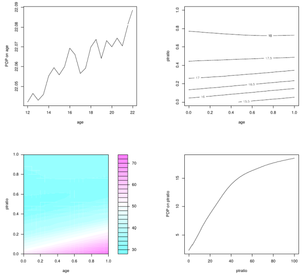
Interpretable Machine Learning

Introduction to Functional Decomposition



Learning goals

- Basic idea of additive functional decompositions
- Motivation and usefulness of functional decompositions
- Difficulty of obtaining or even defining a functional decomposition
- Several examples

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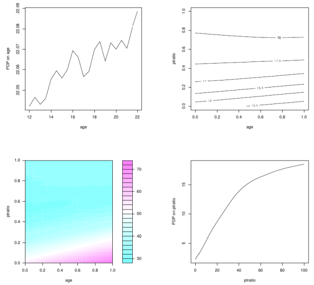
Functional Decompositions
Introduction



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- Interactions between features: Effect of one feature on the prediction output depends on (one or more) other features
- Definition: Features x_j and x_k are considered to interact, if

$$\mathbb{E}\left[\left(\frac{\partial^2 f(\mathbf{x})}{\partial x_j \partial x_k}\right)^2\right] > 0$$

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- Do not contain any interactions

$$\hat{f}(\mathbf{x}) = \theta_0 + g_1(x_1) + g_2(x_2) + \ldots + g_p(x_p)$$

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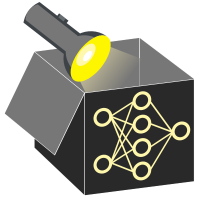

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$$\hat{f}(x_1, x_2) = 4 - 2x_1 + 0.3e^{x_2} + |x_1|x_2$$

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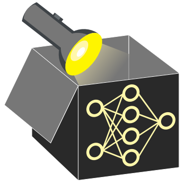

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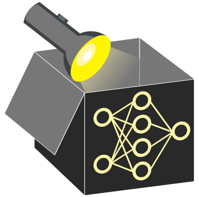

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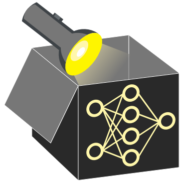

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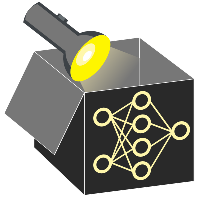

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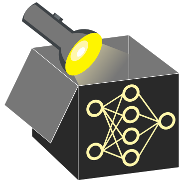

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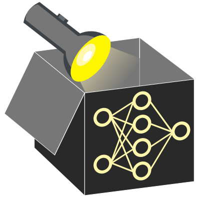

Goal in general: Given a black-box model $\hat{f} : \mathbb{R}^2 \to \mathbb{R}$, find a decomposition

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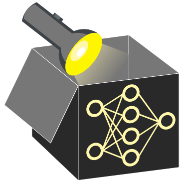

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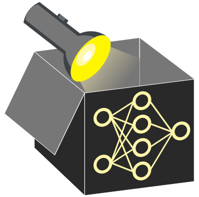

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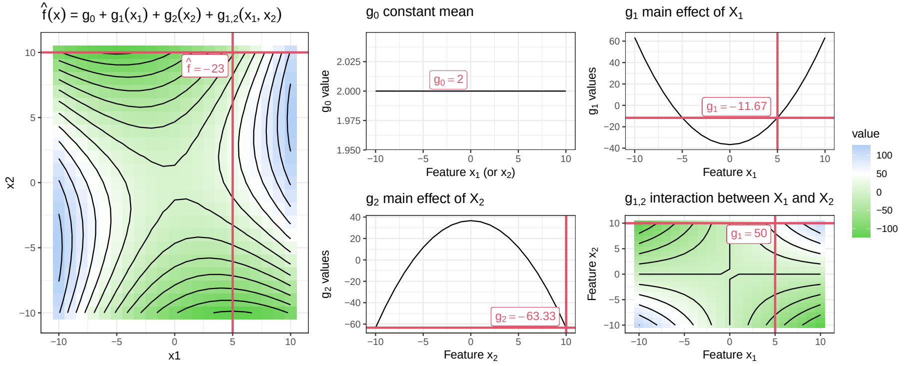

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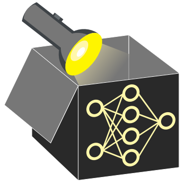
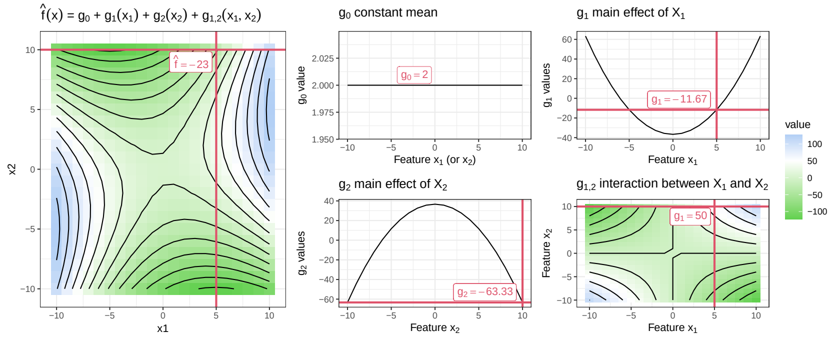
Interpretable Machine Learning – 3 / 11





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$\Rightarrow$ 8 components in total, but some empty $\rightsquigarrow$ Certain interactions not present

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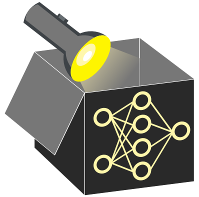
▸ Li and Rabitz (2011) ▸ Chastaing et al. (2012)



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$\rightsquigarrow$ one component for every possible combination S of indices, allowed to formally only depend on these features / be a function of these features

Problems:

- How to find / compute such a decomposition for arbitrary black-box models $\hat{f}$?
- . . . such that the decomposition is useful / has nice properties (w.r.t. the model / w.r.t. the data)?

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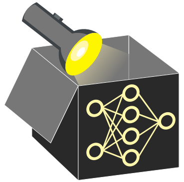

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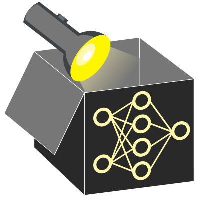

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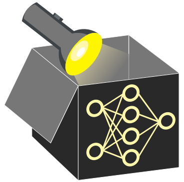

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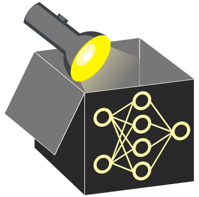

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  $\Longrightarrow$ Any GAM already comes with its decomposition

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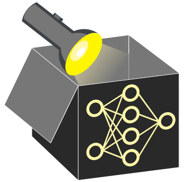

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Interpretable Machine Learning – 7 / 11

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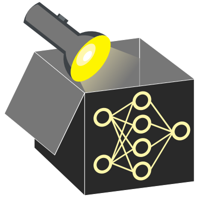

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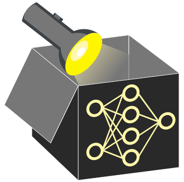

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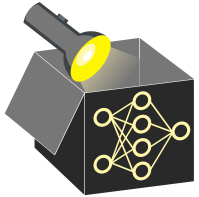

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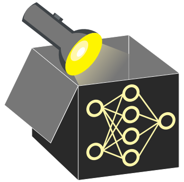

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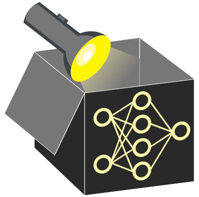

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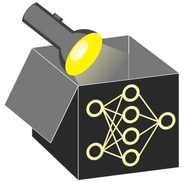

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$$\hat{f}(x_1, x_2, x_3) = -2x_1 - 2\sin(x_3) + |x_1|x_2 + 0.5x_1x_2x_3 - \sin(x_2x_3) + 1$$

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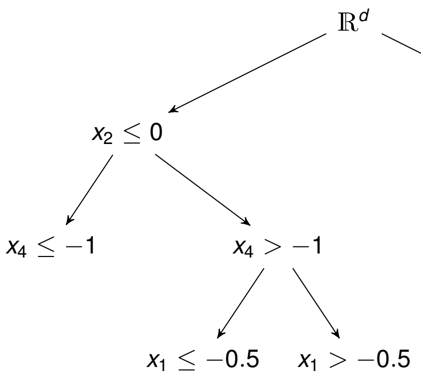

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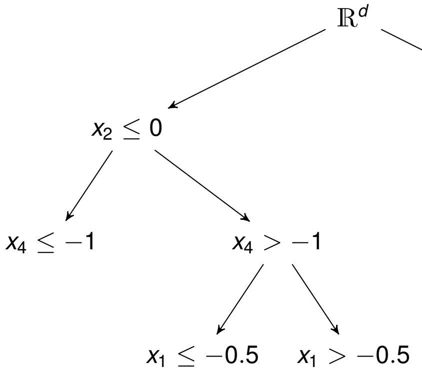

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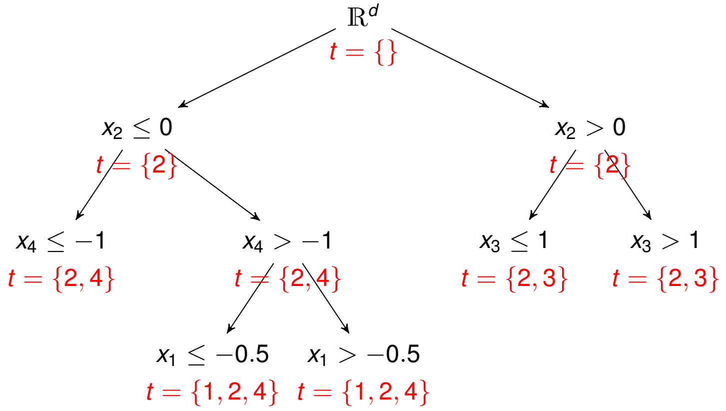

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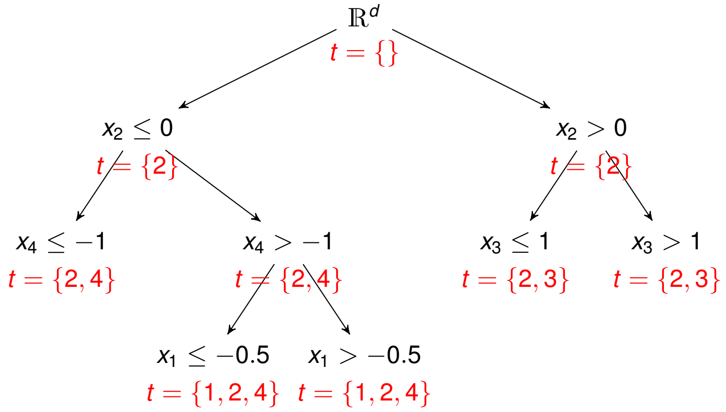

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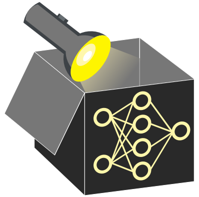

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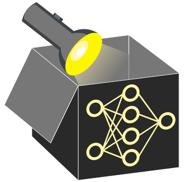

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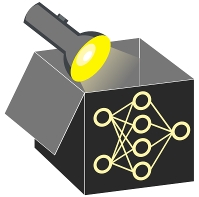

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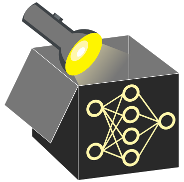

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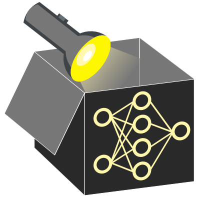

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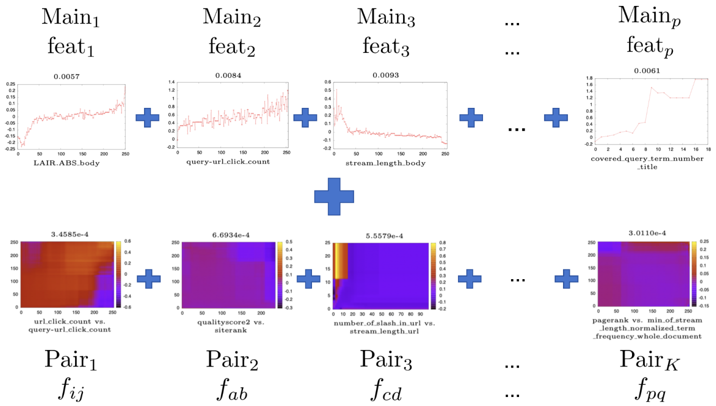

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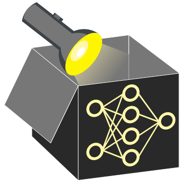

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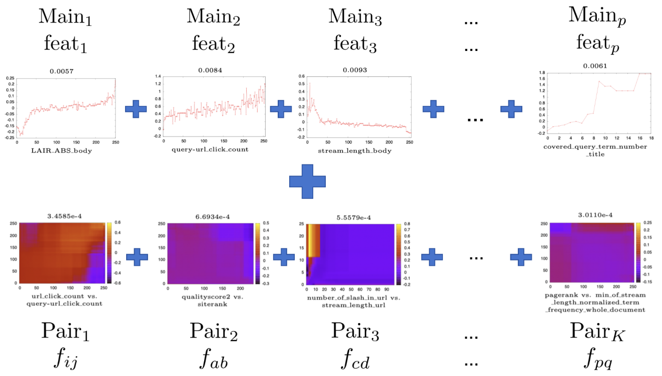

Interpretable Machine Learning – 11 / 11

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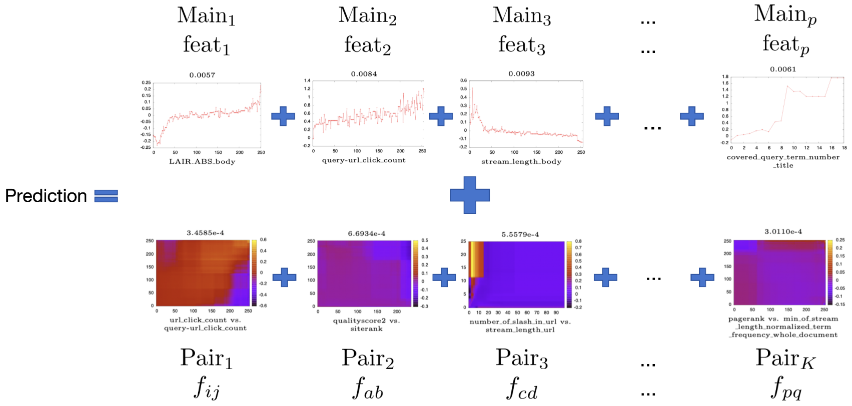

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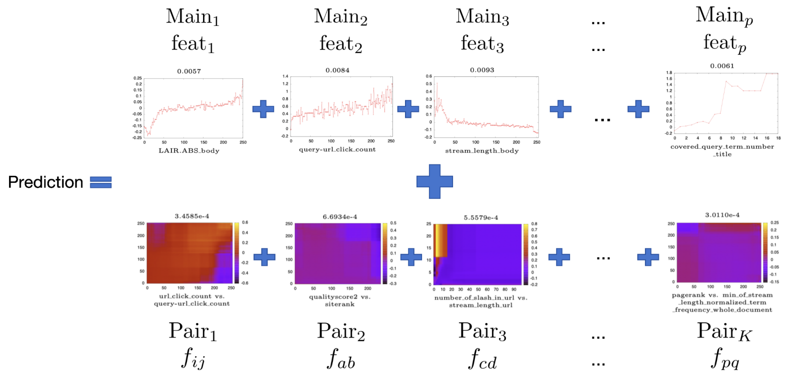

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