Bachelor's Thesis

fANOVA for Interpretable Machine Learning

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Abstract

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Contents

1 Introduction

Questions

- 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? I think 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?
- Denote original model with y or f?
- Connection between the (conditional) expected value, (partial) integral, projections (section 2)?
- 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 4)?
- Hooker (2007) what should the conditional expectation (dotted line) in Figure 2 show? How should it look like for the true data generating process?
- If the general fANOVA formulation is a true generalization then I should be able to take the general form and construct from it the simple form when I use certain constrains (such as independence, uniform distribution, etc.) right?
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- 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 (it might inhibit artefacts and weird behaviour because there was to little data for good model fit in the regions but still that's how the specific model works)
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- 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.*

fANOVA Brainstorming Questions

What happens if...?

- What happens if the function f is linear in all its variables? What do the fANOVA terms look like in that case?
- What happens if some variables are independent? Do any Sobol' terms vanish automatically?
- What happens if you permute the inputs? Do the Sobol' indices change?
- What happens if two variables are strongly collinear? How does that affect the interpretability of fANOVA?

Why is...?

- Why is orthogonality (zero mean and mutual independence of components) important in fANOVA?

- Why is the constant term f_0 equal to the expected value of f?
- Why is fANOVA usually associated with variance-based methods like Sobol indices?
- Why is it necessary to subtract lower-order terms when computing higher-order ones?
- Why is the decomposition hierarchical?

Is it possible to...?

- Is it possible to compute fANOVA in closed form for certain functions (e.g., polynomials)?
- Is it possible to use fANOVA in models where inputs are dependent?
- Is it possible to extend fANOVA to time-series models or dynamic systems?
- Is it possible to use fANOVA ideas in neural networks? How would you interpret interactions then?

What does this remind you of? (Analogies and Parallels)

- fANOVA reminds me of *Fourier decomposition*: projecting a function onto orthogonal basis functions.
- It feels similar to *PCA*, but in the input space instead of the output space.
- fANOVA terms are like *partial derivatives* in symbolic differentiation — quantifying localized influence.
- It's analogous to *ANOVA in statistics*, but instead of experimental groups, you decompose function behavior.
- In machine learning, it reminds me of *feature importance* in random forests or *Shapley values.*
- fANOVA's additive structure is similar to *GAMs (Generalized Additive Models).*

How does fANOVA compare to...?

- How does fANOVA compare to Shapley values? (Shapley is axiomatic, fANOVA is Hilbert space projection-based.)
- How does fANOVA compare to LIME/SHAP in interpretability?
- How does fANOVA compare to gradient-based sensitivity methods?
- How does fANOVA compare to partial dependence plots?
- How does fANOVA compare to mutual information as a dependence measure?

2 General Definitions

2.1 $\mathcal{L}_2$ space

Let $(X, \mathcal{F}, \nu)$ be a measure space, where X is a sample space, $\mathcal{F}$ is a $\sigma-$algebra for X and ν is a general measure. Then the vector space of all square-integrable functions is given by

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

$\mathcal{L}^2$ 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?

Orthogonal projection

$\mathcal{G} \subset \mathcal{L}^2$ denotes 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.

3 Foundations

3.1 Early Work on fANOVA

Hoeffding decomposition 1948

- The idea of fANOVA decomposition dates back to Hoeffding (1948).
- Introduces Hoeffding decomposition (or U-statistics ANOVA decomposition).
- Math-workings: involves orthogonal sums, projection functions, orthogonal kernels, and subtracting lower-order contributions.
- Assupmtions: unclear about all but one assumptions is (mututal?) independence of input variables, which is unrealistic in practice (different generalizations to dependent variables follow, e.g. Il Idrissi et al. (2025))
- Relevance: shows that U-statistics or any symmetric function of the data can be broken down into simpler pieces (e.g., main effects, two-way interactions) without overlap.
- Pieces can be used to dissect/explain the variance.
- fANOVA performs a similar decomposition, not for U-statistics but for functions.

⇒fANOVA and U-statistics

Sobol Indices 1993, 2001

- In "Sensitivity Estimates for Nonlinear Mathematical Models" (1993), Sobol first introduces decomposition into summands of different dimensions of a (square) integrable function.
- Does not cite Hoeffding nor discuss U-statistics.
- "Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates" (2001) builds on his prior work (Sobol, 2001).
- Math-workings: similar to Hoeffding, involving orthogonal projections, sums, and independent terms.
- Sobol focuses on sensitivity analysis for deterministic models, while Hoeffding is concerned with estimates of probabilistic models.

I think in his 1993 paper Sobol mainly introduces fANOVA decomposition (definition, orthogonality, L1 integrability), already speaks of L2 integrability and variance decomp-soition, which leads to Sobol indices, gives some analytical examples and MC algorithm for calculations. In the 2001 paper he focuses on illustrating three usecases of the sobol indices + the decomposition

- ranking of variables
- fixing unessential variables
- deleting high order members

For each of the three there are some mathematical statements, sometimes an algorithm or an example. ⇒
textbffANOVA and sensitivity analysis

Efron and Stein (1981)

- Use idea to proof a famous lemma on jackknife variances (Efron and Stein, 1981)

Stone 1994

- Stone (1994)
- Math-workings: sum of main terms, lower-order terms, etc., with an identifiability constraint (zero-sum constraint); follows the same principle as the decomposition frameworks by Hoeffding (1948) and Sobol (2001).
- All of them work independently, do not cite each other, and use the principle with different goals/build different tools on it.
- Stone's work is part of a broader body of fANOVA models.

⇒fANOVA and smooth regression models / GAMs
I think the main focus of this paper is to extend the theoretical framework of GAMs with interactions. So the baseline is logistic regression with smooth terms but only univariate components are considered. Now the paper goes deeper into the theory where multivariate terms are also considered. For this they refer to the "ANOVA decomposition"of a function. The focus of the paper is on how the smooth multivariate interaction terms can be estimated, what mathematical properties they have, etc.

3.2 Modern Work on fANOVA

- Rabitz and Alis¸ (1999) see ANOVA decomposition as a specific high dimensional model representation (HDMR); the goal is to decompose the model iteratively from main effects, to lower order interactions and so on, but to do this in an efficient way and seletect only interaction terms that are necessary (most often lower-order interactions are sufficient). → chemistry paper

- Work of Hooker (2007) can be seen as an attempt to generalize Hoeffding decomposition (or the Hoeffding principle) to dependent variables. According to Slides to talk on Shapley and Sobol indices

- At least in his talk which is based on the paper Il Idrissi et al. (2025) he puts his work in a broader context of modern attempts to generalize Hoeffding indices. So Il Idrissi et al. (2025) can be seen as one attempt to generalize Hoeffding decomposition to dependent variables.

3.3 Formal Introduction to fANOVA

fANOVA decomposition

This chapter is based on the formal introductions by Sobol (1993, 2001), Hooker (2004), Owen, Muehlenstaedt et al. (2012). Where suitable we show both formulations of the fANOVA, via the integral and via the expected value. Let $i_1, \dots, i_s$ denote a set of indices. For now, we assume that $X_i \overset{\text{i.i.d.}}{\sim} \mathcal{U}[0,1]$ and work in the measure space $(X, \mathcal{F}, \nu) = ([0,1]^n, \mathcal{B}([0,1]^n), \lambda_n)$. $\mathcal{B}([0,1]^n)$ is the Borel σ-algebra on the n-dimensional unit interval and λ_n is the n-dimensional Lebesgue measure. The general inner product and norm we defined earlier simplify under these assumptions.
The inner product under uniform distribution assumption:

$$\langle f, g \rangle = \int f(x)g(x)\, d(x) \quad \forall f, g \in \mathcal{L}^2$$

The norm under uniform distribution assumption:

$$\|f\| = \sqrt{\langle f, f \rangle} = \sqrt{\int f^2(x)\, d(x)} \quad \forall f \in \mathcal{L}^2$$

Definition. Let $f(x)$ be a mathematical model with input X_i as described above. We can represent such a model f as a sum of specific basis functions

$$f(x) = f_0 + \sum_{s=1}^{n} \sum_{i_1<...<i_s}^{n} f_{i_1...i_s}(x_{i_1}, ..., x_{i_s}) \tag{1}$$

To ensure identifiability and interpretation, we set the zero-mean constraint. It requires 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:

$$\int_0^1 f_{i_1...i_s}(x_{i_1}, ..., x_{i_s})\, d\nu(x_k) = 0 \quad \forall k = i_1, ..., i_s \tag{2}$$

In combination with the zero-mean constraint (Equation 2), Sobol (1993) calls Equation 1 initially the “Expansion into Summands of Different Dimensions”. In Sobol (2001) he renames the decomposition to the “ANOVA-representation”. Now, it is mostly referred to as the “functional ANOVA decomposition”(Hooker, 2004).
The individual terms that make up Equation 1 are defined in the following. To get the constant term, we take the integral of f w.r.t. all variables:

$$f_0(x) = \int_{[0,1]^n} f(x) d\nu(x) = \mathbb{E}[f(X)] \tag{3}$$

The constant term f_0 captures the overall mean of f and serves as a baseline. Since the the remaining effects are centred around zero, they quantify the deviation from the overall mean. Next, we take the integral of y w.r.t. all variables except for x_i. This represents f as the sum of the constant term and the isolated effect of one variable x_i (main effect of x_i). This partial integral is equivalent to the expected value conditioned on the variable of interest x_i.

$$f_0 + f_i(x_i) = \int f(x) \prod_{k \neq i} \nu(d_{x_k}) = \mathbb{E}[f(X)|X_i = x_i] \tag{4}$$

Following the same principle, we can take the integral of f w.r.t. all variables except for x_i and x_j. With this we capture everything up to the interaction effect of x_i and x_j. This is equivalent to the expected value conditioned on both variables x_i and x_j:

$$f_0 + f_i(x_i) + f_j(x_j) + f_{ij}(x_i, x_j) = \int f(x) \prod_{k \neq i,j} \nu(d_{x_k}) = \mathbb{E}[f(X)|X_i = x_i, X_j = x_j] \tag{5}$$

For a successive construction of the fANOVA decomposition, we can generally write:

$$\int f(x) \prod_{k \notin u} \nu(d_{x_k}) = \mathbb{E}[f(X)|X_u = x_u] \tag{6}$$

With these partial integrations (or conditional expected values) we build up the fANOVA decomposition in a cumulative way. To actually see the fANOVA terms defined in isolation, it is clearer to rearrange terms. When we rearrange Equation 4 we see that the main effect of x_i is calculated by taking the marginal effect while explicitly accounting for what was already explained by lower-order terms, in this case the intercept:

$$f_i(x_i) = \int f(x) \prod_{k \neq i} \nu(d_{x_k}) - f_0 \tag{7}$$

The two-way interactions can then be seen as the marginal effects of the involved variables, while accounting for all main effects and the constant term:

$$f_{ij}(x_i, x_j) = \int f(x) \prod_{k \neq i,j} \nu(d_{x_k}) - f_0 - f_i(x_i) - f_j(x_j) \tag{8}$$

Therefore, it is also common to formulate the fANOVA decomposition in the following way (Hooker, 2007, 2004):

$$f_u(x) = \int_{[0,1]^{d-|u|}} \left(f(x) - \sum_{v \subsetneq u} f_v(x) \right) d\nu(x_{-u}). \tag{9}$$

This means we subtract all lower-order terms from the original function f and then integrate over all the variables not in u to get the effect of x_u. Using the linearity of the integral, we can also first take the partial integral of the original function w.r.t. all variables not in u and then subtract all the lower-order terms, as we did above for the main effects and two-way interaction effects. So generally we write:

$$f_u(x) = \int_{[0,1]^{d-|u|}} f(x)\, d\nu(x_{-u}) - \sum_{v \subsetneq u} f_v(x). \tag{10}$$

The basis 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.

Example

Before moving to properties of the fANOVA decomposition, let us introduce a simple function g as running example. It contains a constant term a, isolated linear effects of two variables x_1 and x_2 and their interaction.

$$g(x_1, x_2) = a + x_1 + 2x_2 + x_1 x_2 \quad \text{for} \quad a, x_1, x_2 \in \mathbb{R}$$

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 instead of the integral for notational simplicity:

$$f_0 = \mathbb{E}[g(x_1, x_2)] = \mathbb{E}[a + x_1 + 2x_2 + x_1 x_2] = \mathbb{E}[a] + \mathbb{E}[x_1] + 2\mathbb{E}[x_2] + \mathbb{E}[x_1 x_2]$$

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:

$$f_0 = \mathbb{E}[a] + \mathbb{E}[x_1] + 2\mathbb{E}[x_2] + \mathbb{E}[x_1]\mathbb{E}[x_2] = a$$

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

$$\begin{aligned}
f_1(x_1) &= \mathbb{E}_{X_2}[g(x_1, X_2)] - f_0 \\
&= \mathbb{E}_{X_2}[a + x_1 + 2x_2 + x_1 x_2] - a \\
&= x_1 + 2\mathbb{E}[x_2] + x_1\mathbb{E}[x_2] = x_1 \\
f_2(x_2) &= \mathbb{E}_{X_1}[g(X_1, x_2)] - f_0 \\
&= \mathbb{E}_{X_1}[a + x_1 + 2x_2 + x_1 x_2] - a \\
&= \mathbb{E}_{X_1}[x_1] + 2x_2 + x_2\mathbb{E}_{X_1}[x_1] = 2x_2 \\
f_{12}(x_1, x_2) &= \mathbb{E}[g(x_1, x_2)] - f_0 - f_1(x_1) - f_2(x_2) \\
&= a + x_1 + 2x_2 + x_1 x_2 - a - x_1 - 2x_2 = x_1 x_2
\end{aligned}$$

It comes as no surprise that in this simple case the fANOVA decomposition does not provide any additional insights. This is because the model consists of only linear terms, constant terms, and an interaction. We show this simple example nevertheless to illustrate at which step we use which assumption. Understanding this will be relevant for the generalization of the method to dependent inputs later on.

Orthogonality of the fANOVA terms

Orthogonality of the fANOVA terms follows using the zero-mean constraint (Equation 2). If two sets of indices are not completely equivalent $(i_1, \ldots, i_s) \neq (j_1, \ldots, j_l)$ then

$$\int f_{i_1,\ldots,i_s} f_{j_1,\ldots,j_l} d(x) = 0 \tag{11}$$

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. In our example from before we can test this for $i = 1$ and $j = 2$:

$$\int f_1(x_1) f_2(x_2) d(x) = \int x_1 \cdot 2x_2 \, dx_1 \, dx_2 = \mathbb{E}[x_1 2x_2] = \mathbb{E}[x_1] \cdot 2\mathbb{E}[x_2] = 0$$

To write the expected value of a product as the product of the expected values we needed the independence assumption. To state that the product of the expected values is equal to zero, we used the zero-mean constraint. This shows that the independence assumption and zero-mean constraint are critical to ensure orthogonality in this traditional formulation of the fANOVA decomposition. This is of course also true for terms of different order, e.g. $f_{1,2}(x_1, x_2)$ and $f_1(x_1)$. Orthogonality ensures that the effects do not overlap and each term represents the isolated contribution.

Variance decomposition

The variance decomposition is Sobol's major use of fANOVA. He built the Sobol indices for sensitivity analysis on it. We sketch the variance decomposition here and note that it is only possible under independence assumption.
If $f \in \mathcal{L}^2$, then $f_{i_1,\ldots,i_n} \in \mathcal{L}^2$ 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:

$$\begin{aligned}
\sigma &= \int f^2(x) d\nu(x) - (f_0)^2 \\
&= \int f^2(x) d\nu(x) - (\int f(x) d\nu(x))^2 \\
&= \mathbb{E}[f^2(x)] - \mathbb{E}[f(x)]^2
\end{aligned}$$

The variance of the fANOVA components is then defined as

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

Because of the zero-mean constraint (Equation 2) the second term vanishes and we get

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

With the definition of the total variance D and the component-wise variance $D_{i_1,\dots,i_n}$ we can now see that the total variance can be decomposed into the sum of the component-wise variances.
We come back to our example $g(x_1, x_2)$ to illustrate the variance decomposition.

$$\begin{aligned}\sigma &= \int g^2(x_1, x_2) \, d\nu(x) - f_0^2 \\ &= \mathbb{E}[g^2(x_1, x_2)] - a^2 \\ &= \mathbb{E}[(x_1 + 2x_2 + x_1x_2 + a)^2] - a^2 \\ &= \mathbb{E}\left[x_1^2 + 4x_2^2 + x_1^2x_2^2 + a^2 + 4x_1x_2 + 2x_1^2x_2 + 2ax_1 + 4x_1x_2^2 + 4ax_2 + 2ax_1x_2\right] - a^2 \\ &= \mathbb{E}[x_1^2] + 4\mathbb{E}[x_2^2] + \mathbb{E}[x_1^2x_2^2] + 4\mathbb{E}[x_1x_2] + 2\mathbb{E}[x_1^2x_2] + 2a\mathbb{E}[x_1] + 4\mathbb{E}[x_1x_2^2] + 4a\mathbb{E}[x_2] + 2a\mathbb{E}[x_1x_2] \\ &= \sigma^2(x_1) + 4\sigma^2(x_2) + \sigma^2(x_1x_2) + 2\mathbb{E}[x_1^2x_2] + 4\mathbb{E}[x_1x_2^2]\end{aligned}$$

This holds because:

$$\begin{aligned}\sigma(X_1) &= \mathbb{E}[X_1^2] - (\mathbb{E}(X_1))^2 = \mathbb{E}[X_1^2] \\ 4\sigma(X_2) &= \sigma(2X_2) = \mathbb{E}[(2X_2)^2] - (\mathbb{E}(2X_2))^2 = \mathbb{E}[(2X_2)^2] \\ \sigma(X_1X_2) &= \mathbb{E}[X_1^2X_2^2] - (\mathbb{E}[X_1X_2])^2 = \mathbb{E}[X_1^2X_2^2]\end{aligned}$$

Notice that we used the independence assumption and the zero-mean constraint again for the variance decomposition.

fANOVA as projection

Referring to the general connection between the expected value and orthogonal projections presented in section 2, the fANOVA terms can also be understood from a viewpoint of projections. This will also help to understand the generalization of fANOVA in section 4.

f_0 is the projections of the original function f onto the space of all constant functions $\mathcal{G}_0 = \{g(x) = a; a \in \mathbb{R}\}$. It is an unconditional expected value and the best approximation of f given a constant function:

$$\begin{aligned}\Pi_{\mathcal{G}_0} f &= \arg\min_{g \in \mathcal{G}_0} \|f(x) - g\|^2 \\ &= \arg\min_{g \in \mathcal{G}_0} \mathbb{E}[\|f(x) - g\|^2] \\ &= \mathbb{E}[f(X)]\end{aligned}$$

The main effect $f_i(x_i)$ is the projection of f 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 $\mathcal{G}_i = \{g(x) = g_i(x_i); \int g(x) d\nu(x_i) = 0\}$.

$$\begin{aligned}\Pi_{\mathcal{G}_i} f - f_0 &= \arg\min_{g \in \mathcal{G}_i} \|f(x) - g(x_i)\|^2 - f_0 \\ &= \arg\min_{g \in \mathcal{G}_i} \mathbb{E}_{-x_i}[\|f(x) - g(x_i)\|^2] - \mathbb{E}[f(x)] \\ &= \mathbb{E}_{-x_i}[f(X_1, \dots, x_i, \dots, X_n)] - \mathbb{E}[f(X)]\end{aligned}$$

The two-way interaction effect $f_{ij}(x_i, x_j)$ is the projection of f 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:

$$\begin{aligned}\Pi_{\mathcal{G}_{ij}} f - f_0 - f_1(x_i) - \dots &= \arg\min_{g \in \mathcal{G}_{ij}} \|f(x) - g(x_i, x_j)\|^2 - f_0 - f_1(x_i) - \dots \\ &= \arg\min_{g \in \mathcal{G}_{ij}} \mathbb{E}_{-x_i, -x_j}[\|f(x) - g(x_i, x_j)\|^2] - \mathbb{E}[f(x)] - \mathbb{E}_{-x_i}[f(x)] \\ &= \mathbb{E}_{-x_i, -x_j}[f(X_1, \dots, x_i, x_j, \dots, X_n)] - \mathbb{E}[f(x)] - \mathbb{E}_{-x_i}[f(X)]\end{aligned}$$

I think Hilbert space theorem tells us that the orthogonal projection minimizes the squared difference in a Hilbert space? So the projection is the solution to the minimization problem that wants to minimize the squared differences between two elements of the vector space. This would be the first equality. The last equality that the solution is equal to the (conditional) expected value also has to be shown, still have to look which theorem this is proven by.

In general, general we can write:

$$f_u(x) = \Pi_{\mathcal{G}_u} f - \sum_{v \subsetneq u} f_v(x) \tag{12}$$

We project f onto the subspace spanned by the own terms of the fANOVA component to be defined, while accounting for all lower-order terms.

4 Generalization

The chapter is based on Hooker (2007). We want to let go of two key assumptions of the classical fANOVA decomposition (as introduced by Sobol (1993)): We widen the input domain to the multidimensional reel number line, i.e. we now work in the measure space $(X, \mathcal{F}, \nu) = (\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n), dw(x))$. This goes hand in hand with dropping the assumption about the uniform distribution of the X_i. Further, we investigate what happens when the variables are no longer independent of each other.
The inner product on $\mathcal{L}^2(\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n), dw(x))$ is now defined more generally as the integral of a weighted product:

$$\langle f, g\rangle = \int f(x)g(x)\, d\nu(x) \quad \forall f, g \in \mathcal{L}^2 \quad \text{with} \quad \nu(dx) = w(x)dx$$

The norm is given by

$$\|f\|_w = \sqrt{\langle f, f\rangle_w} = \sqrt{\int f^2(x)\, w(x)dx} \quad \forall f \in \mathcal{L}^2$$

The general definition of the function $f(x)$ as a weighted sum stays the same (see Equation 1). What changes is the definition of the fANOVA components. The components are simultaneously defined as:

$$\{f_u(x_u) \,|\, u \subseteq d\} = \arg \min_{\{g_u \in L^2(\mathbb{R}^u)\}_{u \subseteq d}} \int \left(\sum_{u \subseteq d} g_u(x_u) - f(x) \right)^2 w(x)\, dx \tag{13}$$

There is a key difference to the classical definition: All the components are defined simultaneously via the orthogonal projections of the original function $f(x)$. This means the components f_u are a set of functions that jointly minimize the weighted squared difference to the original function $f(x)$ and fulfil the generalized zero-mean constraint and hierarchical orthogonality (both defined in the following). A natural choice for the weights $w(x)$ is the probability distribution of the x_i (Hooker, 2007).
We require the fANOVA terms to be centred around the grand mean, in the same way as we did for the classical approach. Hooker (2007) formulates this in a generalized zero-mean condition for dependent variables:

$$\forall u \subseteq d,\ \forall i \in u: \quad \int f_u(x_u)\, w(x)\, dx_i\, dx_{-u} = 0 \tag{14}$$

Orthogonality of the fANOVA terms plays and important role. It ensures that they represent isolated effects which makes the interpretation of fANOVA so useful in practice. In contrast to the classical fANOVA, we set a hierarchical orthogonality constraint (instead of a general orthogonality constraint):

$$\forall v \subseteq u,\ \forall g: \quad \int f_u(x_u)\ g_v(x_v) w(x)\ dx = 0 \tag{15}$$

I am always puzzled by this definition because v could theoretically be equal to u which would require the function to be orthogonal to itself. But wanting this for all functions g somehow changes something, but I am not super clear why. Would it be correct to write:

$$\forall v \subset u: \quad \int f_u(x_u)\ g_v(x_v) w(x)\ dx = 0 \tag{16}$$

Category	**Classical**	**Generalized**
Measure space	$([0,1]^n, \mathcal{B}([0,1]^n))$	$(\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n))$
Measure	$\mathbb{P}: \mathcal{B}([0,1]^n) \to [0,1]$	$\mu: \mathcal{B}(\mathbb{R}^n) \to [0,\infty)$, where $\mu(A) = \int_A w(x)\,dx$, $w(x) = \frac{d\mu}{d\lambda}$
Distribution assumption	$\mathbf{X} = (X_1,\ldots,X_n) \overset{\text{iid}}{\sim} \mathcal{U}([0,1])$	$\mathbf{X} = (X_1,\ldots,X_n) \sim$ any distribution
Random Variable	$\mathbf{X}: \Omega \to [0,1]^n$, $\mu := \mathbf{X}_\# \mathbb{P}$	$\mathbf{X}_*: \Omega \to \mathbb{R}^n$, $w(x)\,dx = \mathbf{X}_\# \mathbb{P}$
Inner product	$\langle f,g\rangle = \int f(x)g(x)\,dx$	$\langle f,g\rangle_w = \int f(x)g(x)\,w(x)\,dx$
Norm	$\Vert f\Vert = \left(\int f(x)^2\,dx\right)^{1/2} = \sqrt{\mathbb{E}[f(\mathbf{X})^2]}$	$\Vert f\Vert_w = \left(\int f(x)^2 w(x)\,dx\right)^{1/2} = \sqrt{\mathbb{E}[f(\mathbf{X})^2]}$
fANOVA components	$f_u(x) = \int_{x_{-u}} \left(F(x) - \sum_{v \subset u} f_v(x)\right) dx_{-u}$	$\{f_u(x_u)\}_{u \subset d} = \arg\min_{\{g_u \in L^2(\mathbb{R}^u)\}} \int \left(\sum_{u \subset d} g_u(x_u) - F(x)\right)^2 w(x)\,dx$
Zero-mean constraint	$\int f_u(x_u)\,dx_u = 0$ for $u \neq \emptyset$	$\forall u \subset d, \forall i \in u: \int f_u(x_u)\,w(x)\,dx_i\,dx_{-u} = 0$
Orthogonality	$\int f_u(x_u) f_v(x_v)\,dx = 0$ for $u \neq v$	$\forall v \subset u,\ \forall g_v: \int f_u(x_u) g_v(x_v) w(x)\,dx = 0$

Table 1: Comparison of classical and generalized functional ANOVA (fANOVA) decompositions.

5 Simulation Study

5.1 Software implementations

- Suitable but currently problems installing locally: fanova
- Context of kriging models; create own graphs (not super informative): fanovaGraph
- mlr3 function
- tntorch
- shapley values implementation python

6 Method Comparison

This chapter will investigate the mathematical and conceptual parallels between fANOVA decomposition and other IML methods. Goal: get a better understanding for the role fANOVA plays in IML method landscape - When is it suitable? What are the advantages/ limitations compared to other methods?

6.1 fANOVA and Shapley values

paper by Andrew Nii Anang et al. (2024)

7 Conclusion

A Appendix

B Electronic appendix

Data, code and figures are provided in electronic form.

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