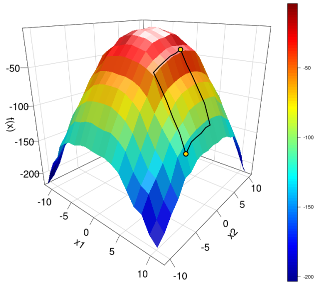
# Interpretable Machine Learning

## 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

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## Feature Effects

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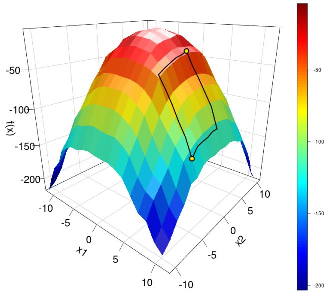


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# INTERPRETATION OF SIMPLE MODELS

- **Linear Models**:
  - Change in $x_j$ by $\Delta x_j$ results in change in $y$ by $\Delta y = \Delta x_j \cdot \theta_j$
  - Model equation:

$$y = \theta_0 + \theta_1 x_1 + \cdots + \theta_p x_p + \epsilon$$

  - Default interpretations correspond to $\Delta x_j = 1$, i.e., $\Delta y = \theta_j$
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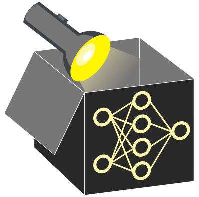

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- **Non-Linear Models with Interactions**:
  - For models with higher-order or interaction terms, single coefficients are not sufficient:
$$y = \theta_0 + \theta_1 x_1^2 + \theta_2 x_2^2 + \theta_{1,2} x_1 x_2 + \epsilon$$
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  - Interactions depend on the values of other features



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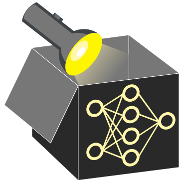

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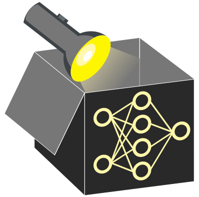

- MEs measure changes in predictions due to changes in *one/several* features.
- **How to compute it?**
  1. **Derivative Marginal Effects (dMEs)**: *numeric derivative* (slope of tangent)
     $\rightsquigarrow$ needs differentiability, fails for step-wise models.
  2. **Forward Marginal Effects (fMEs)**: *forward difference* $\hat{f}(\mathbf{x} + \mathbf{h}) - \hat{f}(\mathbf{x})$
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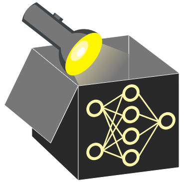

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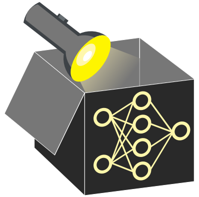

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- **Local instantiations (one number per data point)**
  - **ME** (at observed point $\boldsymbol{x}^{(i)}$): Individual, observation-specific "what-if" effect.
  - **MEM** (at mean $\bar{\boldsymbol{x}}$): Effect at artificial profile ("average obs.").
  - **MER** (at representative value $\boldsymbol{x}^*$): Effect at a user-defined profile.
- **Global summary – Average Marginal Effect (AME)**:
  Expectation of the (d/f)MEs; captures the *global overall* effect.



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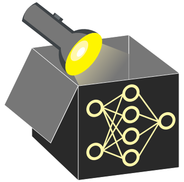

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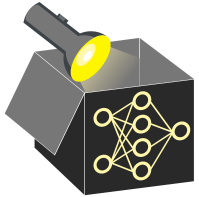
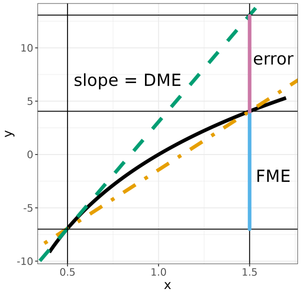


- **dME (tangent, green)**
  - slope of the tangent at $x$;
  - delivers a *rate* of change $\frac{\partial \hat{f}}{\partial x}$.
- **fME (secant, orange)**
  - vertical gap between two model evaluations;
  - always *exact* change in predicted outcome.
  - Non-linearity measure (pink band, bottom): quantifies deviation of secant and true curve
- **When the two differ**
  - Curvature makes the tangent overshoot or undershoot $\Rightarrow$ dME may be badly biased.
  - fME is robust to kinks, plateaus, trees, ...

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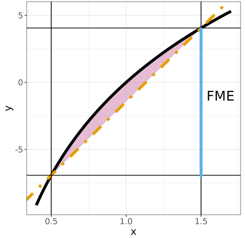




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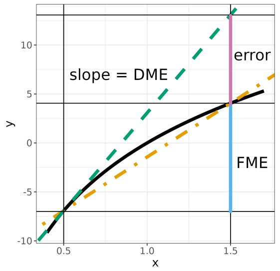


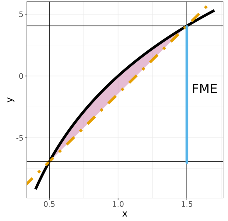


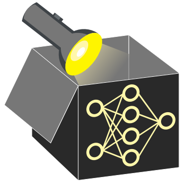

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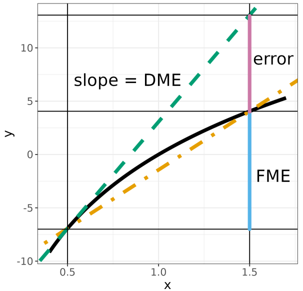
- Use fME for any non-linear or non-smooth model
- Use dME for lin. functions or analytic convenience

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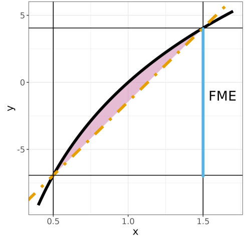




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**Recommendations**

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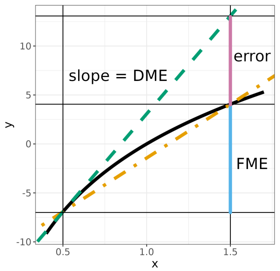


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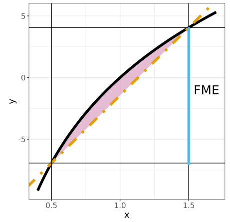
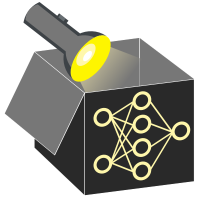


# MARGINAL EFFECTS FOR CONTINUOUS FEATURES



- **Derivative Marginal Effect (dME)**:

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- **Forward Marginal Effect (fME)**:

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- **Note:** fME is not scale-invariant – halving the step size does not halve the effect.
- **Additive Recovery:** dME and fME isolate terms involving the target feature.
  - **Example:** For $\widehat{f}(\mathbf{x}) = ax_1 + bx_2$: $\text{dME}_1(\mathbf{x}) = a, \quad \text{fME}_1(\mathbf{x}, h_1) = ah_1$
  - Effects from additively linked features (e.g., $x_2$) are canceled.
  - Enables focus on direct feature-specific influence in $\widehat{f}$.



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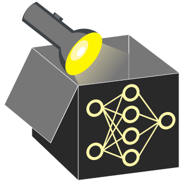

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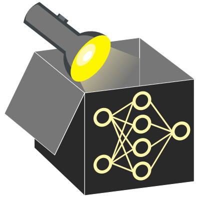

- **Traditional Approach**:
  - Choose a baseline category for the categorical feature $x_j$
    $\rightsquigarrow$ Either the observed value $x_j$ or a fixed reference $x_j^{\text{ref}}$
  - Replace $x_j$ with an alternative category $x_j^{\text{new}}$
  - Compute the change in prediction, keeping all other features $\mathbf{x}_{-j}$ fixed
- **fME Definition for Categorical Features**:

$$\text{fME}_j(\mathbf{x}; x_j^{\text{new}}) = \widehat{f}(x_j^{\text{new}}, \mathbf{x}_{-j}) - \widehat{f}(x_j, \mathbf{x}_{-j})$$

  - $x_j$: original category of feature $j$ in obs. $\mathbf{x}$ (or reference category $x_j^{\text{ref}}$)
  - $x_j^{\text{new}}$: new category to evaluate
  - $\mathbf{x}_{-j}$: all other features held fixed
- **Advantages**:
  - Mirrors continuous feature fME: measures discrete change in prediction.
  - Any level can act as baseline - no fixed reference needed.



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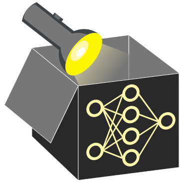

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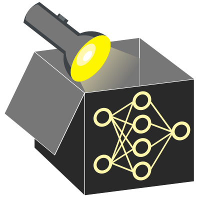

**Definition (based on fMEs with step $h_S$, can also be based on dMEs)**:

$$\text{AME}_S = \frac{1}{n}\sum_{i=1}^{n}\left[\hat{f}(\mathbf{x}_S^{(i)} + \mathbf{h}_S, \mathbf{x}_{-S}^{(i)}) - \hat{f}(\mathbf{x}^{(i)})\right]$$

**Why they work in GLMs**:

- Link function is monotonic $\Rightarrow$ direction of effect stable.
- Averaging gives sensible results (e.g., logit, probit).

**Why they fail on non-parametric models**:

- AMEs assume a consistent effect across the feature space.
- Non-parametric models can model complex, non-linear relationships.
- Averaging effects can obscure important heterogeneities.

**Takeaway:** AMEs can be useful summaries for smooth, monotonic models. For black-boxes, use **local fMEs** and support them with a non-linearity measure.



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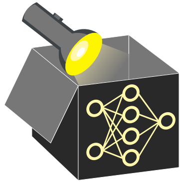

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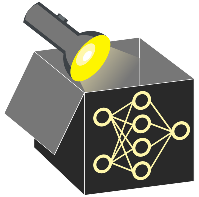

- **Single, formal number:** One scalar per observation; can be averaged (AME), reported with CIs, audited, stored easily.
- **Multivariate changes** Simultaneously perturb multiple *continuous/categorical* features. Still yields a scalar (unlike PD/ICE, which require multivariate plots).
- **Model-faithful, assumption-light** Measured at the *actual data point*. Captures interactions, no independence or surrogate-model assumptions (LIME).
- **Non-Linearity Measure:** Quantifies how well local linear approximation holds (e.g., via a normalized squared deviation from the secant).
  $\rightsquigarrow$ Local reliability measure, something PD/ICE plots cannot quantify.
- **Computationally cheap** Just two forward passes (or $k-1$ for a $k$-level factor) per observation vs. grid$\times n$ for PD/ICE.

**Conclusion: Plots let you *see* the landscape; ME give numbers you can *use*.**



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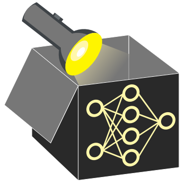

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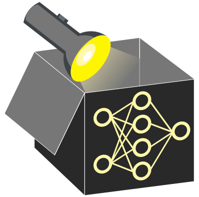
# USE-CASE: SCALAR VS. VISUAL ESTIMATION



**Setting:** A clinical model predicts heart attack risk from patient features, e.g., $x_1$ : systolic blood pressure (BP), $x_2$ : LDL cholesterol, $x_3$ : age, ...

**Clinician's questions**

- *"What if this patient's systolic BP increases by 10 mmHg?"*
- *"What if BP increases by 10 mmHg & LDL by 15 mg/dL?"*

**Route A – ICE / PD**

- Plot prediction as a function of BP (1-D) or BP+LDL (2-D) on a grid.
- Manual interpretation of change by looking at curve/surface.

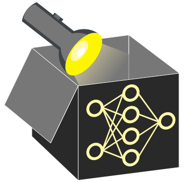
$\rightarrow$ Visual and local; limited to 1–2 features at a time.

**Route B – Forward Marginal Effect**: $\mathrm{fME} = \widehat{f}(\mathbf{x} + \mathbf{h}) - \widehat{f}(\mathbf{x})$

- **1-D case: h** $= (10, 0, 0, \dots)$ $\Rightarrow$ risk increases by **+3 percentage points**
- **2-D case: h** $= (10, 15, 0, \dots)$ $\Rightarrow$ risk increases by **+4.1 percentage points**
- One scalar answer per query, extensible to higher dimensions.



# USE-CASE: SCALAR VS. VISUAL ESTIMATION



**Setting:** A clinical model predicts heart attack risk from patient features, e.g., $x_1$ : systolic blood pressure (BP), $x_2$ : LDL cholesterol, $x_3$ : age, ...

**Clinician's questions**

- *"What if this patient's systolic BP increases by 10 mmHg?"*
- *"What if BP increases by 10 mmHg & LDL by 15 mg/dL?"*

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- **Individual Conditional Expectation (ICE)**:
  - Visualizes predictions for an observation across a range of feature values.
  - fME corresponds to vertical differences between points on an ICE curve.
- **Partial Dependence (PD)**:
  - Shows average predictions across a range of feature values.
  - AME is equivalent to vertical differences on PD for linear models.
- **Advantages of fMEs**:
  - Provide exact change in prediction.
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