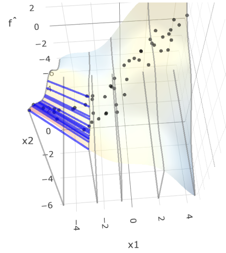

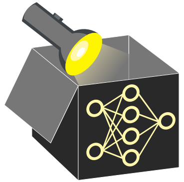

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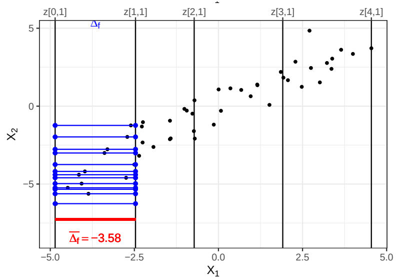

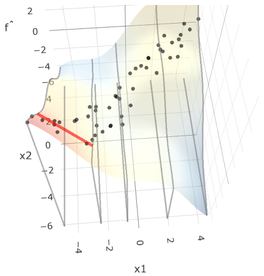

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- Average these finite differences over all observations in each interval
  $\rightsquigarrow$ Approximates **inner integral** $\mathbb{E}_{\mathbf{x}_{-S}|x_S=z_S}\left[\partial\hat{f}/\partial z_S\right]$
- Accumulate these averages from z_0 to the point of interest $x \in \mathcal{X}_S$
  $\rightsquigarrow$ Approximates **outer integral** over $z_S \in [z_0, x] \Rightarrow$ uncentered ALE function

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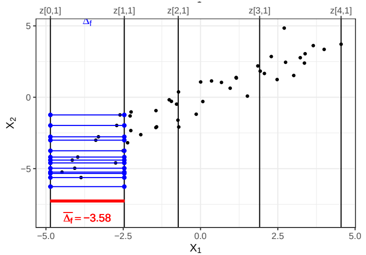

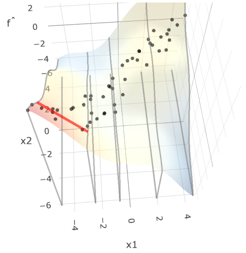

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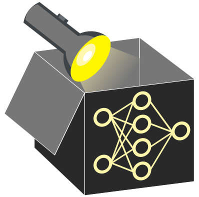

Estimated uncentered ALE: For a point $x \in \mathcal{X}_S$, define:

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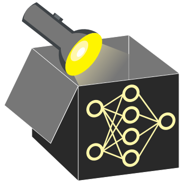

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Centering: Ensure identifiability by subtracting mean uncentered ALE (constant c):

$$\hat{f}_{S,\text{ALE}}(x) = \hat{\tilde{f}}_{S,\text{ALE}}(x) \ - \ c, \qquad c = \tfrac{1}{n} \textstyle\sum_{i=1}^{n} \hat{\tilde{f}}_{S,\text{ALE}}\left(x_S^{(i)}\right).$$

Efficient centering (used in implementations): Use weighted trapezoidal averaging of interval-wise boundary values (avoids redundant re-evaluation at all n points):

$$c = \textstyle\sum_{k=1}^{K} \frac{1}{2} \cdot \left(\hat{\tilde{f}}_{S,\text{ALE}}(z_{k-1,S}) + \hat{\tilde{f}}_{S,\text{ALE}}(z_{k,S})\right) \cdot \frac{n_S(k)}{n}$$

Plotting ALE: Visualize the pairs $\left(z_{k,S}, \hat{f}_{S,\text{ALE}}(z_{k,S})\right)$ for all interval boundaries $z_{k,S}$.

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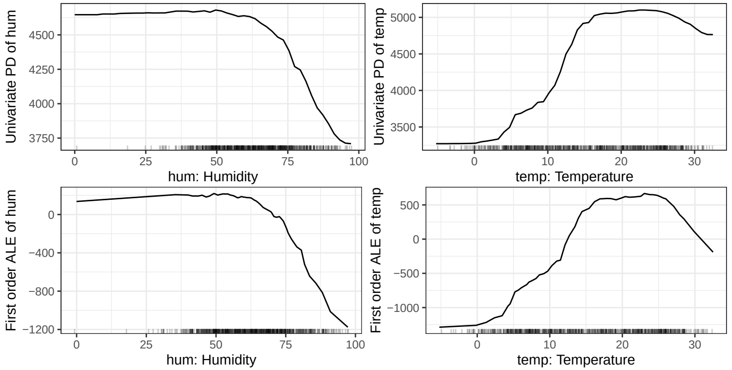
BIKE SHARING DATASET: FIRST ORDER ALE

- **Visual comparison:** PD plot (top) vs. First-order ALE plot (bottom)
- **Shape:** Both plots show similar trends, but differ in y-axis scale due to centering
- **Interpretation:** ALE accounts for feature dependencies and avoids extrapolation into unsupported regions
  - ⇝ PD reflects model behavior in entire feature space ("true to the model")
  - ⇝ ALE focuses on effects in data-supported regions ("true to the data")



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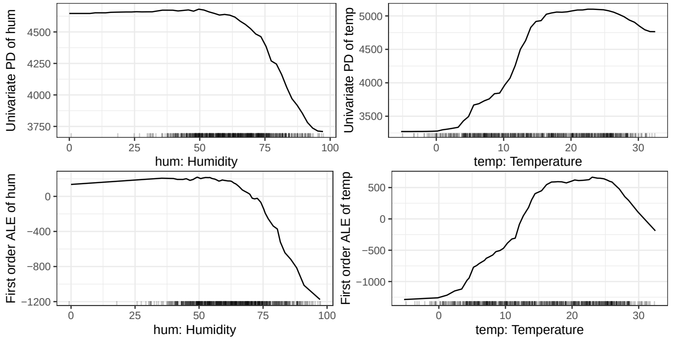
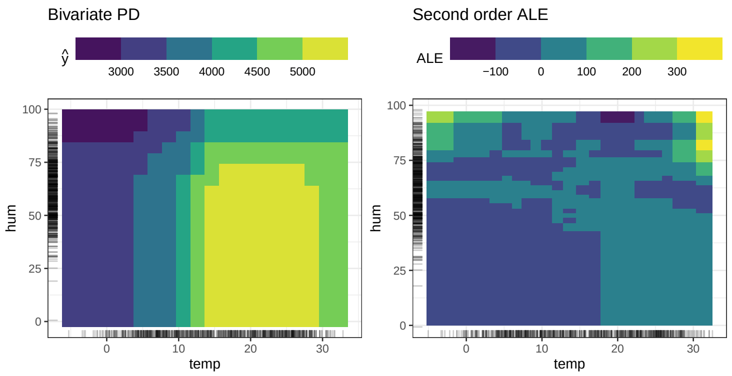


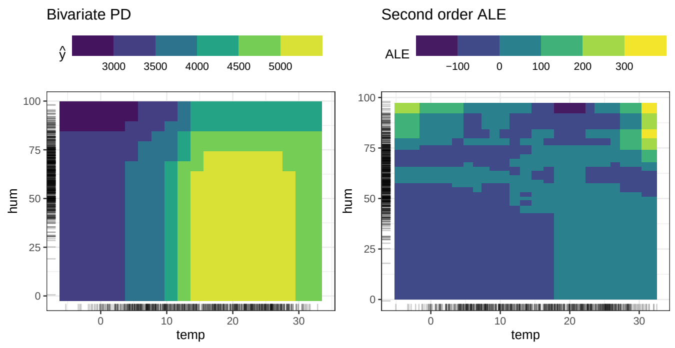
BIKE SHARING DATASET: SECOND ORDER ALE

Unlike bivariate PD plots, 2nd-order ALE plots only estimate pure interaction between two features (1st-order effects are not included).



BIKE SHARING DATASET: SECOND ORDER ALE

Unlike bivariate PD plots, 2nd-order ALE plots only estimate pure interaction between two features (1st-order effects are not included).



PD VS. ALE

PD:

$$f_{S,PD}(x_S) = \mathbb{E}_{\mathbf{x}_{-S}}\left(\hat{f}(x_S, \mathbf{x}_{-S})\right)$$

ALE:

$$f_{S,\text{ALE}}(x) = \int_{z_0}^{x} \mathbb{E}_{\mathbf{x}_{-S}|x_S = z_S}\left(\frac{\partial \hat{f}(z_S, \mathbf{x}_{-S})}{\partial z_S}\right) dz - \text{const}$$

- Recall: PD directly averages predictions over marginal distribution of $\mathbf{x}_{-S}$
- ALE is faster: Needs $O(2 \cdot n)$ model calls vs. $O(n \cdot g)$ for PD with g grid points
- Difference 1: ALE averages
  - prediction changes (via partial derivatives, estimated by finite differences)
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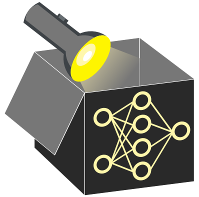

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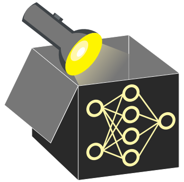
  $\rightsquigarrow$ isolates effect of x_S and removes main effect of other dependent features

PD VS. ALE



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