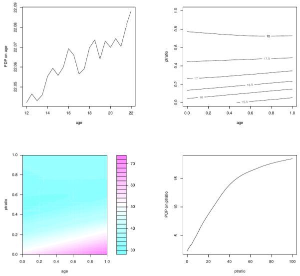
Interpretable Machine Learning

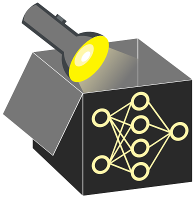
Introduction to Functional Decomposition



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

PRELIMINARIES

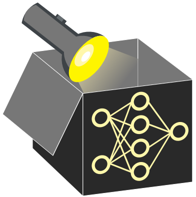


Recap: Interactions

- 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

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

PRELIMINARIES



Recap: Interactions

- 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

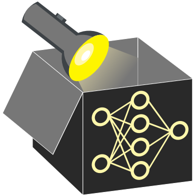
$$\mathbb{E}\left[\left(\frac{\partial^2 f(\mathbf{x})}{\partial x_j \partial x_k}\right)^2\right] > 0$$

Recap: GAMs

- Decomposition into only main effects
- Do not contain any interactions

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

FIRST EXAMPLE: ADDITIVE DECOMPOSITION



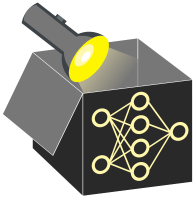
Example

Consider

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

- Idea: Additive decomposition depending on which features used:

FIRST EXAMPLE: ADDITIVE DECOMPOSITION



Example

Consider

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

- Idea: Additive decomposition depending on which features used:

$$g_\emptyset(x_1, x_2) = 4 \qquad \text{Part depending on no features at all (intercept)}$$

$$\left.\begin{aligned} g_1(x_1, x_2) &= 2x_1 \\ g_2(x_1, x_2) &= 0.3e^{x_2} \end{aligned}\right\} \quad \text{Parts depending on a single feature (main effects)} \tag{1}$$

$$g_{1,2}(x_1, x_2) = |x_1|x_2 \qquad \text{Part depending on both features (interaction)}$$

$\leadsto$ single terms with immediate interpretation, full understanding of the model

FIRST EXAMPLE: ADDITIVE DECOMPOSITION

Example

Consider

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

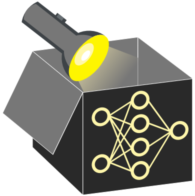
- Idea: Additive decomposition depending on which features used:

$$
\begin{aligned}
&g_{\emptyset}(x_1, x_2) = 4 && \text{Part depending on no features at all (intercept)} \\
&\left.\begin{aligned} g_1(x_1, x_2) &= 2x_1 \\ g_2(x_1, x_2) &= 0.3e^{x_2} \end{aligned}\right\} && \text{Parts depending on a single feature (main effects)} \quad (1) \\
&g_{1,2}(x_1, x_2) = |x_1|x_2 && \text{Part depending on both features (interaction)}
\end{aligned}
$$

$\rightsquigarrow$ single terms with immediate interpretation, full understanding of the model

$\leftrightarrow$ Not possible with effects of single features (e.g. PDPs) or GAM surrogate model (miss interaction part)

ANOTHER EXAMPLE: ADDITIVE DECOMPOSITION



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

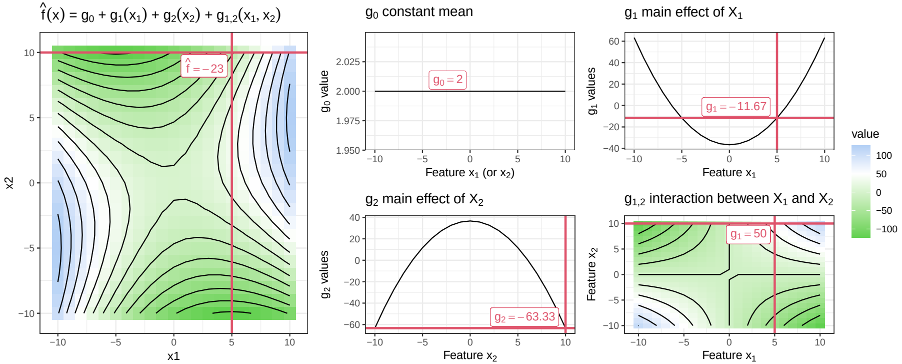
$$\hat{f}(x_1, x_2) = g_\emptyset + g_1(x_1) + g_2(x_2) + g_{1,2}(x_1, x_2) \quad (2)$$

ANOTHER EXAMPLE: ADDITIVE DECOMPOSITION

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

$$\hat{f}(x_1, x_2) = g_\emptyset + g_1(x_1) + g_2(x_2) + g_{1,2}(x_1, x_2) \tag{2}$$

Example



$\rightsquigarrow$ More details on this example later

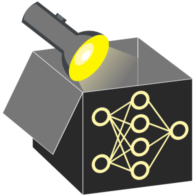
ANOTHER EXAMPLE: ADDITIVE DECOMPOSITION

Example

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

Again, read additive decomposition from formula:

ANOTHER EXAMPLE: ADDITIVE DECOMPOSITION



Example

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

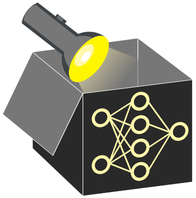
Again, read additive decomposition from formula:

$$\begin{aligned}
&g_\emptyset(x_1, x_2, x_3) = 1 && \text{constant part, no effects} \\
&\left.\begin{aligned} g_1(x_1, x_2, x_3) &= -2x_1 \\ g_2(x_1, x_2, x_3) &= 0 \\ g_3(x_1, x_2, x_3) &= -2\sin(x_3) \end{aligned}\right\} && \text{main effects, no interactions} \\
&\left.\begin{aligned} g_{1,2}(x_1, x_2, x_3) &= |x_1|x_2 \\ g_{1,3}(x_1, x_2, x_3) &= 0 \\ g_{2,3}(x_1, x_2, x_3) &= -\sin(x_2x_3) \end{aligned}\right\} && \text{2-way interactions (depending on 2 features)} \\
&g_{1,2,3}(x_1, x_2, x_3) = 0.5x_1x_2x_3 && \text{3-way interactions}
\end{aligned} \tag{3}$$

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

GENERAL FORM OF FUNCTIONAL DECOMPOSITION

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



Definition

Functional decomposition: Additive decomposition of a function $\hat{f} : \mathbb{R}^p \mapsto \mathbb{R}$ into a sum of components of different dimensions w.r.t. inputs $x_1, \ldots, x_p$:

$$\begin{aligned}\hat{f}(\mathbf{x}) &= \sum_{S \subseteq \{1,\ldots,p\}} g_S(\mathbf{x}_S) \\ &= g_\emptyset + g_1(x_1) + g_2(x_2) + \cdots + g_p(x_p) + \\ &\quad g_{1,2}(x_1, x_2) + \cdots + g_{p-1,p}(x_{p-1}, x_p) + \cdots + \\ &\quad g_{1,2,3}(x_1, x_2, x_3) + \cdots + g_{1,2,3,4}(x_1, x_2, x_3, x_4) + \cdots + g_{1,\ldots,p}(x_1, \ldots, x_p)\end{aligned}$$

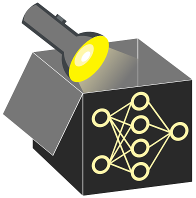
$\leadsto$ one component for every possible combination S of indices, allowed to formally only depend on these features / be a function of these features

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)?

GENERAL FORM OF FUNCTIONAL DECOMPOSITION

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



Definition

Functional decomposition: Additive decomposition of a function $\hat{f} : \mathbb{R}^p \mapsto \mathbb{R}$ into a sum of components of different dimensions w.r.t. inputs $x_1, \ldots, x_p$:

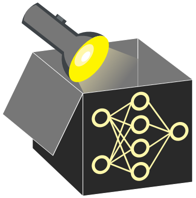
$$\begin{aligned}
\hat{f}(\mathbf{x}) &= \sum_{S \subseteq \{1,\ldots,p\}} g_S(\mathbf{x}_S) \\
&= g_\emptyset + g_1(x_1) + g_2(x_2) + \cdots + g_p(x_p) + \\
&\quad g_{1,2}(x_1, x_2) + \cdots + g_{p-1,p}(x_{p-1}, x_p) + \cdots + \\
&\quad g_{1,2,3}(x_1, x_2, x_3) + \cdots + g_{1,2,3,4}(x_1, x_2, x_3, x_4) + \cdots + g_{1,\ldots,p}(x_1, \ldots, x_p)
\end{aligned}$$

$\leadsto$ one component for every possible combination S of indices

Sort terms according to degree of interaction:

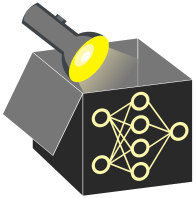
- $g_\emptyset \hat{=}$ Constant mean (intercept)
- $g_j \hat{=}$ first-order or main effect of j-th feature alone on $\hat{f}(\mathbf{x})$
- $g_{j,k} \hat{=}$ second-order interaction effect of features j and k w.r.t. $\hat{f}(\mathbf{x})$
- $g_S(\mathbf{x}_S) \hat{=} |S|$-order effect, depends **only** on features in S

PROPERTIES OF THE DEFINITION



- **Interpretability**: Extremely powerful decomposition, reveals complete interaction structure

PROPERTIES OF THE DEFINITION

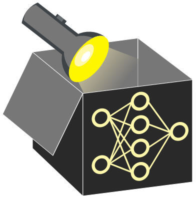


- **Interpretability**: Extremely powerful decomposition, reveals complete interaction structure
- Compare to GAM: Same decomposition, but without interactions
  $\Longrightarrow$ Any GAM already comes with its decomposition

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

- Same for LMs: Decomposition explicitly modeled

PROPERTIES OF THE DEFINITION

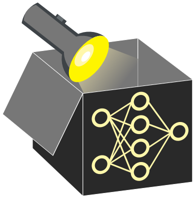


- **Interpretability**: Extremely powerful decomposition, reveals complete interaction structure
- Compare to GAM: Same decomposition, but without interactions
  $\Longrightarrow$ Any GAM already comes with its decomposition

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

- Same for LMs: Decomposition explicitly modeled
- Easy decomposition also for decision trees and tree ensembles (see below)

PROPERTIES OF THE DEFINITION

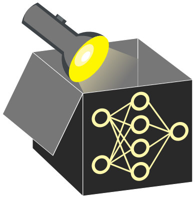


- **Interpretability**: Extremely powerful decomposition, reveals complete interaction structure
- Compare to GAM: Same decomposition, but without interactions
  $\Longrightarrow$ Any GAM already comes with its decomposition

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

- Same for LMs: Decomposition explicitly modeled
- Easy decomposition also for decision trees and tree ensembles (see below)
- **Problem 1:** Calculating decomposition extremely difficult, often infeasible
  - For p features: Decomposition with 2^p terms $\rightarrow$ too many different terms, difficult to interpret

PROPERTIES OF THE DEFINITION



- **Interpretability**: Extremely powerful decomposition, reveals complete interaction structure
- Compare to GAM: Same decomposition, but without interactions
  $\Longrightarrow$ Any GAM already comes with its decomposition

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

- Same for LMs: Decomposition explicitly modeled
- Easy decomposition also for decision trees and tree ensembles (see below)
- **Problem 1:** Calculating decomposition extremely difficult, often infeasible
  - For p features: Decomposition with 2^p terms $\rightarrow$ too many different terms, difficult to interpret
- **Problem 2:** Definition not complete: Decomposition not unique, many trivial decompositions not useful
  $\rightarrow$ More requirements or constraints needed to ensure decomposition is meaningful
  - Even worse once features are dependent or correlated (see later)

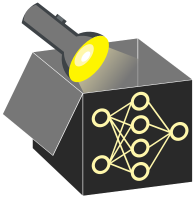
PROBLEM 2: DEFINITION NOT ENOUGH

Example

Again consider

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

PROBLEM 2: DEFINITION NOT ENOUGH



Example

Again consider

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

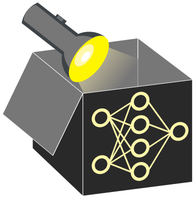
Two possible decompositions (valid according to definition):

$$g_{1,\ldots,p}(x_1, \ldots, x_p) := \hat{f}(\mathbf{x}) \text{ and for all other terms } g_S(\mathbf{x}_S) := 0,$$

or:

$$g_\emptyset = 1\,; \quad g_1(x_1) = x_1\,; \; g_2(x_2) = 2x_2\,; \; g_3(x_3) = 3x_3\,;$$
$$g_{1,2}(x_1, x_2) = \frac{1}{2}x_1x_2\,; \; g_{1,3}(x_1, x_3) = \frac{1}{3}x_1x_3\,; \; g_{2,3}(x_2, x_3) = \frac{2}{3}x_2x_3\,;$$
$$\text{and} \quad g_{1,2,3}(x_1, x_2, x_3) = \hat{f}(x_1, x_2, x_3) - \sum_{S \subsetneq \{1,2,3\}} g_S(\mathbf{x}_S)$$

PROBLEM 2: DEFINITION NOT ENOUGH



Example

Again consider

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

Two possible decompositions (valid according to definition):

$$g_{1,\dots,p}(x_1, \dots, x_p) := \hat{f}(\mathbf{x}) \text{ and for all other terms } g_S(\mathbf{x}_S) := 0,$$

or:

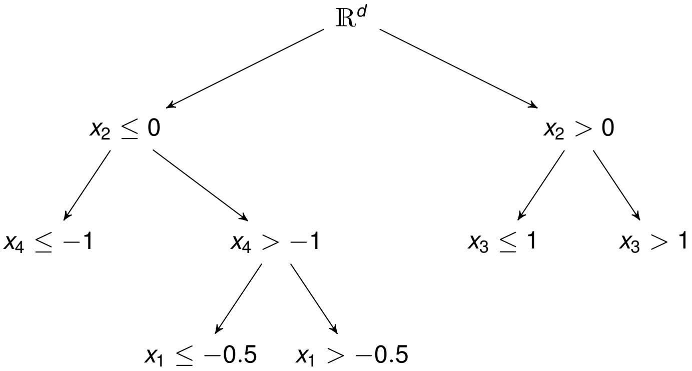
$$g_\emptyset = 1\,; \quad g_1(x_1) = x_1\,;\; g_2(x_2) = 2x_2\,;\; g_3(x_3) = 3x_3\,;$$
$$g_{1,2}(x_1, x_2) = \frac{1}{2}x_1x_2\,;\; g_{1,3}(x_1, x_3) = \frac{1}{3}x_1x_3\,;\; g_{2,3}(x_2, x_3) = \frac{2}{3}x_2x_3\,;$$
$$\text{and} \quad g_{1,2,3}(x_1, x_2, x_3) = \hat{f}(x_1, x_2, x_3) - \sum_{S \subsetneqq \{1,2,3\}} g_S(\mathbf{x}_S)$$

$\Longrightarrow$ Definition of decomposition not unique

EXAMPLE: DECISION TREES

Define *interaction type t* of a node: subset of features involved in constructing this node.

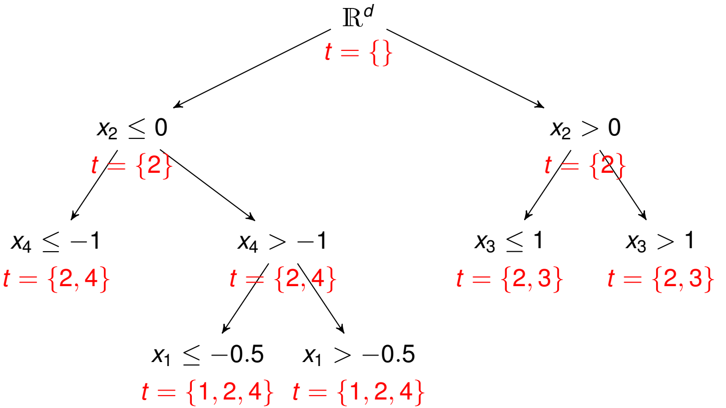
Example:



EXAMPLE: DECISION TREES

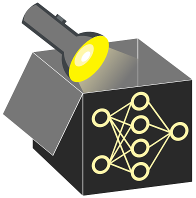
Define *interaction type t* of a node: subset of features involved in constructing this node.

Example:



$\Rightarrow$ Degree of interaction in each node is $|t|$.

DECOMPOSITION FOR DECISION TREES



Here: Decomposition via indicator functions

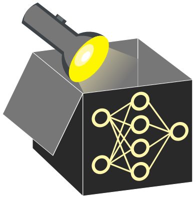
$$\hat{f}(\mathbf{x}) = g_{\emptyset} + g_{2,4}(x_2, x_4) + g_{2,3}(x_2, x_3) + g_{1,2,4}(x_1, x_2, x_4)$$

$\implies$ Decomposition has no main effect, but model certainly contains an effect of e.g. x_2

$\implies$ Lower-order effects “hidden” inside higher-order terms

$\rightsquigarrow$ reading from decision tree not enough, “bad decomposition”

DECOMPOSITION FOR DECISION TREES



Here: Decomposition via indicator functions

$$\hat{f}(\mathbf{x}) = g_{\emptyset} + g_{2,4}(x_2, x_4) + g_{2,3}(x_2, x_3) + g_{1,2,4}(x_1, x_2, x_4)$$

$\Longrightarrow$ Decomposition has no main effect, but model certainly contains an effect of e.g. x_2

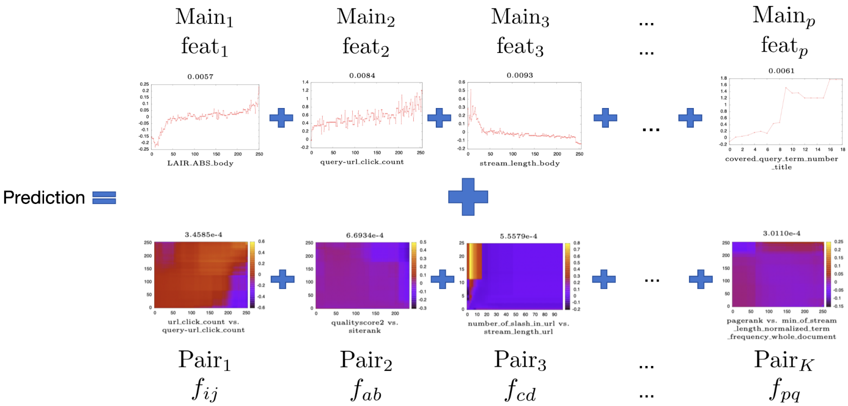
$\Longrightarrow$ Lower-order effects “hidden” inside higher-order terms

$\rightsquigarrow$ reading from decision tree not enough, “bad decomposition”

Note: ▸ Yang (2024) propose a (quite complicated) solution for this case

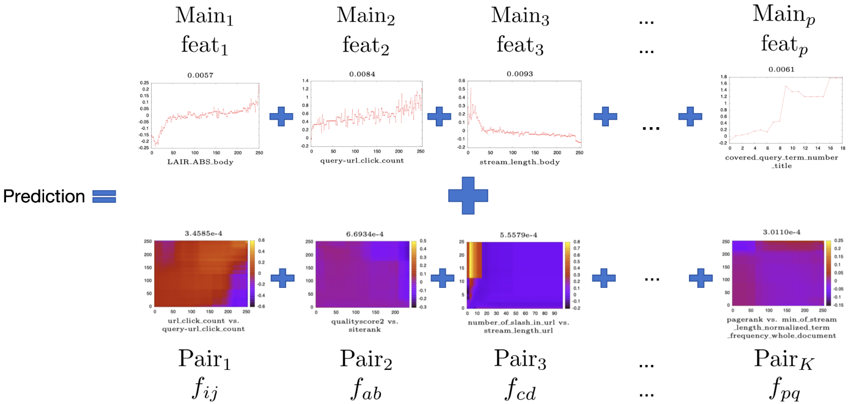
EXAMPLE: EBM

- See before: **GAMs** have functional decomposition by definition
- **EBMs:** Sum of the final one- and two-dimensional components



EXAMPLE: EBM

- See before: **GAMs** have functional decomposition by definition
- **EBMs:** Sum of the final one- and two-dimensional components



- In general: Model with functional decomposition up to max. order 2 is always "inherently interpretable"
- **Reason:** Visualization of all components