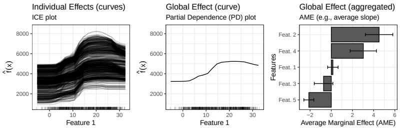
# Interpretable Machine Learning

# Individual Conditional Expectation (ICE) Plot



Individual Effects (curves)
ICE plot

Global Effect (curve)
Partial Dependence (PD) plot

Global Effect (aggregated)
AME (e.g., average slope)

## Learning goals

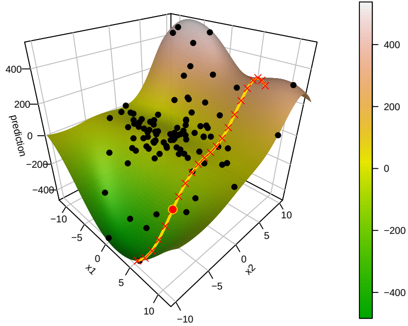
- ICE curves as local effect method
- How to sample grid points for ICE curves

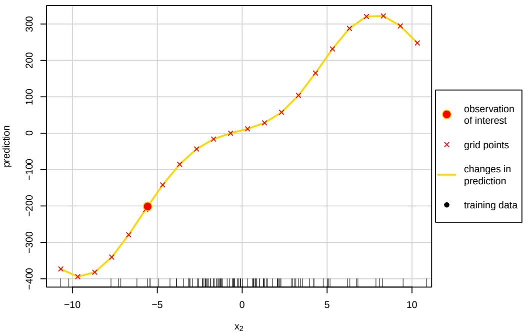
# MOTIVATION

**Question:** How does changing values of a single feature of an observation affect model prediction?

**Idea:** Change values of observation and feature of interest, and visualize how prediction changes

**Example:** Prediction surface of a model (left), select observation and visualize changes in prediction for different values of $x_2$ while keeping $x_1$ fixed ⇒ **local interpretation**





# INDIVIDUAL CONDITIONAL EXPECTATION (ICE)

▸ Goldstein et. al (2013)

Partition each observation $\mathbf{x}$ into $\mathbf{x}_S$ (features of interest) and $\mathbf{x}_{-S}$ (remaining feat.)

⇝ In practice, $\mathbf{x}_S$ consists of one or two features (i.e., $|S| \leq 2$ and $-S = S^{\complement}$).

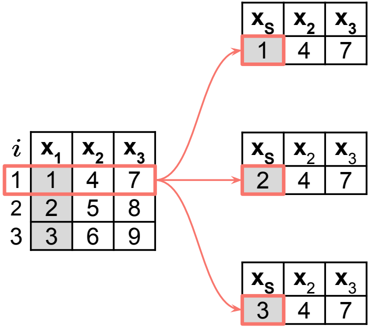
|  | $\mathbf{x}_S$ | $\mathbf{x}_{-S}$ |  |
|---|---|---|---|
| $i$ | $\mathbf{x}_1$ | $\mathbf{x}_2$ | $\mathbf{x}_3$ |
| 1 | 1 | 4 | 7 |
| 2 | 2 | 5 | 8 |
| 3 | 3 | 6 | 9 |

Formal definition of ICE curves:

- Choose grid points $\mathbf{x}_S^* = \mathbf{x}_S^{*^{(1)}}, \dots, \mathbf{x}_S^{*^{(g)}}$ to vary $\mathbf{x}_S$
- Plot point pairs $\left\{\left(\mathbf{x}_S^{*^{(k)}}, \hat{f}_S^{(i)}(\mathbf{x}_S^{*^{(k)}})\right)\right\}_{k=1}^{g}$ where $\hat{f}_S^{(i)}(\mathbf{x}_S^*) = \hat{f}(\mathbf{x}_S^*, \mathbf{x}_{-S}^{(i)})$
- For each $k$ connect point pairs to obtain **ICE curve**

⇝ ICE curves visualize how prediction of $i$-th observation changes after varying its feature values indexed by $S$ using grid points $\mathbf{x}_S^*$ while keeping all values in $-S$ fixed:

# ICE CURVES - ILLUSTRATION



| $i$ | $\mathbf{x}_1$ | $\mathbf{x}_2$ | $\mathbf{x}_3$ |
|---|---|---|---|
| 1 | 1 | 4 | 7 |
| 2 | 2 | 5 | 8 |
| 3 | 3 | 6 | 9 |

| $\mathbf{x}_S$ | $\mathbf{x}_2$ | $\mathbf{x}_3$ |
|---|---|---|
| 1 | 4 | 7 |

| $\mathbf{x}_S$ | $\mathbf{x}_2$ | $\mathbf{x}_3$ |
|---|---|---|
| 2 | 4 | 7 |

| $\mathbf{x}_S$ | $\mathbf{x}_2$ | $\mathbf{x}_3$ |
|---|---|---|
| 3 | 4 | 7 |

**1. Step - Grid points:**

Sample grid values $\mathbf{x}_S^{*^{(1)}}, \ldots, \mathbf{x}_S^{*^{(g)}}$ along feature of interest $\mathbf{x}_S$ and replace vector $\mathbf{x}^{(i)}$ in data with grid
$\Rightarrow$ Creates new artificial points for the *i*-th observation (here: $\mathbf{x}_S^* = x_1^* \in \{1, 2, 3\}$ is a scalar)

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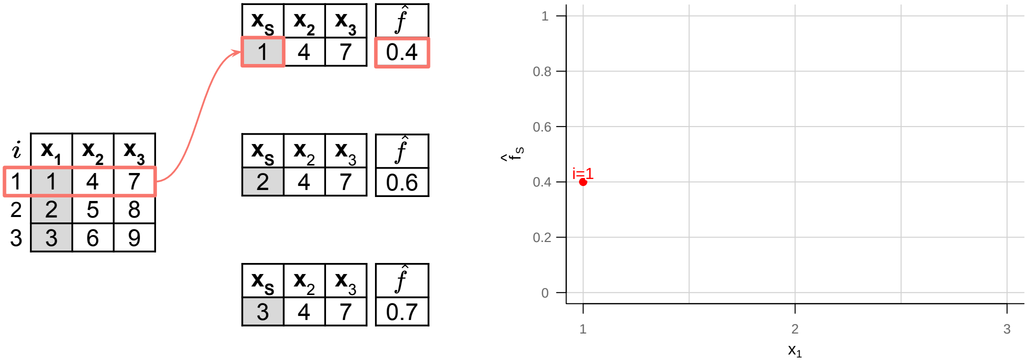

| $i$ | $x_1$ | $x_2$ | $x_3$ |
|---|---|---|---|
| 1 | 1 | 4 | 7 |
| 2 | 2 | 5 | 8 |
| 3 | 3 | 6 | 9 |

| $x_S$ | $x_2$ | $x_3$ | $\hat{f}$ |
|---|---|---|---|
| 1 | 4 | 7 | 0.4 |

| $x_S$ | $x_2$ | $x_3$ | $\hat{f}$ |
|---|---|---|---|
| 2 | 4 | 7 | 0.6 |

| $x_S$ | $x_2$ | $x_3$ | $\hat{f}$ |
|---|---|---|---|
| 3 | 4 | 7 | 0.7 |

**2. Step - Predict and visualize:**

For each artificially created data point of $i$-th observation, plot prediction $\hat{f}_S^{(i)}(\mathbf{x}_S^*)$ vs. grid values $\mathbf{x}_S^*$:

$$\hat{f}_1^{(i)}(x_1^*) = \hat{f}(x_1^*, \mathbf{x}_{2,3}^{(i)}) \text{ vs. } x_1^* \in \{1, 2, 3\}$$

# ICE CURVES - ILLUSTRATION

| $i$ | $\mathbf{x}_1$ | $\mathbf{x}_2$ | $\mathbf{x}_3$ |
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| $\mathbf{x}_S$ | $\mathbf{x}_2$ | $\mathbf{x}_3$ | $\hat{f}$ |
|---|---|---|---|
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| $\mathbf{x}_S$ | $\mathbf{x}_2$ | $\mathbf{x}_3$ | $\hat{f}$ |
|---|---|---|---|
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| $\mathbf{x}_S$ | $\mathbf{x}_2$ | $\mathbf{x}_3$ | $\hat{f}$ |
|---|---|---|---|
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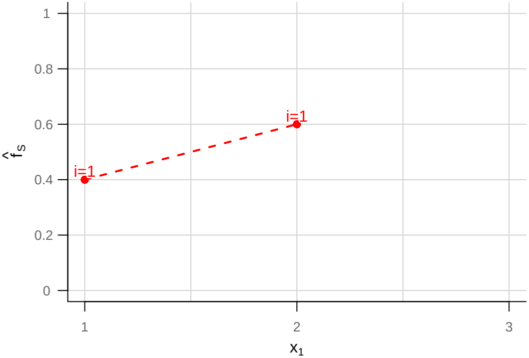

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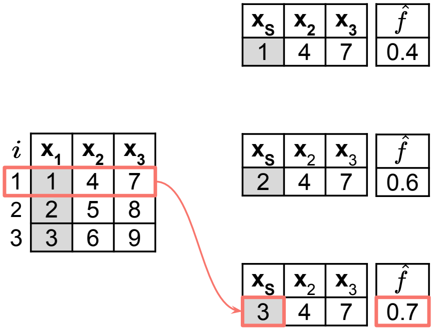

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|---|---|---|---|
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| 3 | 3 | 6 | 9 |

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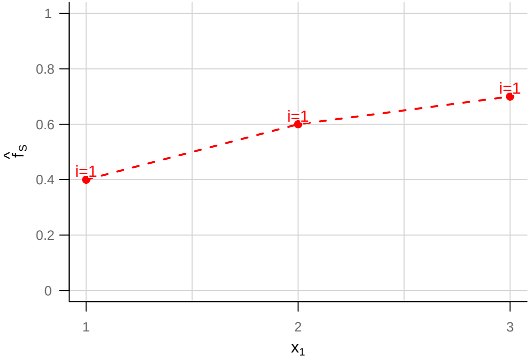
|---|---|---|---|
| 1 | 4 | 7 | 0.4 |

| $x_S$ | $x_2$ | $x_3$ | $\hat{f}$ |
|---|---|---|---|
| 2 | 4 | 7 | 0.6 |

| $x_S$ | $x_2$ | $x_3$ | $\hat{f}$ |
|---|---|---|---|
| 3 | 4 | 7 | 0.7 |



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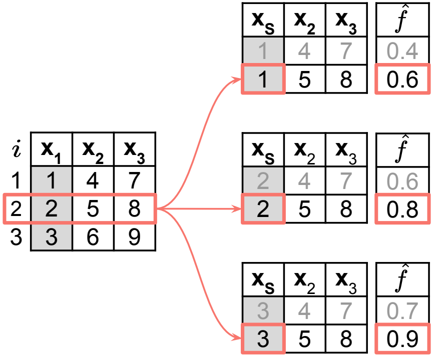
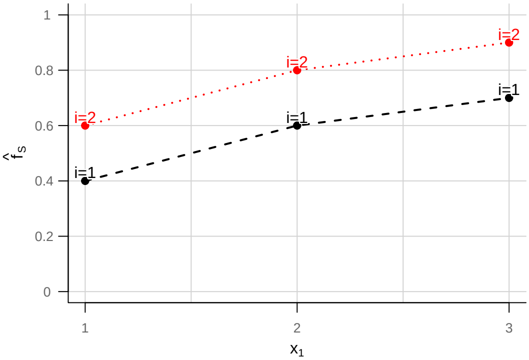


| $i$ | $x_1$ | $x_2$ | $x_3$ |
|---|---|---|---|
| 1 | 1 | 4 | 7 |
| 2 | 2 | 5 | 8 |
| 3 | 3 | 6 | 9 |

| $x_S$ | $x_2$ | $x_3$ | $\hat{f}$ |
|---|---|---|---|
| 1 | 4 | 7 | 0.4 |
| 1 | 5 | 8 | 0.6 |

| $x_S$ | $x_2$ | $x_3$ | $\hat{f}$ |
|---|---|---|---|
| 2 | 4 | 7 | 0.6 |
| 2 | 5 | 8 | 0.8 |

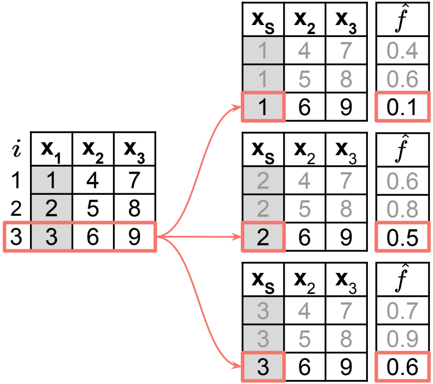
| $x_S$ | $x_2$ | $x_3$ | $\hat{f}$ |
|---|---|---|---|
| 3 | 4 | 7 | 0.7 |
| 3 | 5 | 8 | 0.9 |



**3. Step - Repeat for other observations:**

ICE curve for $i = 2$ connects all predictions at grid values associated to $i$-th observation.

# ICE CURVES - ILLUSTRATION



| $i$ | $x_1$ | $x_2$ | $x_3$ |
|---|---|---|---|
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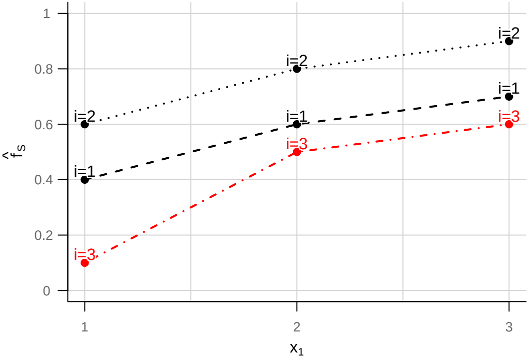
| 2 | 2 | 5 | 8 |
| 3 | 3 | 6 | 9 |

| $x_S$ | $x_2$ | $x_3$ | $\hat{f}$ |
|---|---|---|---|
| 1 | 4 | 7 | 0.4 |
| 1 | 5 | 8 | 0.6 |
| 1 | 6 | 9 | 0.1 |

| $x_S$ | $x_2$ | $x_3$ | $\hat{f}$ |
|---|---|---|---|
| 2 | 4 | 7 | 0.6 |
| 2 | 5 | 8 | 0.8 |
| 2 | 6 | 9 | 0.5 |

| $x_S$ | $x_2$ | $x_3$ | $\hat{f}$ |
|---|---|---|---|
| 3 | 4 | 7 | 0.7 |
| 3 | 5 | 8 | 0.9 |
| 3 | 6 | 9 | 0.6 |



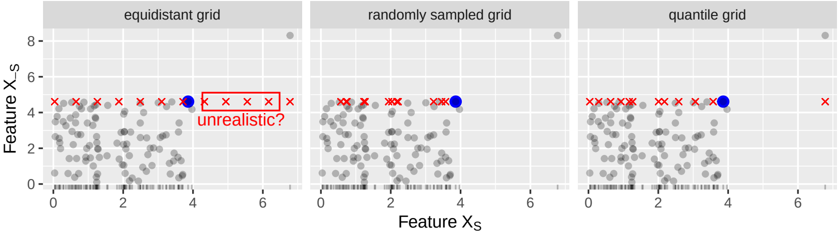
**3. Step - Repeat for other observations:**

ICE curve for $i = 3$ connects all predictions at grid values associated to $i$-th observation.

# COMMENTS ON GRID VALUES

- Plotting ICE curves involves generating grid values $\mathbf{x}_S^*$ that are visualized on the x-axis
- Common choices for grid values are
  - equidistant grid values within feature range
  - randomly sampled values or quantile values of observed feature values
- Except equidistant grid, the other two options preserve (approximately) the marginal distribution of feature of interest $\Rightarrow$ Avoids unrealistic feature values for distributions with outliers

Grid points for $X_S$ (red) for highlighted observation (blue)



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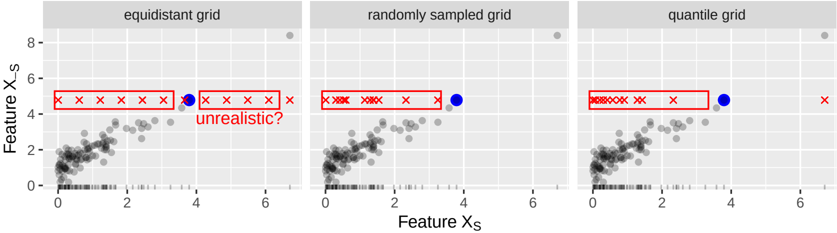
equidistant grid
randomly sampled grid
quantile grid
unrealistic?
Feature X_-S
Feature $X_S$