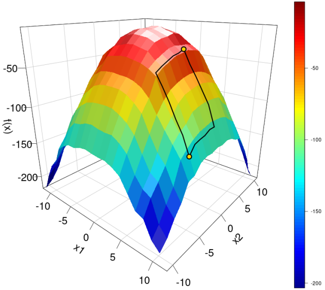
Interpretable Machine Learning

Marginal Effects



Learning goals

- Why parameter-based interpretations are not always possible for parametric models
- How marginal effects can be used in such cases
- Drawbacks of marginal effects
- Model-agnostic applicability

INTERPRETATIONS OF LINEAR MODELS

- The LM can be directly interpreted by evaluating the model coefficients:

$$y = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p + \dots + \epsilon$$

- A change in x_1 by Δx_1 results in a change in y by $\Delta y = \Delta x_1 \cdot \beta_1$.

- Default interpretations correspond to $\Delta x_1 = 1$, i.e., $\Delta y = \beta$.

- All interpretations are done ceteris paribus, i.e., all remaining features are kept constant.

INTERPRETATIONS OF POLYNOMIAL MODELS

- If higher-order terms or interactions are present, parameter-based interpretations are not possible anymore:

$$y = \beta_0 + \beta_1 x_1^2 + \beta_2 x_2^2 + \beta_{1,2} x_1, x_2 + \epsilon \tag{1}$$

- The isolated main effects of both features vary across different values

- The interaction depends on values of the remaining feature

- The marginal effect (ME) allows us to determine a feature effect nonetheless.

MARGINAL EFFECTS

- The most common definition of the marginal effect (ME) corresponds to the derivative of the prediction function w.r.t. a feature. In this lecture, we refer to this variant as the derivative ME (dME). The dME can be computed model-agnostically via numeric differentiation, e.g., with a symmetric difference quotient:

$$dME_j(x) = \frac{\partial f(x)}{\partial x_j}$$
$$dME_j(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

- For Eq. (1), the dME corresponds to:

$$dME_j(x) = 2\beta_1 x_1 + \beta_{1,2} x_2$$

MARGINAL EFFECTS

- A less commonly known definition corresponds to the change in predicted outcome due to an intervention in the data, e.g., by increasing a feature value by one unit. As this variant corresponds to a forward difference, we refer to it as a forward ME (fME) in this lecture:

$$fME_j(x, h_j) = f(x_1, \dots, x_j + h_j, \dots, x_p) - f(x)$$

- For Eq. (1), the fME of x_1 with step size 1 correspond to:

$$fME_j(x, h_j) = 2\beta_1 h_1^2 + \beta_{1,2} x_2 h_1$$

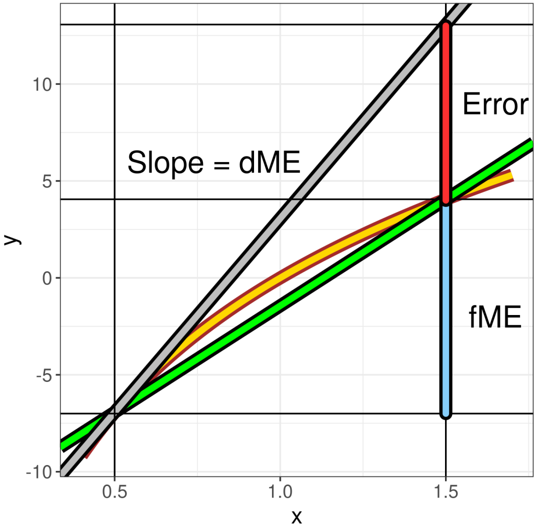
DERIVATIVE VERSUS FORWARD DIFFERENCE

- The dME is not suited to interpret non-linear prediction functions, as the derivative of the prediction function at one point may be substantially different at another.

- The fME is better suited for non-linear prediction functions. It essentially corresponds to a movement on the prediction function, indicating changes in predicted outcome regardless of the function's shape.

- However, with both variants, we lose information about the prediction function along the finite difference.

DERIVATIVE VERSUS FORWARD DIFFERENCE



ADDITIVE RECOVERY

- Due being based on a finite difference, both variants only recover terms within the prediction function that depend on the feature(s) of interest.

- Consider a prediction function $\widehat{f}(x) = ax_1 + bx_2$. It follows that:

$$dME_1(x) = a$$
$$fME_1(x, h_1) = ah_1$$

- The ME removes effects of other features that are linked additively, regardless of how many remaining features exist, and their effect structure.

MODEL-AGNOSTIC APPLICABILITY

- MEs are traditionally used to interpret parametric models such as GLMs. However, both dME and fME can be used as model-agnostic interpretation tools for non-parametric models. As the fME is better suited for non-linear prediction functions, it is the natural choice for black box ML models.

- The fME essentially correspond to an exploration of the prediction function. We can also use multivariate changes in feature values to explore the prediction surface in various directions simultaneously.

- One needs to keep in mind that the shape of the prediction function may vary considerably along the forward difference, i.e., an fME with half the step size may not result in half the fME.