Bachelor's Thesis

fANOVA for Interpretable Machine Learning

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Abstract

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Contents

1 Introduction

Questions

Clarifying the connection between fANOVA, expected value, and projection & bringing together different definitions

When I start from Muehlenstaedt et al. (2012) and basically go the way: *fANOVA term* $\rightarrow$ *expected value* $\rightarrow$ *projection*, I arrive at the formulation where we first compute the projection and afterwards subtract lower order terms. For example following the definition by Muehlenstaedt et al. (2012) and using the parallel between (conditional) expected value and the projection (Van Ravenzwaaij et al., 2018) we can write for example for $u = \{1, 2\}$:

$$\begin{aligned} y_{12}(.;.) &:= \mathbb{E}[y(\boldsymbol{X}) \mid X_1, X_2] - y_\emptyset - y_{\{1\}}(\cdot) - y_{\{2\}}(\cdot) \\ &= \arg\min_{g_{\{1,2\}} \in \mathcal{G}_{\{1,2\}}} \mathbb{E}\left[(y(\boldsymbol{X}) - g_{\{1,2\}}(X_1, X_2))^2\right] - y_\emptyset - y_{\{1\}}(\cdot) - y_{\{2\}}(\cdot) \\ &= (\Pi_{\mathcal{G}_{\{1,2\}}} y)(.;.) - y_\emptyset - y_{\{1\}}(\cdot) - y_{\{2\}}(\cdot) \end{aligned}$$

But when I get it correctly Hooker (2007) writes his generalized fANOVA components as the projection of the differences. Also, he goes the other way around, starting from the projections (and we could restate this as the conditional expected value).
Because Hooker defines the fANOVA terms as:

$$\{f_u(x_u) \mid u \subseteq d\} = \arg\min_{\{g_u \in L^2(\mathbb{R}^u)\}_{u \subseteq d}} \int \left(y(\boldsymbol{x}) - \sum_{u \subseteq d} g_u(x_u) \right)^2 w(\boldsymbol{x})\, d\boldsymbol{x} \tag{1}$$

And I think we can rewrite this as the conditional expected value. For example for $u = \{1, 2\}$:

$$\begin{aligned} y_{12}(.;.) &:= \arg\min_{g_{\{1,2\}} \in L^2(\mathbb{R}^2)} \int \left(y(\boldsymbol{x}) - \sum_{\{1,2\}} g_{\{1,2\}}(.;.) \right)^2 w(\boldsymbol{x})\, d\boldsymbol{x} \\ &= \arg\min_{g_{\{1,2\}} \in L^2(\mathbb{R}^2)} \int \left(y(\boldsymbol{x}) - y_\emptyset - y_{\{1\}}(\cdot) - y_{\{2\}}(\cdot) - g_{\{1,2\}}(.;.) \right)^2 w(\boldsymbol{x})\, d\boldsymbol{x} \\ &= \arg\min_{g_{\{1,2\}} \in L^2(\mathbb{R}^2)} \mathbb{E}[(y(\boldsymbol{X}) - y_\emptyset - y_{\{1\}}(X_1) - y_{\{2\}}(X_2) - g_{\{1,2\}}(X_1, X_2))^2] \\ &= (\Pi_{\mathcal{G}_{\{1,2\}}}(y - y_\emptyset - y_{\{1\}}(\cdot) - y_{\{2\}}(\cdot)))(.;.) \\ &= \mathbb{E}[y(\boldsymbol{X}) - y_\emptyset - y_{\{1\}}(X_1) - y_{\{2\}}(X_2) | X_1 = x_1, X_2 = x_2] \end{aligned}$$

So Hooker (2007) defines the fANOVA terms via the projection *fANOVA term* $\rightarrow$ *projec-*

tion → expected value (not in Hooker). But he takes the projection of the differences.

- Could it happen that based on fANOVA decomposition we build a model which uses the interaction effect of i, j but not the main effects i and/or j?
- Can I really compute the generalized fANOVA terms a proposed by Hooker (2007) by hand? Molnar writes: "The estimation is done on a grid of points in the feature space and is stated as a minimization problem that can be solved using regression techniques. However, the components cannot be computed independently of each other, nor hierarchically, but a complex system of equations involving other components has to be solved. The computation is therefore quite complex and computationally intensive." *If he would write he generalized fANOVA as conditional expected values it is actually not that complicated and we simply would need to solve regression problems hierarchically.*
- I am still confused if setting the zero-mean constraint for $X_i \overset{\text{i.i.d.}}{\sim} \mathcal{U}[0, 1]$ is essentially saying that we centre the distribution and now assume $X_i \overset{\text{i.i.d.}}{\sim} \mathcal{U}[-1, 1]$. So can we, instead of explicitly stating the zero-mean constraint just assume $X_i \overset{\text{i.i.d.}}{\sim} \mathcal{U}[-1, 1]$? And following the same principle we would shift other distributions by altering their parameters, not by explicitly stating the zero-mean constraint? Then for the standard normal distribution we wouldn't need to do anything, it is already centred around 0. For other distributions we would need to change, and for some it doesn't make inhaltlichen Sinn e.g. Poisson distribution? *No generally zero-mean constraint and distribution assumption of the variables has no connection. The zero-mean constraint is sth. we set for the fANOVA terms y_u while distribution assumption is about the input variables X_i. We don't set the zero-mean constraint for the variables"*
-
- fANOVA decomposition via the integral, how would the zero mean constraint look here? (see "General_fANOVA_handnotes")
- Can you reconstruct the function from only the fANOVA terms? I think it can be reconstructed only if variables are independent, have zero-mean, are orthogonal?
- Is it possible to perform fANOVA for non-square-integrable functions? *in general yes but the variance decomposition doesn't work then or might have problems.*
- fANOVA decomposition for discrete variables possible? Does it make sense even?

- Connection between the (conditional) expected value, (partial) integral, projections (section **??**)?
- In the hierarchical orthogonality condition (4.2) formulated in Hooker (2007) for the gerneralized fAVNOA framework, shouldn't we explicitly exclude the case that $v = u$, because then, we would require that the inner product of the fANOVA component is zero wouldn't we (section 5)?
- Why is it a problem, when explainability methods also place large emphasis on regions of low probability mass when dependencies between variables exist - because in the end explainability is about explaining the model, not the data generating process; and after all it is how the model works in these regions. [But as the Hooker example illustrates, how the model works and what it estimates in these regions is wrong and then it's better to not report any model behaviour or come closer to the DGP than to give wrong estimations?]
-
- Use of AI tools?
- Do we need to restrict ourselves to the unit hypercube? Or does fANOVA decomposition work in general, but maybe with some constraints? Originally it was constructed for models on the unit hypercube $[0, 1]$, but other papers also use models from R^d *Generally no restriction, so next step could be to generalize, to* $\mathbb{R}^n$*, other measures, dependent variables*
- Still unclear: Are the terms fully orthogonal or hierarchically? See subsection on Orthogonality of the fANOVA terms (especially the example) I think in the original fANOVA decomposition the terms are orthogonal but in the generalized fANOVA (Hooker, 2007) they are hierarchically orthogonal. *fully orthogonal when independence assumption, probably partially when no independence*
- $x_1, \ldots, x_k$ are simply the standardized features, right? *Yes*
- My current understanding: we need independence of $x_1, \ldots x_k$ so that fANOVA decomposition is unique (and orthogonality holds). We need zero-mean constraint for the orthogonality of the components. We need orthogonality for the variance decomposition.*zero-mean* $\rightarrow$ *orthogonality* $\rightarrow$ *uniqueness; Lemma 1 im Hooker 2007 ist verallgemeinerg ds zero-mean constraint*

- Next step might be to investigate the (mathematical) parallels of fANOVA decomposition and other IML methods (PDP, ALE, SHAP), e.g. there is definitely a strong relationship between Partial dependence (PD) and fANOVA terms, and PD is itself again related to other IML methods; Also look how are other IML models studied and study fANOVA in a similar way (e.g. other IML methods are defined, checked for certain properties, examined under different conditions (dependent features, independent features) etc.) (see dissertation by Christoph Molnar for this); Also I would be very interested in investigating the game theory paper further (Fumagalli et al., 2025) but still a bit unsure if it is too complex.

- Why does a fANOVA decomposition of a simple GAM not lead to the "true" coefficients? https://christophm.github.io/interpretable-ml-book/decomposition.html talks about this a bit in the subchapter "Statistical regression models" *It should actually lead to the GAM; at least under all the constraint like zero-mean constraint and orthogonality*

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- In Hooker (2004) they work with $F(x)$ and $f(x)$, but in Sobol (2001) they only work with $f(x)$. I think this is only notation? *Only notation.*

- Does orthogonality in fANOVA context mean that all terms are orthogonal to each other? Or that a term is orthogonal to all lower-order terms ("Hierarchical orthogonality ")? *The terms are hierarchically orthogonal, so each term is orthogonal to all lower-order terms, but not to the same-order terms! So f_1 is not necessarily orthogonal to f_2 but it is orthogonal to f_{12}, f_0.*

- Do the projections here serve as approximations? (linalg skript 2024 5.7.4 Projektionen als beste Annäherung) *Yes, they can be interpreted as sort of approximation.*

- Which sub-space are we exactly projecting onto? Are the projections orthogonal by construction (orthogonal projections) or only when the zero-mean constraint is set? *The subspace we project onto depends on the component. For f_0 we project onto the subspace of constant functions, for f_1 we project onto the subspace of all functions that involve x_1 and have an expected value of 0 (zero-mean constraint to ensure orthogonality). It depends on the formulation of the fANOVA decomposition if you need to explicitly set the zero-mean constraint for orthogonality or if it is met by construction.*

- How "far"should I go back, formally introduce L^2 space, etc. or assume that the reader is familiar with it? *Yes, space, the inner product on this space should be formally introduced.*

2 Background Knowledge

Basic Setup

Let $(\Omega, \mathcal{F}, \nu)$ be a measure space, where Ω is a sample space, $\mathcal{F}$ is a $\sigma-$algebra on Ω and $\nu : \mathcal{F} \to [0,1]$ is a probability measure. $\mathcal{B}^N$ is the Borel σ-algebra on $\mathbb{R}^N, N \in \mathbb{N}$. $\boldsymbol{X} = (X_1, \ldots, X_N) : (\Omega, \mathcal{F}) \to (\mathbb{R}^N, \mathcal{B}^N)$ denotes a $\mathbb{R}^N$-valued random vector.
We assume that the probability distribution of $\boldsymbol{X}$ is continuous and completely defined by the joint probability density function $f_{\boldsymbol{X}} : \mathbb{R}^N \to \mathbb{R}_0^+$.
Let u denote a subset of indices $\{1, \ldots, N\}$, and $-u := \{1, \ldots, N\} \backslash u$ its compliment. $\boldsymbol{X_u} = (X_1, \ldots, X_{|u|}), u \neq \emptyset, 1 \leq i_1 < \cdots < i_{|u|} \leq N$ is a subvector of $\boldsymbol{X}$ and $\boldsymbol{X}_{-u} = \boldsymbol{X}_{\{1,\ldots,N\}\backslash u}$ is the complement of $\boldsymbol{X}_u$.
The marginal density function is $f_u(\boldsymbol{x_u}) := \int f_{\boldsymbol{X}}(\boldsymbol{x}) d\boldsymbol{x_{-u}}$ for a given set $\emptyset \neq u \subseteq \{1, \ldots N\}$. $f(\boldsymbol{X}) := f(X_1, \ldots, X_N)$ is a mathematical model with random variables as inputs. We write a vector space of square-integrable functions as

$$\mathcal{L}^2(\Omega, \mathcal{F}, \nu) = \left\{ f : \Omega \to \mathbb{R} \; s.t. \; \mathbb{E}[f^2(\boldsymbol{X})] < \infty \right\}$$

.
$\mathcal{L}^2(\Omega, \mathcal{F}, \nu)$ is a Hilbert space with the inner product defined as:

$$\langle f, g \rangle = \int f(x) g(x) \, d\nu(x) = \mathbb{E}[fg], \quad \forall f, g \in \mathcal{L}^2.$$

The norm is then defined as:

$$\|f\| = \sqrt{\langle f, f \rangle} = \sqrt{\int f^2(x) \, d\nu(x)} = \mathbb{E}[f^2], \quad \forall f \in \mathcal{L}^2.$$

Which resource should I cite for these "general" definitions? e.g. https://apachepersonal.miun.se/ andrli/Bok.pdf?

Conditional expectation

In general, we define the conditional expectation of a vector of random variables $\boldsymbol{X} = (X_1, X_2)$ as follows:

$$\mathbb{E}[g(X_1, X_2) \mid X_1 = x_1] = \int g(x_1, s_2) \, p_{X_2|X_1}(s_2 \mid x_1) \, ds_2.$$

Only when X_1 and X_2 are independent can we write

$$\mathbb{E}[g(X_1, X_2) \mid X_1 = x_1] = \int g(x_1, s_2)\, p_{X_2|X_1}(s_2 \mid x_1)\, ds_2 = \int g(x_1, s_2)\, p_{X_2}(s_2)\, ds_2 = \mathbb{E}_{X_2}[g(x_1, X_2)].$$

Extended to n random variables it looks as follows. Without loss of generality, we condition on $X_1 = x_1$:

$$\begin{aligned}\mathbb{E}[g(X_1, \ldots, X_n) \mid X_1 = x_1] &= \int g(x_1, s_2, \ldots, s_n)\, p_{X_2,\ldots,X_n|X_1}(s_2, \ldots, s_n \mid x_1)\, ds_2 \ldots ds_n \\ &= \int g(x_1, s_2, \ldots, s_n)\, p_{X_2}(s_2, \ldots, s_n)\, ds_2 \ldots, ds_n \\ &= \mathbb{E}_{X_2,\ldots,X_n}[g(x_1, X_2, \ldots, X_n)]\end{aligned}$$

Orthogonal projection

Let $\mathcal{G} \subset \mathcal{L}^2$ denote a linear subspace. The projection of f onto $\mathcal{G}$ is defined by the function $\Pi_{\mathcal{G}} f$ which minimizes the distance to f in $\mathcal{L}^2$:

$$\Pi_{\mathcal{G}} f = \arg\min_{g \in \mathcal{G}} \|f - g\|^2\, d\nu = \arg\min_{g \in \mathcal{G}} \mathbb{E}[(f - g)^2].$$

I think this is closely related to Hilbert projection theorem?
Definition of $\mathcal{L}^2$ space and projection modified from https://tnagler.github.io/mathstat-lmu-2024.pdf.

Properties of the Multivariate Normal Distribution

Let $\boldsymbol{X} = (X_1, \ldots, X_d)^\top \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ be a d-dimensional multivariate normal (MVN) random vector, where $\boldsymbol{\mu} \in \mathbb{R}^d$ is the mean vector and $\boldsymbol{\Sigma} \in \mathbb{R}^{d \times d}$ is the symmetric positive semi-definite covariance matrix.
The marginal distribution of X_i is generally given by an univariate normal distribution:

$$X_i \sim \mathcal{N}(\mu_i, \Sigma_{ii}) \quad \text{for all } i = 1, \ldots, d.$$

If we condition on a subset of the variables, we can also make statements about the conditional distribution. For this we partition the random vector $\boldsymbol{X}$ into two parts, $\boldsymbol{X}_A$ and $\boldsymbol{X}_B$, where $\boldsymbol{X}_A$ contains the variables we condition on and $\boldsymbol{X}_B$ contains the remaining variables. The joint distribution of $\boldsymbol{X}$ can be expressed as:

$$\boldsymbol{X} = \begin{pmatrix} \boldsymbol{X}_A \\ \boldsymbol{X}_B \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} \boldsymbol{\mu}_A \\ \boldsymbol{\mu}_B \end{pmatrix}, \begin{pmatrix} \boldsymbol{\Sigma}_{AA} & \boldsymbol{\Sigma}_{AB} \\ \boldsymbol{\Sigma}_{BA} & \boldsymbol{\Sigma}_{BB} \end{pmatrix} \right).$$

The conditional distribution of $\boldsymbol{X}_B$ given $\boldsymbol{X}_A = \boldsymbol{x}_A$ is

$$\boldsymbol{X}_B \mid \boldsymbol{X}_A = \boldsymbol{x}_A \sim \mathcal{N}\left(\boldsymbol{\mu}_B + \boldsymbol{\Sigma}_{BA}\boldsymbol{\Sigma}_{AA}^{-1}(\boldsymbol{x}_A - \boldsymbol{\mu}_A), \boldsymbol{\Sigma}_{BB} - \boldsymbol{\Sigma}_{BA}\boldsymbol{\Sigma}_{AA}^{-1}\boldsymbol{\Sigma}_{AB}\right).$$

For normally distributed random variables, we also know that $\mathrm{Cov}(X_i, X_j) = 0$, implies $X_i \perp X_j$. Lastly, for any real vector $\boldsymbol{a} \in \mathbb{R}^d$, the linear combination $\boldsymbol{a}^\top \boldsymbol{X}$ is normally distributed:

$$\boldsymbol{a}^\top \boldsymbol{X} \sim \mathcal{N}(\boldsymbol{a}^\top \boldsymbol{\mu}, \boldsymbol{a}^\top \boldsymbol{\Sigma} \boldsymbol{a}).$$

Find official resource for these properties; review how this can be shown.

3 History of fANOVA

3.1 Early Work on fANOVA

The main idea of the fANOVA decomposition is to decompose a statistical model into the sum of the main effects and interaction effects of its input variables. The underlying principle of fANOVA decomposition dates back to Hoeffding (1948). In his seminal work(?) on estimators with asymptotical normal distribution, he introduced U-statistics, along with the "Hoeffding decomposition", which allows to write a symmetric function of the data as a sum of orthogonal components. Sobol (1993) used the same principle and applied it to deterministic mathematical models. He built on the originally called "decomposition into summands of different dimension" in Sobol (2001), where he introduces Sobol indices and renames the method to the "ANOVA-representation". For Sobol decomposing the function into the sum of fANOVA terms is actually not central, but what he is mostly interested is the variance decomposition which he shows follows from the fANOVA decomposition of a function. This variance decomposition allows quantifying how much the variance of a single input variable contributes to the overall variance of the function. Thus, Sobol indices are commonly used in sensitivity analysis. Sobol builds his main contributions around fANOVA on the 1) variance decomposition, but also proposes to use fANOVA for 2) variable selection/ dimensionality reduction (terms that contribute a lot to overall variance should be in the model).
Efron and Stein (1981) use the idea of the decomposition to proof their famous lemma on jackknife variances.
A true wave of fANOVA literature around the 1990s, where authors investigate fANOVA-based models, establish parallels to splines, study their theoretical properties (convergence, consistency, etc.), and prectical use cases (dimensionality reduction, etc.). All cited in Huang (1998b). Stone (1994) mainly uses fANOVA decomposition to base smooth regression models with interactions on it and his paper is the building block for a broader body of work of fANOVA-based models (see for example Huang (1998a,b))

3.2 Modern Work on fANOVA

The fANOVA decomposition has a long history with roots in mathematical statistics and non-parametric estimation theory.
Owen (2013) formal intro to fANOVA decomposition and generalization of Sobol indices. Owen has generally a lot of work related to fANOVA decomposition, either lecture notes explaining the decomposition, methods based on it Owen (2003), or deeper into sensitivity analysis and fANOVA Owen (2013).

Since the assumptions of independent variables in classical fANOVA is often too restrictive in practice, Hooker (2007) generalizes the method to dependent variables. A recent paper by Il Idrissi et al. (2025) can be seen as another approach to generalize the principle of fANOVA decomposition to dependent inputs.
In more recent years, the method has been rediscovered by the machine-learning community, especially in the context of interpretable machine learning (IML) and explainable AI (XAI). Hooker (2004) introduces the fANOVA decomposition with the goal of providing a global explanation method for black-box models. And recent work discovered interesting mathematical parallels between fANOVA and other IML methods, such as PDP Friedman (2001), or Shapley values (Fumagalli et al. (2025), Herren, Owen preprint).
There are specific domains of statistics, such as geostatistics, that explicitly build models on fANOVA framework (see Muehlenstaedt et al. (2012) for fANOVA Kriging models). Liu and Owen (2006) use of fANOVA and sensitivity analysis for functions arising in computational finance.

4 Classical fANOVA

4.1 Formal Introduction to fANOVA

This chapter is based on the formal introductions by Rahman (2014), Sobol (1993, 2001), Hooker (2004), Owen (2013), Muehlenstaedt et al. (2012). We show both formulations of the fANOVA, via the integral and via the expected value and in general prefer the expected value formulation as it is more intuitive in a probabilistic setting. Originally, Sobol (1993) presented the fANOVA decomposition with independent input variables with support bounded to the unit interval, i.e. he considered the measure space $([0,1]^n, \mathcal{B}([0,1]^n), \nu)$. Later work shows that this restriction is not necessary, and we can work with the Borel σ-algebra on the n-dimensional real number line, i.e. $(\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n), \nu)$, and with a general measure ν defined on it (see e.g. Rahman (2014)). Since we assume independence of the input variables, their joint distribution is given by the product over the marginal distributions, i.e. $f_{\boldsymbol{X}}(\boldsymbol{x})\, d\nu(\boldsymbol{x}) = \prod_{i=1}^{N} f_{X_i}(x_i)\, d\nu(x_i)$. $f_{X_i} : \mathbb{R} \to \mathbb{R}_0^+$ is the marginal probability density function of X_i defined on $(\Omega_i, \mathcal{F}_i, \nu_i)$.

Definition 4.1. *Let y denote a mathematical model with realizations of independent random variables $x_1, \ldots, x_N$ as input. We can represent such a model y as the hierarchical sum of specific basis functions with increasing dimensionality:*

$$y(\boldsymbol{X}) = \sum_{u \subseteq \{1,\ldots,N\}} y_u(\boldsymbol{X}_u), \tag{2}$$

If $|u| = 0$ it describes the constant term, if $|u| = 1$ it describes the main effects, if $|u| > 1$ it describes the interaction effects of the variables in u. The expansion consists of 2^N terms.

Construction of the fANOVA Terms

The individual fANOVA term for the variables with indices in u are constructed from integrating the original function $y(\boldsymbol{X})$ w.r.t all variables expect for the ones in u, and subtracting the lower order terms. Intuitively the integral is averaging the original function over all other variables expect the ones of interest, which makes sense as we are then left with a function of the variables of interest only. Subtracting lower order terms corresponds to accounting for effects that are already explained by other variables or interactions so that we obtain the isolated effects.

Since $u = \emptyset$ for the constant term, we integrate w.r.t all variables:

$$y_\emptyset = \int y(\boldsymbol{x}) \prod_{i=1}^{N} f_{X_i}(x_i)\, d\nu(x_i) = \mathbb{E}[y(\boldsymbol{X})]. \tag{3}$$

For all other effects $\emptyset \neq u \in \{1, \ldots, N\}$ we can write:

$$y_u(\boldsymbol{X}_u) = \int y(\boldsymbol{X}_u, \boldsymbol{x}_{-u}) \prod_{i=1, i \notin u}^{N} f_{X_i}(x_i)\, d\nu(x_i) - \sum_{v \subsetneq u} y_v(\boldsymbol{X}_v), \tag{4}$$

Notice that this definition relies on a product-type measure rooted in the independence of the variables. We will see what changes when we let got of this assumption in the next section.

The fANOVA components offer a clear interpretation of the model, decomposing it into main effects, two-way interaction effects, and so on. This is why fANOVA decomposition has received increasing attention in the IML and XAI literature, holding the potential for a global explanation method of black box models.

The fANOVA terms should be constructed in such a way that they have two specific properties crucial for identifiability and interpretation.

Proposition 4.1. *The zero-mean property states that all effects, except for the constant terms, are centred around zero. Mathematically this means that the effects integrate to zero w.r.t. their own variables:*

$$\int y_u(\boldsymbol{x}_u) f_{\boldsymbol{X}}(\boldsymbol{x})\, d\nu(\boldsymbol{x}) := \mathbb{E}[y_u(\boldsymbol{X}_u)] = 0 \tag{5}$$

Proposition 4.2. *The second property is the orthogonality of the fANOVA terms. If two sets of indices are not completely equivalent, i.e.* $\emptyset \neq u \subseteq \{1, \ldots, N\}, \emptyset \neq v \subseteq \{1, \ldots, N\}$, *and* $u \neq v$, *then it holds that their fANOVA terms are orthogonal to each other:*

$$\int y_u(\boldsymbol{x_u}) y_v(\boldsymbol{x_v}) f_{\boldsymbol{X}}(\boldsymbol{x}) d\nu(\boldsymbol{x}) = \mathbb{E}[y_u(\boldsymbol{X}_u) y_v(\boldsymbol{X}_v)] = 0 \tag{6}$$

This means that fANOVA terms are "fully orthogonal" to each other, meaning not only terms of different order are orthogonal to each other but also terms of the same order are. Rahman (2014) derives these two properties (Equation 5, Equation 6)from a more general condition, he calls the "strong annihilating conditions".

The strong annihilating conditions require that the fANOVA terms integrate to zero w.r.t the individual variables contained in u and weighted by the individual marginal

probability density functions:

$$\int y_u(\boldsymbol{x}_u) f_{X_i}(x_i)\, d\nu(x_i) = 0, \quad \text{for } i \in u \neq \emptyset. \tag{7}$$

We can reassure ourselves that the properties in fact follow from the strong annihilating conditions. For the zero-mean constraint we can write:

$$\begin{aligned}
\mathbb{E}[y_u(\boldsymbol{X}_u)] :== & \int_{\mathbb{R}^N} y_u(\boldsymbol{x_u}) f_{\boldsymbol{X}}(\boldsymbol{x})\, d\nu(\boldsymbol{x}) \\
&= \int_{\mathbb{R}^{|u|}} y_u(\boldsymbol{x_u}) f_{\boldsymbol{X}_u}(\boldsymbol{x}_u)\, d\nu(\boldsymbol{x}_u) \\
&= \int_{\mathbb{R}^{|u|}} y_u(\boldsymbol{x_u}) \prod_{i \in \boldsymbol{u}} f_{X_i}(x_i)\, d\nu(\boldsymbol{x}_u) \\
&= \int_{\mathbb{R}^{|u|-1}} \int_{\mathbb{R}} y_u(\boldsymbol{x_u}) f_{X_i}(x_i)\, dx_u \prod_{j \in u, j \neq i} f_{X_j}(x_j) = 0
\end{aligned}$$

One can follow the same reasoning for the orthogonality condition:

$$\begin{aligned}
\mathbb{E}[y_u(\boldsymbol{X}_u) y_v(\boldsymbol{X}_v)] &= \int_{\mathbb{R}^{\mathbb{N}}} y_u(\boldsymbol{x_u}) y_v(\boldsymbol{x_v}) f_{\boldsymbol{X}}(\boldsymbol{x})\, d\nu(\boldsymbol{x}) \\
&= \int_{\mathbb{R}^{\mathbb{N}}} y_u(\boldsymbol{x_u}) y_v(\boldsymbol{x_v}) \prod_{i=1}^{N} f_{X_i}(x_i)\, d\nu(x_i) \\
&= \int_{\mathbb{R}^{\mathbb{N}-1}} \int_{\mathbb{R}} y_u(\boldsymbol{x_u}) y_v(\boldsymbol{x_v}) f_{X_i}(x_i)\, dx_u \prod_{j \in \{1,\ldots,N\}, j \neq i} f_{X_j}(x_j) = 0
\end{aligned}$$

4.2 Example: Multivariate Normal Inputs

Before further investigating the fANOVA decomposition, let us consider the following function as example: $g = a + X_1 + 2X_2 + X_1 X_2$. We assume that $\boldsymbol{X} = (X_1, X_2)^T$ follows a standard MVN distribution, i.e.:

$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho_{12} \\ \rho_{12} & 1 \end{pmatrix} \right).$$

From the properties of the MVN, we know that marginal distributions are standard normal:

$$X_i \sim \mathcal{N}(0, 1) \quad \text{for } i = 1, 2$$

We also know that the conditional distributions are given by:

$$X_1 \mid X_2 = x_2 \sim \mathcal{N}(\rho_{12} x_2, 1 - \rho_{12}^2), \quad X_2 \mid X_1 = x_1 \sim \mathcal{N}(\rho_{12} x_1, 1 - \rho_{12}^2)$$

Case 1: Independent Inputs

The classical fANOVA decomposition we covered so far assumes $\rho_{12} = 0$. Computing the fANOVA decomposition of $g(x_1, x_2)$ by hand, we start with the constant term and make use of formulation via the expected value:

$$y_0 = \mathbb{E}[g_1(X_1, X_2)] = \mathbb{E}[a + X_1 + 2X_2 + X_1X_2] = \mathbb{E}[a] + \mathbb{E}[X_1] + 2\mathbb{E}[X_2] + \mathbb{E}[X_1X_2]$$

Making use of the independence assumption of X_1 and X_2, the last term can be written as the product of the expected values. Additionally, given the zero-mean constraint, all terms, except for the constant, vanish and we obtain:

$$y_0 = \mathbb{E}[a] + \mathbb{E}[X_1] + 2\mathbb{E}[X_2] + \mathbb{E}[X_1]\mathbb{E}[X_2] = a$$

Under zero-mean constraint and independence, the main effects and the interaction effect can be computed as follows:

$$\begin{aligned}
y_1(x_1) &= \mathbb{E}_{X_2}[g_1(x_1, X_2)] - y_0 \\
&= \mathbb{E}_{X_2}[a + x_1 + 2X_2 + x_1X_2] - a \\
&= x_1 + 2\mathbb{E}[X_2] + x_1\mathbb{E}[X_2] = x_1 \\
y_2(x_2) &= \mathbb{E}_{X_1}[g_1(X_1, x_2)] - y_0 \\
&= \mathbb{E}_{X_1}[a + X_1 + 2x_2 + X_1x_2] - a \\
&= \mathbb{E}_{X_1}[X_1] + 2x_2 + x_2\mathbb{E}_{X_1}[X_1] = 2x_2 \\
y_{12}(x_1, x_2) &= \mathbb{E}[g_1(x_1, x_2)] - y_0 - y_1(x_1) - y_2(x_2) \\
&= a + x_1 + 2x_2 + x_1x_2 - a - x_1 - 2x_2 = x_1x_2
\end{aligned}$$

It comes as no surprise that in this simple case the fANOVA decomposition does not provide any additional insights, as the isolated effects can be directly seen from the function. We show this simple example nevertheless to illustrate at which step which assumption is used. This will make clearer what breaks down when we generalize to dependent variables.

fANOVA as projection

In the following we revisit the fANOVA decomposition from the view of orthogonal projections. The section is based on Vaart (1998). This will also help to understand the generalization of fANOVA in section 5.
When we define the constant term $y_\emptyset$ our goal is to best approximate the original function y by a constant function. In other words, we want to minimize the squared difference

between y and a constant function $g(x) = a$ over all possible constant functions. The solution is the orthogonal projection of y onto the linear subspace of all constant functions $\mathcal{G}_0 = \{g(x) = a; a \in \mathbb{R}\}$. In a probabilistic context, we want to minimize the expected squared different between the random variables $y(\boldsymbol{X})$ and a, which turns out to be equivalent to the expected value of the random variable (Vaart, 1998). So intuitively, in the absence of any additional information, the expected value is our best approximation of y. More formally we can write:

$$\begin{aligned}\Pi_{\mathcal{G}_0} y &= \arg\min_{g_0 \in \mathcal{G}_0} \|y - g_0\|^2 \\ &= \arg\min_{a_0 \in \mathbb{R}} \mathbb{E}[(y(\boldsymbol{X}) - a)^2] \\ &= \mathbb{E}[y(\boldsymbol{X})] = y_0\end{aligned}$$

The main effect $y_i(x_i)$ is the projection of y onto the subspace of all functions that only depend on x_i and have an expected value of zero while accounting for the lower-order effects. The subspace we project onto is $\mathcal{G}_i = \{g(x) = g_i(x_i); \int g(x) d\nu(x_i) = 0\}$. The conditional expected value of $\mathbb{E}[y(\boldsymbol{X}) \mid X_i = x_i]$ is the solution to the minimization problem (Vaart, 1998), and the conditional expected value is also a way to express the fANOVA terms (Muehlenstaedt et al., 2012):

$$\begin{aligned}(\Pi_{\mathcal{G}_i} y) - (y_0) &= \arg\min_{g_i \in \mathcal{G}_i} \|y - g_i\|^2 - y_0 \\ &= \arg\min_{g_i \in \mathcal{G}_i} \mathbb{E}[(y(\boldsymbol{X}) - g_i(X_i))^2] - y_0 \\ &= \mathbb{E}[y(\boldsymbol{X}) \mid X_i = x_i] - y_0 = y_i\end{aligned}$$

The two-way interaction effect $y_{ij}(x_i, x_j)$ is the projection of y onto the subspace of all functions that depend on x_i and x_j and have an expected value of zero in each of it's single components, i.e. $\mathcal{G}_{i,j} = \{g(x) = g_{ij}(x_i, x_j); \int g(x) d\nu(x_i) = 0 \wedge \int g(x) d\nu(x_j) = 0\}$. Again, we account for lower-order effects by subtracting the constant term and all main effects:

$$\begin{aligned}(\Pi_{\mathcal{G}_{ij}} y) - (y_0 + y_i(x_i) + y_j(x_j)) &= \arg\min_{g_{ij} \in \mathcal{G}_{ij}} \|y - g_{i,j}\|^2 - (y_0 + y_i(x_i) + y_j(x_j)) \\ &= \arg\min_{g_{ij} \in \mathcal{G}_{ij}} \mathbb{E}[(y(\boldsymbol{X}) - g(X_i, X_j))^2] - (y_0 + y_i(x_i) + y_j(x_j)) \\ &= \mathbb{E}[y(\boldsymbol{X}) | X_j = x_j, X_i = x_i] - (y_0 + y_i(x_i) + y_j(x_j)) = y_{ij}(x_i, x_j)\end{aligned}$$

In general, we can write for a subset of indices $u \subseteq \{1, \dots, N\}$ and the subspace $\mathcal{G}_u = \{g(\boldsymbol{x}) = g_u(\boldsymbol{x}_u); \int g(\boldsymbol{x}) d\nu(\boldsymbol{x}_u) = 0\}$:

$$\begin{aligned}(\Pi_{\mathcal{G}_u} y) - \sum_{v \subsetneq u} y_v(x) &= \arg\min_{g_u \in \mathcal{G}_u} \|y - g_u\|^2 - y_0 \\ &= \arg\min_{g_u \in \mathcal{G}_u} \mathbb{E}[(y(\boldsymbol{X}) - g(X_u))^2] \\ &= \mathbb{E}[y(\boldsymbol{X}) | X_u = x_u] - \sum_{v \subsetneq u} y_v(x) = y_u(\boldsymbol{x}_u),\end{aligned}$$

which means that we project y onto the subspace spanned by the own terms of the fANOVA component to be defined, while accounting for all lower-order terms.

Notes & Questions

Situation: $y(\boldsymbol{X}) \in \Omega, \mathcal{G} \subseteq \Omega, g(\boldsymbol{X}) \in \mathcal{G}$.
Vaart (1998) tells us that the expected value is equivalent to the projection Muehlenstaedt et al. (2012) tells us that the fANOVA terms are equivalent to the conditional expected value.

Second-moment statistics

We already established that $\mathbb{E}[y(\boldsymbol{X})] = y_\emptyset$. For the variance of $y(\boldsymbol{X})$, we find that the total variance can be decomposed into the sum of the fANOVA term variances. The variance decomposition is a major result in Sobol (1993) and forms the basis for the Sobol indices in sensitivity analysis. We sketch the variance decomposition here and note that it is only possible under independence assumption.
If $y \in \mathcal{L}^2$, then $y_{i_1,\dots,y_n} \in \mathcal{L}^2$ proof? reference?; Sobol 1993 says it is easy to show using Schwarz inequality and the definition of the single fANOVA terms. Therefore, we define the variance of f as follows:

$$\begin{aligned}\sigma^2 &:= \int y^2(\boldsymbol{X}) f_{\boldsymbol{X}}(\boldsymbol{x}) d\nu(\boldsymbol{x}) - (y_0)^2 \\ &= \int y^2(\boldsymbol{X}) f_{\boldsymbol{X}}(\boldsymbol{x}) d\nu(\boldsymbol{x}) - (\int y(\boldsymbol{X}) f_{\boldsymbol{X}}(\boldsymbol{x}) d\nu(\boldsymbol{x}))^2 \\ &= \mathbb{E}[y^2(\boldsymbol{X})] - \mathbb{E}[y(\boldsymbol{X})]^2\end{aligned}$$

The variance of the fANOVA components is then defined as

$$\begin{aligned}\sigma^2_{x_{i_1},\dots,x_{i_n}} &= \int \cdots \int y^2_{i_1,\dots,i_n} f_{\boldsymbol{X}}(\boldsymbol{x}) d\nu(x_1) \cdots d\nu(x_n) - \left(\int \cdots \int f_{i_1,\dots,i_n} f_{\boldsymbol{X}}(\boldsymbol{x}) d\nu(x_1) \cdots d\nu(x_n) \right)^2 \\ &= \mathbb{E}[y^2_{i_1,\dots,i_n}] - \mathbb{E}[y_{i_1,\dots,i_n}]^2\end{aligned}$$

Because of the orthogonality property, the second term vanished and we get:

$$\begin{aligned}\sigma^2_{x_{i_1},\dots,x_{i_n})} &= \int \cdots \int y^2_{i_1,\dots,i_n} f_{\boldsymbol{X}}(\boldsymbol{x}) d\nu(x_1) \cdots d\nu(x_n) \\ &= \mathbb{E}[y^2_{i_1,\dots,i_n}]\end{aligned}$$

With the definition of the total variance σ^2 and the component-wise variance $\sigma^2_{x_{i_1},\dots,x_{i_n}}$ we can now see that the total variance can be decomposed into the sum of the component-wise variances.
Alternatively we can formulate this via the expected value. We write the sum over u for the sum over $\emptyset \neq u \subseteq \{1,\dots,N\}$ and the sum over $u \neq v$ for the sum over $\emptyset \neq u \subseteq \{1,\dots,N\}, \emptyset \neq v \subseteq \{1,\dots,N\}, u \neq v$.

$$\begin{aligned}\sigma^2 := \mathbb{E}[(y(\boldsymbol{X}) - \mu])^2] &= \mathbb{E}[(y_\emptyset + \sum_u y_u(\boldsymbol{X}_u) - y_\emptyset)^2] \\ &= \mathbb{E}[(\sum_u y_u(\boldsymbol{X}_u))^2] \\ &= \mathbb{E}[\sum_u y^2_u(\boldsymbol{X}_u)] + 2\mathbb{E}[\sum_{u \neq v} y_u(\boldsymbol{X}_u) y_v(\boldsymbol{X}_v)] \\ &= \sum_u \mathbb{E}[y^2_u(\boldsymbol{X}_u)]\end{aligned}$$

5 Generalized fANOVA

5.1 Motivating Example

Recall our example setup of standard MVN input variables and $g = a + X_1 + 2X_2 + X_1X_2$ from the previous section 4.2. For classical fANOVA we make the assumption of independent inputs, which is often violated in practice. Let us therefore investigate what happens, when we allow for dependency between variables.

Case 2: Dependent Inputs (weak)

Now $\rho_{12} \neq 0$, while keeping everything else the same. We follow the exact same logic as above to calculate the constant terms under dependent inputs. Notice that the fANOVA components look more complicated and involve the correlation ρ. maybe call these components $\tilde{y}_i$ or sth. like this to emphasize that it is not the same as above (and that they turn out to not be fANOVA components after all):

$$
\begin{aligned}
\tilde{y}_0 &= \mathbb{E}[g(X_1, X_2)] = a + \mathbb{E}[X_1] + 2\mathbb{E}[X_2] + \mathbb{E}[X_1X_2] \\
&= a + \mathbb{E}[X_1X_2] = a + (\mathrm{Cov}(X_1, X_2) + \mathbb{E}[X_1]\mathbb{E}[X_2]) \\
&= a + \rho_{12} \\
\tilde{y}_1(x_1) &= \mathbb{E}[g(X_1, X_2)|X_1 = x_1] - \tilde{y}_0 \\
&= \mathbb{E}[a + x_1 + 2X_2 + x_1X_2|X_1 = x_1] - (a + \rho_{12}) \\
&= a + x_1 + 2\mathbb{E}[X_2|X_1 = x_1] + x_1\mathbb{E}[X_2|X_1 = x_1] - a - \rho_{12} \\
&= x_1 + \rho_{12}(2x_1 + x_1^2 - 1) \\
\tilde{y}_2(x_2) &= \mathbb{E}[g(X_1, X_2) \mid X_2 = x_2] - \tilde{y}_0 \\
&= \mathbb{E}[a + X_1 + 2x_2 + X_1x_2 \mid X_2 = x_2] - (a + \rho_{12}) \\
&= a + 2x_2 + x_2\mathbb{E}[X_1 \mid X_2 = x_2] - a - \rho_{12} \\
&= 2x_2 + \rho_{12}(x_2 + x_2^2 - 1) \\
\tilde{y}_{12}(x_1, x_2) &= g(x_1, x_2) - \tilde{y}_0 - \tilde{y}_1(x_1) - \tilde{y}_2(x_2) \\
&= a + x_1 + 2x_2 + x_1x_2 - (a + \rho_{12}) \\
&\quad - (x_1 + \rho_{12}(2x_1 + x_1^2 - 1)) - (2x_2 + \rho_{12}(x_2 + x_2^2 - 1)) \\
&= x_1x_2 - 2\rho_{12}x_1 - \rho_{12}x_2 - \rho_{12}x_1^2 - \rho_{12}x_2^2 + \rho_{12}
\end{aligned}
$$

The fANOVA components are characterized by two central properties zero mean and orthogonality which follow from Equation 7. When we check if the components $\tilde{y}_0, \tilde{y}1, \tilde{y}_2, \tilde{y}_{1,2}$ satisfy the properties, we find out that all components are zero-centred, but not all are

hierarchical to each other. We can, for example, immediately see that checking orthogonality between $\tilde{y}_1, \tilde{y}_{1,2}$ will yield the expectation over the constant term $\rho_{1,2}$ exactly once, meaning even if all the other expectations cancel out, this constant will remain and the entire expression will be unequal to zero.

$$\begin{aligned}\mathbb{E}(\tilde{y}_1(X_1)\tilde{y}_{1,2}(X_1, X_2)) &= \mathbb{E}[(X_1 + 2\rho_{12}X_1 + \rho_{12}X_1^2 - \rho_{12}) \\ &\quad \cdot (X_1X_2 - 2\rho_{12}X_1 - \rho_{12}X_2 - \rho_{12}X_1^2 - \rho_{12}X_2^2 + \rho_{12})] \\ &= \mathbb{E}[X_1^2X_2] \ldots - \mathbb{E}[\rho_{12}^2] \neq 0\end{aligned}$$

When we no longer have independent inputs naively computing the "fANOVA decomposition" does not yield the fANOVA components as it turns out. What we performed in this example is not the fANOVA decomposition for dependent variables. It is Hoeffding decomposition and results in zero mean but not mutually orthogonal component functions. This shows the need for a more involved approach for generalizing fANOVA.

5.2 Formal Introduction to Generalized fANOVA

We base this chapter mainly on the generalization of Rahman (2014), while there exists other work from Hooker (2007) or Chastaing et al. (2012).
Letting go of the independence assumption means that we no longer work with a product-type probability measure. $f_{\boldsymbol{X}} : \mathbb{R} \to \mathbb{R}_0^+$ denotes an arbitrary probability density function and $f_{\boldsymbol{X}_u} : \mathbb{R}^u \to \mathbb{R}_0^+$ the marginal probability density function of the subset of variables $u \subseteq d$. Classical fANOVA boils down to integration w.r.t. the uniform measure and in generalized fANOVA we integrate w.r.t. the distribution of $(X_1, \ldots, X_n)$.

Definition 5.1. ***Generalized fANOVA decomposition.*** *We denote the generalized functional fANOVA decomposition as:*

$$y(\boldsymbol{X}) = \sum_{u \subseteq \{1,\ldots,N\}} y_{u,G}(\boldsymbol{X}_u) \tag{8}$$

The subscript G indicates that we are working with the generalized fANOVA components. The main question is, how one can build fANOVA components that still satisfy the desired properties of zero mean and orthogonality under dependent inputs.

Construction of the Generalized fANOVA Terms

While the constant term requires no change in definition, the motivating example in the beginning of this section showed that the non-constant terms need some additional terms

to ensure orthogonality. Rahman (2014) defines the generalized components as follows:

$$y_{\emptyset,G} = \int_{\mathbb{R}^N} y(\boldsymbol{x}) f_{\boldsymbol{X}}(\boldsymbol{x})\, d\boldsymbol{x}, \tag{4.5a}$$

$$\begin{aligned} y_{u,G}(\boldsymbol{X}_u) = &\int_{\mathbb{R}^{N-|u|}} y(\boldsymbol{X}_u, \boldsymbol{x}_{-u}) f_{\boldsymbol{X}_{-u}}(\boldsymbol{x}_{-u})\, d\boldsymbol{x}_{-u} - \sum_{v \subset u} y_{v,G}(\boldsymbol{X}_v) \\ &- \sum_{\substack{\emptyset \neq v \subseteq \{1,\ldots,N\} \\ v \cap u \neq \emptyset, v \not\subset u}} \int_{\mathbb{R}^{|v \cap -u|}} y_{v,G}(\boldsymbol{X}_{v \cap u}, \boldsymbol{x}_{v \cap -u}) f_{v \cap -u}(\boldsymbol{x}_{v \cap -u})\, d\boldsymbol{x}_{v \cap -u}. \end{aligned} \tag{4.5b}$$

The first part of the non-constant components looks very similar to the classical formulation, but instead of the product pdf we use the joint pdf of all variables except for the ones of interest. The terms we subtract include not only lower order fANOVA terms but also (not yet computed) higher order fANOVA terms, which depend on the variable of interest. This means, we account for all the terms in which the term of interest is somehow involved in. This is necessary to ensure a form of orthogonality under dependent inputs but also means that solving the terms sequentially, as in the classical case and our naive approach, is not working anymore.
If components are constructed in this way, we can ensure that they have zero mean and satisfy a milder from of orthogonality - hierarchical orthogonality, which means that components of different order are orthogonal to each other while components of the same order are not.

Proposition 5.1. *The generalized fANOVA components $y_{u,G}$, with $\emptyset \neq u \subseteq \{1, \ldots, N\}$, are centred around zero:*

$$\mathbb{E}[y_{u,G}(\boldsymbol{X}_u)] := \int y_{u,G}(\boldsymbol{x}_u) f_{\boldsymbol{X}}(\boldsymbol{x})\, d\nu(\boldsymbol{x}) = 0 \tag{9}$$

Proposition 5.2. *The fANOVA components are hierarchically orthogonal. This means that for two components $y_{u,G}$ and $y_{v,G}$ with $u \subset v, \emptyset \neq u \subseteq \{1, \ldots, N\}, \emptyset \neq v \subseteq \{1, \ldots, N\}$ it holds that:*

$$\mathbb{E}[y_{u,G}(\boldsymbol{X}_u) y_{v,G}(\boldsymbol{X}_v)] := \int y_{u,G}(\boldsymbol{x}_u) y_{v,G}(\boldsymbol{X}_v) f_{\boldsymbol{X}}(\boldsymbol{x})\, d\nu(\boldsymbol{x}) = 0 \tag{10}$$

To ensure that these statements hold for the generalized fANOVA components, we need to set the weak annihilating conditions. They fulfill the same function as the strong annihilating conditions do in the classical case but work with the joint density of the variables of interest, instead of the individual marginal probability density functions.

This makes sense, since for the general case we cannot ensure to recover the marginal densities from the joint density function. Is this really the reason? Or is the reason: When there are dependencies between variables then the individual pdfs would not assign the "correct weight" as they ignore the dependence between features in u.

Proposition 5.3. ***Weak annihilating conditions.*** *To ensure the two desired properties of the generalized fANOVA components (zero mean, hierarchical orthogonality), we require the weak annihilating conditions:*

$$\int_{\mathbb{R}} y_{u,G}(\boldsymbol{x}_u) f_{\boldsymbol{X}_u}(\boldsymbol{x}_u) d\nu(x_i) = 0 \quad \textit{for} \quad i \in u \neq \emptyset \tag{11}$$

To show that zero mean and hierarchical orthogonality follow from the weak annihilating conditions, Rahman (2014) makes use of Fubini's theorem (see his proof in section 4 of his paper - or should I write the commented proof here?).
Hooker (2007) offers an alternative definition of the generalized fANOVA components[1]:

$$\{y_{u,G}(x_u) \,|\, u \subseteq d\} = \arg \min_{\{g_u \in L^2(\mathbb{R}^u)\}_{u \subseteq d}} \int \left(\sum_{u \subseteq d} g_u(x_u) - y(x) \right)^2 f_{\boldsymbol{X}}(\boldsymbol{x}) \, d\nu(\boldsymbol{x}) \tag{12}$$

In Hookers definition we recognize a projection problem. We are simultaneously finding the set of components functions g_u that minimize the weighted squared difference to the original function y (under zero mean and hierarchical orthogonality constraint), which is exactly the definition of a projection of y onto a specific subspace $\mathcal{G}$, which we defined generally in section 2.
A crucial difference both versions of the generalized components have in common is that they are defined in dependence of each other (Equation 4.5b, Equation 12). Since they form a coupled system, which needs to be solved simultaneously, it is clear now why the approach in the beginning was too simple.

[1] We modified the notation from the original work to match the notation of Rahman (2014) and the rest of this thesis.

6 Estimation of fANOVA

In this chapter we will illustrate two approaches to estimate the fANOVA components on a conceptual level. The first approach can be found in Hooker (2007) and is essentially a linear least squares problem. The second approach uses Fourier polynomial expansion and is proposed by Rahman (2014).

7 Examples & Visualizations

8 Conclusion

9 Mathematical Statements

Square Integrability of $f_1(x_1)$

For now we want to show that the single fANOVA term $f_1(x_1)$ is square integrable, given that the original function $f(x) \in \mathcal{L}^2$. We need to show that:

$$\int |f_1(x_1)|^2 \, dx_1 < \infty$$

The single fANOVA term is defined as:

$$f_1(x_1) = \int f(x) \, dx_{-1} - f_0$$

We take the squared norm, and integrate w.r.t. x_1 to use the Cauchy-Schwarz inequality:

$$\int |f_1(x_1)|^2 \, dx_1 = \int \left| \int f(x) \, dx_{-1} - f_0 \right|^2 dx_1$$

$$= \int |(\int f(x) \, dx_{-1})^2 - 2 \int f(x) \, dx_{-1} f_0 + f_0^2 | dx_1$$

Break this into three terms:

$$(1): \quad \int \left| \int f(x) \, dx_{-1} \right|^2 dx_1 \leq \int \left(\int 1^2 \, dx_{-1} \right) \left(\int |f(x)|^2 \, dx_{-1} \right) dx_1 = \int |f(x)|^2 \, dx < \infty$$

$$(2): \quad 2 \int \left(\int f(x) \, dx_{-1} \right) f_0 \, dx_1 = 2 f_0 \int \left(\int f(x) \, dx_{-1} \right) dx_1 = 2 f_0^2 < \infty$$

$$(3): \quad \int f_0^2 \, dx_1 = f_0^2 < \infty$$

Since each term (1)–(3) is finite, and $\int |f_1(x_1)|^2 dx_1$ is a linear combination of them: $\int |f_1(x_1)|^2 dx_1 < \infty$

A Appendix

B Electronic appendix

Data, code and figures are provided in electronic form.

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