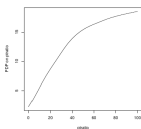
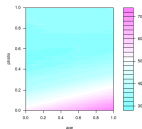
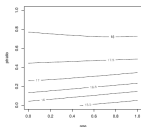
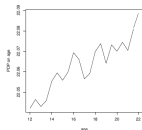
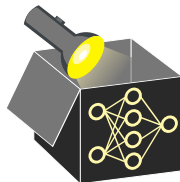


Interpretable Machine Learning

Functional Decompositions

Functional ANOVA

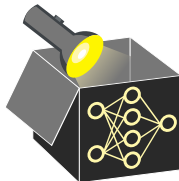


Learning goals

- One method for functional decomposition: Classical functional ANOVA (fANOVA)
- Algorithm for calculating the components in a fANOVA
- Variance decomposition in fANOVA

INTRODUCTION AND HISTORY OF FANOVA

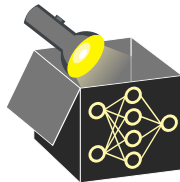
- One possible method to obtain functional decomposition
- Since 1940's: Developed under different names in mathematics and sensitivity analysis
- Since 1990's: Developed for probability distributions or statistical data
- Since 2000's: Applied to machine learning, subsequently alternatives developed extending applicability
- **Assumption:** Independent features



STANDARD FANOVA: IDEA

- Example:

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

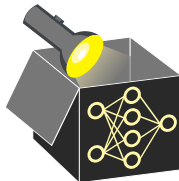


STANDARD FANOVA: IDEA

- Example:

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

- **First idea:** Make sure higher-order terms don't contain lower-order terms
⇒ First compute lower-order terms, then higher-order terms.

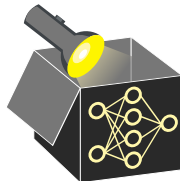


STANDARD FANOVA: IDEA

- Example:

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

- **First idea:** Make sure higher-order terms don't contain lower-order terms
⇒ First compute lower-order terms, then higher-order terms.
- **Second idea:** In 1st step, compute main effects using feat effect methods
Here: PDP + more general PD-functions



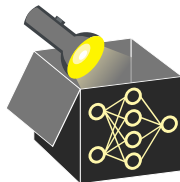
STANDARD FANOVA: IDEA

- Example:

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

- **First idea:** Make sure higher-order terms don't contain lower-order terms
⇒ First compute lower-order terms, then higher-order terms.
- **Second idea:** In 1st step, compute main effects using feat effect methods
Here: PDP + more general PD-functions
- **Idea for fANOVA:** PD-function $\hat{f}_{S;PD}$ = sum of all components $g_{\tilde{S}}$ up to this order

$$\hat{f}_{S;PD}(\mathbf{x}_S) = \sum_{V \subseteq S} g_V(\mathbf{x}_V)$$



STANDARD FANOVA: IDEA

- Example:

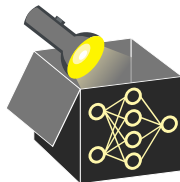
$$\hat{f}(x_1, x_2) = 4 - 2x_1 + 0.3e^{x_2} + |x_1|x_2$$

- **First idea:** Make sure higher-order terms don't contain lower-order terms
⇒ First compute lower-order terms, then higher-order terms.
- **Second idea:** In 1st step, compute main effects using feat effect methods
Here: PDP + more general PD-functions
- **Idea for fANOVA:** PD-function $\hat{f}_{S;PD}$ = sum of all components $g_{\tilde{S}}$ up to this order

$$\hat{f}_{S;PD}(\mathbf{x}_S) = \sum_{V \subseteq S} g_V(\mathbf{x}_V)$$

- **Remember:**
Idea of PDPs or general PD-functions: Average out all other features
⇒ Total formula for calculating the components g_S in the fANOVA algorithm:

$$g_S(\mathbf{x}_S) = (\text{average out all features not contained in } S) \\ - (\text{All lower-order components})$$



FORMAL DEFINITION AND COMPUTATION

► “Hooker” 2004

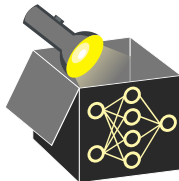
Definition

Recursive computation using PD-functions

(here $-S = \{1, \dots, p\} \setminus S$ denotes all indices not contained in S):

$$\begin{aligned} g_S(\mathbf{x}_S) &= \hat{f}_{S;PD}(\mathbf{x}_S) - \sum_{V \subseteq -S} g_V(\mathbf{x}_V) = \mathbb{E}_{\mathbf{x}_{-S}} \left[\hat{f}(\mathbf{x}_S, \mathbf{x}_{-S}) \right] - \sum_{V \subseteq -S} g_V(\mathbf{x}_V) \\ &= \int \hat{f}(\mathbf{x}_S, \mathbf{x}_{-S}) d\mathbb{P}(\mathbf{x}_{-S}) - \sum_{V \subseteq -S} g_V(\mathbf{x}_V) \end{aligned}$$

- Expectation integrates $\hat{f}(\mathbf{x})$ over all input features except \mathbf{x}_S
- Subtract sum of g_V to remove all lower-order effects and center the effect
- **Note:** If no distribution given: Uniform distribution or plain integral



FORMAL DEFINITION AND COMPUTATION

► "Hooker" 2004

Definition

Recursive computation using PD-functions

(here $-S = \{1, \dots, p\} \setminus S$ denotes all indices not contained in S):

$$g_S(\mathbf{x}_S) = \hat{f}_{S;PD}(\mathbf{x}_S) - \sum_{\substack{V \subseteq S \\ V \neq S}} g_V(\mathbf{x}_V) = \mathbb{E}_{\mathbf{x}_{-S}} \left[\hat{f}(\mathbf{x}_S, \mathbf{x}_{-S}) \right] - \sum_{\substack{V \subseteq S \\ V \neq S}} g_V(\mathbf{x}_V)$$

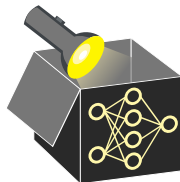
- Recursive computation:

$$g_{\emptyset} = \mathbb{E}_{\mathbf{X}} \left[\hat{f}(\mathbf{X}) \right]$$

$$g_j(x_j) = \mathbb{E}_{\mathbf{x}_{-j}} \left[\hat{f}(\mathbf{X}) \mid X_j = x_j \right] - g_{\emptyset}, \quad \forall j \in \{1, \dots, p\}$$

$$\vdots$$

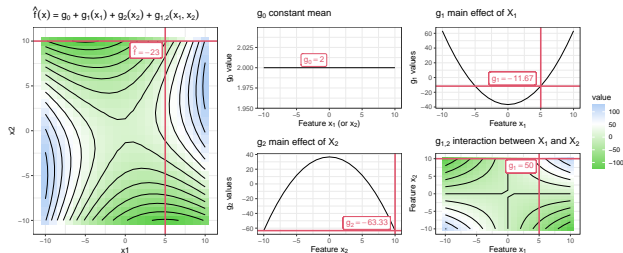
$$\begin{aligned} g_{1,\dots,p}(\mathbf{x}) &= \hat{f}(\mathbf{x}) - \sum_{S \subsetneq \{1,\dots,p\}} g_S(\mathbf{x}_S) \\ &= \hat{f}(\mathbf{x}) - g_{1,\dots,p-1}(x_1, \dots, x_{p-1}) - \dots - g_{1,2}(x_1, x_2) \\ &\quad - g_p(x_p) - \dots - g_2(x_2) - g_1(x_1) - g_{\emptyset} \end{aligned}$$



STANDARD FANOVA – EXAMPLE

Example: $\hat{f}(\mathbf{x}) = 2 + x_1^2 - x_2^2 + x_1 \cdot x_2$ (e.g., for $x_1 = 5$ and $x_2 = 10$ we have $\hat{f}(\mathbf{x}) = -23$)

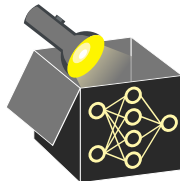
- Computation of components using feature values $x_1 = x_2 = (-10, -9, \dots, 10)^\top$ gives:



For $x_1 = 5$ and $x_2 = 10$:

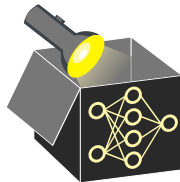
- $g_0 = 2$
- $g_1(x_1) = -9.67$
- $g_2(x_2) = -65.33$
- $g_{1,2}(x_1, x_2) = 50$

$$\Rightarrow \hat{f}(\mathbf{x}) = -23$$



STANDARD FANOVA - EXAMPLE

In-class task



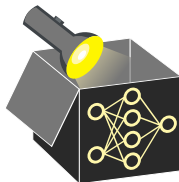
STANDARD FANOVA - EXAMPLE REVISITED

Example

$$\hat{f}(x_1, x_2) = 4 - 2x_1 + 0.3e^{x_2} + |x_1|x_2 \quad (x_1, x_2) \in [0, 1]^2 \quad \text{uniformly distributed}$$

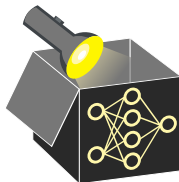
- **Intercept:**

$$\begin{aligned} g_\emptyset &= \mathbb{E}[\hat{f}(x_1, x_2)] = \int_0^1 \int_0^1 4 - 2x_1 + 0.3e^{x_2} + |x_1|x_2 \, dx_1 \, dx_2 \\ &= 4 - \left(\int_0^1 2x_1 \, dx_1 \right) + \left(\int_0^1 0.3e^{x_2} \, dx_2 \right) + \left(\int_0^1 |x_1| \, dx_1 \right) \left(\int_0^1 x_2 \, dx_2 \right) \\ &= 4 - 1 + 0.3(e - 1) + 0.5^2 = 2.95 + 0.3e. \end{aligned}$$



STANDARD FANOVA - EXAMPLE REVISITED

Example



$$\hat{f}(x_1, x_2) = 4 - 2x_1 + 0.3e^{x_2} + |x_1|x_2 \quad (x_1, x_2) \in [0, 1]^2 \quad \text{uniformly distributed}$$

- **First-order components:**

$$\begin{aligned} g_1(x_1) &= \hat{f}_{1;PD}(x_1) - g_\emptyset = \left(\int_0^1 4 - 2x_1 + 0.3e^{x_2} + |x_1|x_2 \, dx_2 \right) - g_\emptyset \\ &= 4 - 2x_1 + 0.3(e - 1) + |x_1| \cdot \frac{1}{2} - (2.95 + 0.3e) \\ &= -2x_1 + 0.5|x_1| + 0.75 \end{aligned}$$

$$\begin{aligned} g_2(x_2) &= \hat{f}_{2;PD}(x_2) - g_\emptyset = \left(\int_0^1 4 - 2x_1 + 0.3e^{x_2} + |x_1|x_2 \, dx_1 \right) - g_\emptyset \\ &= 4 - 1 + 0.3e^{x_2} + \frac{1}{2} \cdot x_2 - (2.95 + 0.3e) \\ &= 0.3e^{x_2} + 0.5x_2 - 0.3e + 0.05 \end{aligned}$$

STANDARD FANOVA - EXAMPLE REVISITED

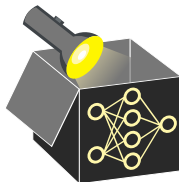
Example

$$\hat{f}(x_1, x_2) = 4 - 2x_1 + 0.3e^{x_2} + |x_1|x_2 \quad (x_1, x_2) \in [0, 1]^2 \quad \text{uniformly distributed}$$

- **Second-order component:**

$$\begin{aligned} g_{12}(x_1, x_2) &= \hat{f}_{\{1,2\};PD}(x_1, x_2) - g_{\emptyset} - g_1(x_1) - g_2(x_2) \\ &= 4 - 2x_1 + 0.3e^{x_2} + |x_1|x_2 - (2.95 + 0.3e) \\ &\quad - (-2x_1 + 0.5|x_1| + 0.75) - (0.3e^{x_2} + 0.5x_2 - 0.3e + 0.05) \\ &= |x_1|x_2 - 0.5|x_1| - 0.5x_2 + 0.25 \end{aligned}$$

- ⇒ All components shifted to have mean 0
- ⇒ Parts of $|x_1|x_2$, which intuitively seems to be the “interaction term”, is attributed to the main effects (correctly, depends on distribution!)



ESTIMATE FANOVA IN PRACTICE

Main part: Calculate all PD-functions $\rightarrow 2^p$ many PD-functions

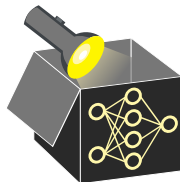
Estimation of a single PD-function: **Sampling**

(so-called **Monte-Carlo integration**)

- Same idea as for PDPs: Fix **grid values** for features \mathbf{x}_S
Here: Same grid for all features over the whole algorithm
- Estimate integral by sampling: for grid value \mathbf{x}_S^* :

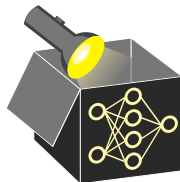
$$\hat{f}_{S,PD}(\mathbf{x}_S^*) = \mathbb{E}_{\mathbf{x}_{-S}} \left[\hat{f}(\mathbf{x}_S^*, \mathbf{x}_{-S}) \right] \approx \frac{1}{n} \sum_{i=1}^n \hat{f}(\mathbf{x}_S^*, \mathbf{x}_{-S}^{(i)})$$

- Or: for each grid value \mathbf{x}_S^* , sample only $n_s < n$ many random samples (e.g. sampling uniformly)



VARIANCE DECOMPOSITION - WHY “FUNCTIONAL ANOVA”?

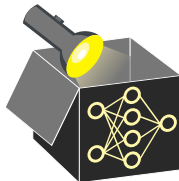
- Decomp. of $\hat{f}(\mathbf{x})$ allows for “functional analysis of variance” (fANOVA)



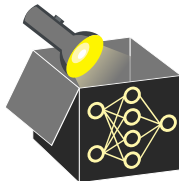
VARIANCE DECOMPOSITION - WHY “FUNCTIONAL ANOVA”?

- Decomp. of $\hat{f}(\mathbf{x})$ allows for “functional analysis of variance” (fANOVA)
- One can prove: If features independent \Rightarrow additive decomposition of variance of \hat{f} possible without covariances:

$$\begin{aligned}\text{Var} \left[\hat{f}(\mathbf{x}) \right] &= \text{Var} \left[g_{\emptyset} + g_1(x_1) + \dots + g_{1,2}(x_1, x_2) + \dots + g_{1,\dots,p}(\mathbf{x}) \right] \\ &= \text{Var} [g_{\emptyset}] + \text{Var} [g_1(x_1)] + \dots + \text{Var} [g_{1,2}(x_1, x_2)] + \dots + \text{Var} [g_{1,\dots,p}(\mathbf{x})]\end{aligned}$$



VARIANCE DECOMPOSITION - WHY “FUNCTIONAL ANOVA”?



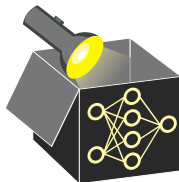
- Decomp. of $\hat{f}(\mathbf{x})$ allows for “functional analysis of variance” (fANOVA)
- One can prove: If features independent \Rightarrow additive decomposition of variance of \hat{f} possible without covariances:

$$\begin{aligned}\text{Var} \left[\hat{f}(\mathbf{x}) \right] &= \text{Var} \left[g_{\emptyset} + g_1(x_1) + \dots + g_{1,2}(x_1, x_2) + \dots + g_{1,\dots,p}(\mathbf{x}) \right] \\ &= \text{Var} [g_{\emptyset}] + \text{Var} [g_1(x_1)] + \dots + \text{Var} [g_{1,2}(x_1, x_2)] + \dots + \text{Var} [g_{1,\dots,p}(\mathbf{x})]\end{aligned}$$

- In other words: Single components uncorrelated (see later)

$$1 = \frac{\text{Var} [g_{\emptyset}]}{\text{Var} [\hat{f}(\mathbf{x})]} + \frac{\text{Var} [g_1(x_1)]}{\text{Var} [\hat{f}(\mathbf{x})]} + \dots + \frac{\text{Var} [g_{1,2}(x_1, x_2)]}{\text{Var} [\hat{f}(\mathbf{x})]} + \dots + \frac{\text{Var} [g_{1,\dots,p}(\mathbf{x})]}{\text{Var} [\hat{f}(\mathbf{x})]}$$

VARIANCE DECOMPOSITION - WHY “FUNCTIONAL ANOVA”?



- Decomp. of $\hat{f}(\mathbf{x})$ allows for “functional analysis of variance” (fANOVA)
- One can prove: If features independent \Rightarrow additive decomposition of variance of \hat{f} possible without covariances:

$$\begin{aligned}\text{Var} [\hat{f}(\mathbf{x})] &= \text{Var} [g_{\emptyset} + g_1(x_1) + \dots + g_{1,2}(x_1, x_2) + \dots + g_{1,\dots,p}(\mathbf{x})] \\ &= \text{Var} [g_{\emptyset}] + \text{Var} [g_1(x_1)] + \dots + \text{Var} [g_{1,2}(x_1, x_2)] + \dots + \text{Var} [g_{1,\dots,p}(\mathbf{x})]\end{aligned}$$

- In other words: Single components uncorrelated (see later)

$$1 = \frac{\text{Var} [g_{\emptyset}]}{\text{Var} [\hat{f}(\mathbf{x})]} + \frac{\text{Var} [g_1(x_1)]}{\text{Var} [\hat{f}(\mathbf{x})]} + \dots + \frac{\text{Var} [g_{1,2}(x_1, x_2)]}{\text{Var} [\hat{f}(\mathbf{x})]} + \dots + \frac{\text{Var} [g_{1,\dots,p}(\mathbf{x})]}{\text{Var} [\hat{f}(\mathbf{x})]}$$

→ **Sobol index**: Fraction of variance explained by some component $g_V(\mathbf{x}_V)$:

$$S_V = \frac{\text{Var} [g_V(\mathbf{x}_V)]}{\text{Var} [\hat{f}(\mathbf{x})]}$$

↪ Usable as importance measure of component $g_V(\mathbf{x}_V)$