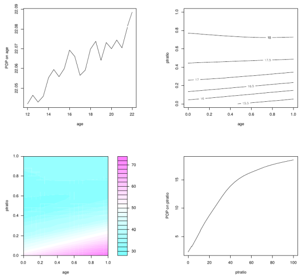
Interpretable Machine Learning

Functional ANOVA

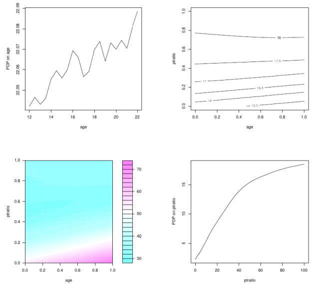


Learning goals

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

Interpretable Machine Learning

Functional Decompositions
Functional ANOVA



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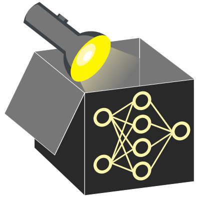
INTRODUCTION AND HISTORY OF FANOVA



- One possible method to obtain functional decomposition
- Since 1940's: Developed under different names in mathematics and sensitivity analysis
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- Since 2000's: Applied to machine learning, subsequently alternatives developed extending applicability
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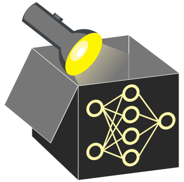

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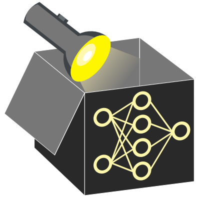

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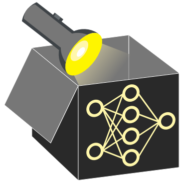

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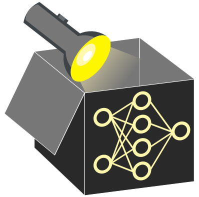

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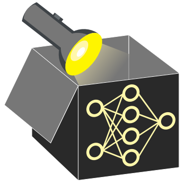

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Idea of PDPs or general PD-functions: Average out all other features

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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):

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

$$= \int \hat{f}(\mathbf{x}_S, \mathbf{x}_{-S}) d\mathbb{P}(\mathbf{x}_{-S}) - \sum_{V \subsetneq S} g_V(\mathbf{x}_V)$$

- 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

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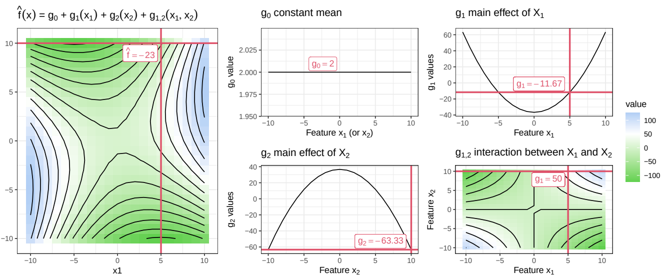
STANDARD FANOVA – EXAMPLE

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 $x_2 = 10$:

- $g_\emptyset = 2$
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- $g_{1,2}(x_1, x_2) = 50$

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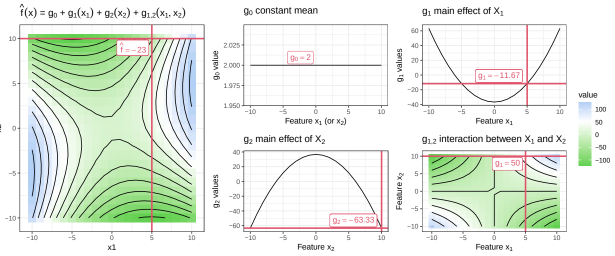

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STANDARD FANOVA - EXAMPLE

In-class task

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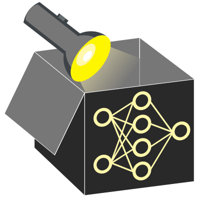
STANDARD FANOVA - EXAMPLE REVISITED



Example

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

- **Intercept:**

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g_{\emptyset} = \mathbb{E}\left[\hat{f}(x_1, x_2)\right] &= \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}
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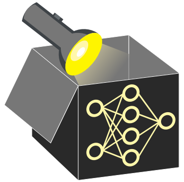
STANDARD FANOVA - EXAMPLE REVISITED



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$\Rightarrow$ All components shifted to have mean 0

$\Rightarrow$ Parts of $|x_1|x_2$, which intuitively seems to be the “interaction term”, is attributed to the main effects (correctly, depends on distribution!)

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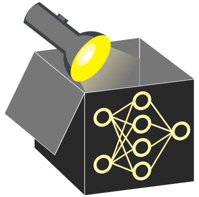

Main part: Calculate all PD-functions $\rightarrow 2^p$ **many PD-functions**
Estimation of a single PD-function: **Sampling**
(so-called **Monte-Carlo integration**)

- Same idea as for PDPs: Fix **grid values** for features 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)

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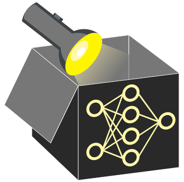

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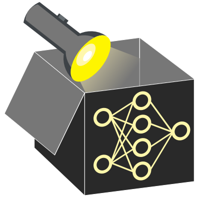
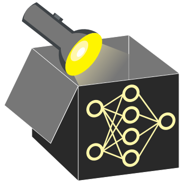


- Decomposition of $\hat{f}(\mathbf{x})$ allows for “functional analysis of variance” (fANOVA)
- One can prove: If features independent $\Rightarrow$ additive decomposition of variance of $\hat{f}$ possible without covariances:

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

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:

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

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

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

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

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

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

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