Bachelor's Thesis

fANOVA for Interpretable Machine Learning

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Supervised by Prof. Dr. Thomas Nagler

Abstract

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Contents

1 Introduction

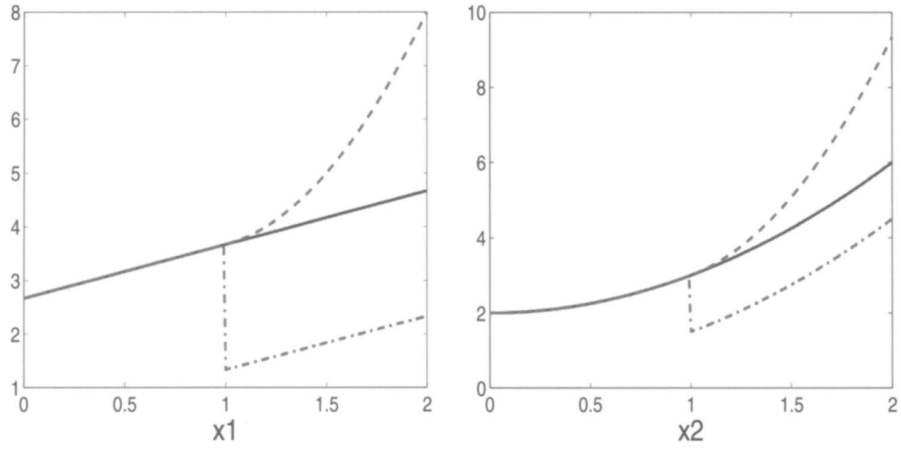

Figure 2. A comparison of Functional ANOVA effects between $F(x_1, x_2)$ (solid) and a learned approximation, $\hat{F}(x_1, x_2)$ (dashed). These two functions are indistinguishable on the data in Figure 1. The left-hand plot provides the effect for x_1, the right for x_2. Dotted lines provide the conditional expectations $E(\hat{F}(x_1, x_2)|x_1)$ and $E(\hat{F}(x_1, x_2)|x_2)$ with respect to the measure in Figure 1.

Questions

- I am confused: I was not clear about the distriction between deterministic input and random variables in the definitions and the examples; and now things are mixed up when it comes to notation, as well as the setup. In general I am now confused if we deal with random variables or deterministic inputs and on which basis fANOVA is really constructed?
- 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?
-
- How is the generalized fANOVA really computed? Could you compute it by hand?
- Effect of non-linear main effects in classical fANOVA (see "General_fANOVA_handnote")

- 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? 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?
- 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 4)?
- I am a bit confused by Figure 2 in Hooker (2007) (see section 1), especially by the dotted line for conditional expectation. What should it tell us? I think what the dashed line (learned approximation) shows is that the model estimates a non-linear effect for x1, even though the true effect is linear. The reasons are the problematic data points in the top right region.
- 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*
-
- 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

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

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

$\mathcal{L}^2$ 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?

2.2 Conditional expectation

In general, we define the conditional expectation of a vector of random variables $X = X_1, X_2$ 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 condi-

tion 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

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

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.

- **Marginal distributions:**
  Each component X_i is univariate normally distributed:

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

  This holds regardless of the dependence structure between the variables.

- **Conditional distributions:**
  Any subset of variables conditioned on another subset is also normally distributed. Partition $\boldsymbol{X}$ as

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

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

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

The conditional mean is a linear function of the conditioning variable, and the conditional covariance does not depend on the conditioning value.

- **Independence and covariance:**
  In the MVN setting, zero covariance implies independence:

  $$\text{If } \operatorname{Cov}(X_i, X_j) = 0, \text{ then } X_i \perp X_j.$$

  This property does not hold in general for arbitrary distributions, but is a special property of the multivariate normal.

- **Linearity of expectations:**
  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 Foundations

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 famous paper 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". Sobol indices are now commonly used in sensitivity analysis. Efron and Stein (1981) use the idea of the decomposition to proof their famous lemma on jackknife variances. 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 example citations needed.

3.2 Modern Work on fANOVA

The fANOVA decomposition has a long history with roots in mathematical statistics and non-parametric estimation theory. 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. 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.
There are specific domains of statistics, such as geostatistics, that explcitly build models on fANOVA framework (see Muehlenstaedt et al. (2012) for fANOVA Kriging 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).
Liu and Owen (2006) use of fANOVA and sensitivity analysis for functions arising in computational finance. Owen (2013) formal intro to fANOVA decomposition and generalization of Sobol indices.

fANOVA and U-statistics, fANOVA and sensitivity analysis, fANOVA and GAMs (with interactions)

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 $i_1, \ldots, i_s$ 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

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

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:

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

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:

$$f_0(x) = \int f(x) d\nu(x) = \mathbb{E}[f(X)] \tag{3}$$

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 1

Before moving to properties of the fANOVA decomposition, let us look at some examples. First, we look at a simple function which takes as input the realization of two continuous independent random variables X_1 and X_2.

$$g_1(x_1, x_2) = a + x_1 + 2x_2 + x_1x_2 \quad \text{for} \quad a, x_1, x_2 \in \mathbb{R}$$

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:

$$f_0 = \mathbb{E}[g_1(X_1, X_2)] = \mathbb{E}[a + X_1 + 2X_2 + X_1X_2] = \mathbb{E}[a] + \mathbb{E}[X_1] + 2\mathbb{E}[X_2] + \mathbb{E}[X_1X_2]$$

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:

$$f_0 = \mathbb{E}[a] + \mathbb{E}[X_1] + 2\mathbb{E}[X_2] + \mathbb{E}[X_1]\mathbb{E}[X_2] = a$$

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

$$\begin{aligned}
f_1(x_1) &= \mathbb{E}_{X_2}[g_1(x_1, X_2)] - f_0 \\
&= \mathbb{E}_{X_2}[a + x_1 + 2X_2 + x_1 X_2] - a \\
&= x_1 + 2\mathbb{E}[X_2] + x_1\mathbb{E}[X_2] = x_1 \\
f_2(x_2) &= \mathbb{E}_{X_1}[g_1(X_1, x_2)] - f_0 \\
&= \mathbb{E}_{X_1}[a + X_1 + 2x_2 + X_1 x_2] - a \\
&= \mathbb{E}_{X_1}[X_1] + 2x_2 + x_2\mathbb{E}_{X_1}[X_1] = 2x_2 \\
f_{12}(x_1, x_2) &= \mathbb{E}[g_1(x_1, x_2)] - f_0 - f_1(x_1) - f_2(x_2) \\
&= a + x_1 + 2x_2 + x_1 x_2 - a - x_1 - 2x_2 = x_1 x_2
\end{aligned}$$

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. Also, it is interesting to compare this example with only linear effects (and an interaction) to the following, which will include a non-linear effect.

Example 2

We now look at the function $g_2 = a + x_1 + x_2^2$ which includes a quadratic effect. We again assume $X_1 \perp X_2$. The constant fANOVA term is given by:

$$f_0 = \mathbb{E}[g_2(X_1, X_2)] = \mathbb{E}[a + X_1 + X_2^2] = a + \mathbb{E}[X_1] + \mathbb{E}[X_2^2] = a + \frac{1}{12}$$

This works because we are still in the setting, in which we assume $X_i \overset{\text{i.i.d.}}{\sim} \mathcal{U}[0, 1]$, in combination with the zero-mean constraint this allows us to state:

$$\mathbb{E}[X_2^2] = \mathbb{V}[X_2] = \frac{1}{12}(1 - 0)^2 = \frac{1}{12}$$

Next, we write the main effects:

$$f_1(x_1) = \mathbb{E}_{X_2}[g_2(x_1, X_2)] - f_0 = \mathbb{E}_{X_2}[a + x_1 + X_2^2] - f_0$$
$$= a + x_1 + \mathbb{E}[X_2^2] - f_0 = a + x_1 + \frac{1}{12} - \left(a + \frac{1}{12}\right) = x_1$$
$$f_2(x_2) = \mathbb{E}_{X_1}[g_2(X_1, x_2)] - f_0 = \mathbb{E}_{X_1}[a + X_1 + x_2^2] - f_0$$
$$= a + \mathbb{E}[X_1] + x_2^2 - f_0 = a + x_2^2 - \left(a + \frac{1}{12}\right) = x_2^2 - \frac{1}{12}$$

Finally, we compute the interaction effect:

$$f_{12}(x_1, x_2) = \mathbb{E}[g_2(x_1, x_2)] - f_0 - f_1(x_1) - f_2(x_2)$$
$$= a + x_1 + x_2^2 - \left(a + \frac{1}{12}\right) - x_1 - \left(x_2^2 - \frac{1}{12}\right) = 0$$

What we observe in this example is that explicit centering of the quadratic effect by subtracting a constant is necessary.

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 $f_{i_1,\dots,i_n} \in \mathcal{L}^2$ 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 **??**, 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 $\mathcal{G}_i = \{g(x) = g_i(x_i); \int g(x) d\nu(x_i) = 0\}$.

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

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:

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

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	$\|f\| = \left(\int f(x)^2\,dx\right)^{1/2} = \sqrt{\mathbb{E}[f(\mathbf{X})^2]}$	$\|f\|_w = \left(\int f(x)^2 w(x)\,dx\right)^{1/2} = \sqrt{\mathbb{E}[f(\mathbf{X})^2]}$
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.

Example 1

Example 2: Multivariate Normal Inputs

We return to our example function $g(x_1, x_2) = a + x_1 + 2x_2 + x_1 x_2$ and assume that:

$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \right), \quad \rho > 0$$

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:

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

The constant term f_0 is given by:

$$\begin{aligned} f_0 &= \mathbb{E}[g(X_1, X_2)] = a + \mathbb{E}[X_1] + 2\mathbb{E}[X_2] + \mathbb{E}[X_1 X_2] \\ &= a + \mathbb{E}[X_1 X_2] = a + (\text{Cov}(X_1, X_2) + \mathbb{E}[X_1]\mathbb{E}[X_2]) \\ &= a + \rho \end{aligned}$$

The main effects can be computed as:

$$\begin{aligned} f_1(x_1) &= \mathbb{E}[g(X_1, X_2)|X_1 = x_1] - f_0 \\ &= \mathbb{E}[a + x_1 + 2X_2 + x_1 X_2 | X_1 = x1] - (a + \rho) \\ &= a + x_1 + 2\mathbb{E}[X_2|X_1 = x_1] + x_1\mathbb{E}[X_2|X_1 = x_1] - a - \rho \\ &= x_1 - \rho + \rho(2 + x_1) \\ f_2(x_2) &= \mathbb{E}[g(X_1, X_2) \mid X_2 = x_2] - f_0 \\ &= \mathbb{E}[a + X_1 + 2x_2 + X_1 x_2 \mid X_2 = x_2] - (a + \rho) \\ &= a + 2x_2 + x_2\mathbb{E}[X_1 \mid X_2 = x_2] - a - \rho \\ &= 2x_2 + x_2^2\rho + \rho \end{aligned}$$

Finally, the interaction effect $f_{12}(x_1, x_2)$ is given by:

$$\begin{aligned} f_{12}(x_1, x_2) &= g(x_1, x_2) - f_0 - f_1(x_1) - f_2(x_2) \\ &= a + x_1 + 2x_2 + x_1 x_2 - (a + \rho) - (x_1 - \rho + 2\rho x_1 + \rho x_1^2) - (2x_2 + x_2^2\rho + \rho) \\ &= x_1 x_2 - 2\rho x_1 - \rho x_1^2 - \rho x_2^2 - \rho \end{aligned}$$

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 Conclusion

7 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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