Your Title

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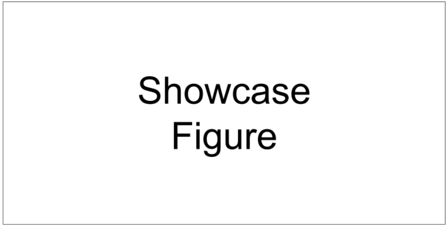
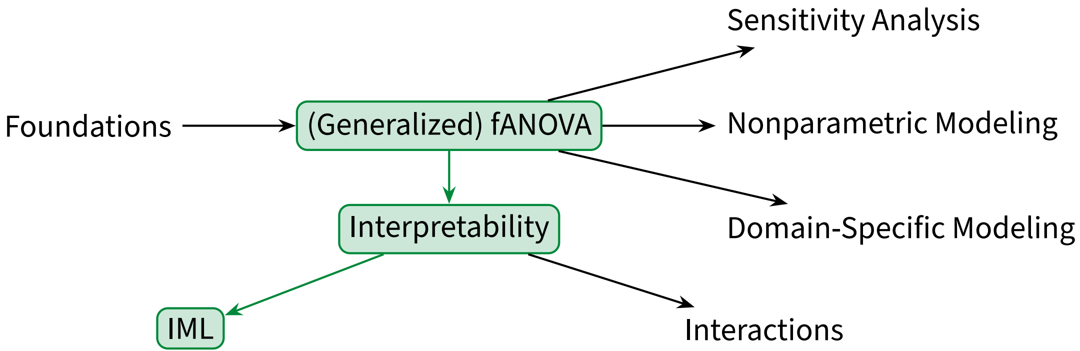
August 1, 2025



Outline

Overview of the fANOVA Research Field



References: [1, 2, 5, 7, 6, 4, 3]

Outline

Formal Setting

- measure space, probability measure, random vector, subvector, complementary vector, pdf
- measure space of square integrable functions
- inner product
- norm

Classical fANOVA Decomposition

General Form

$$y(\boldsymbol{X}) = \sum_{u \subseteq \{1,\ldots,N\}} y_u(\boldsymbol{X}_u) = y_\emptyset + y_{\{1\}}(\boldsymbol{X}_1) + \cdots + y_{\{1,2\}}(\boldsymbol{X}_1, \boldsymbol{X}_2) + \ldots$$

- y : Model
- y_u : Component functions for subset u
- Assumption: $X_1, \ldots, X_N$ are independent

Conditions for Classical fANOVA

Strong Annihilating Conditions

$$\int_{\mathbb{R}} y_u(\boldsymbol{x}_u) f_{\{i\}}(x_i)\, d\nu(x_i) = 0 \quad \text{for } i \in u \neq \emptyset.$$

- Ensures unique component functions
- Applies under independent (product-type) input distributions

Key Properties

$$\mathbb{E}[y_u(\boldsymbol{X}_u)] = 0$$

$$\mathbb{E}[y_u(\boldsymbol{X}_u)y_v(\boldsymbol{X}_v)] = 0 \quad (u \neq v)$$

- Zero mean components
- Mutual orthogonality

Component Construction

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

$$y_u(x_u) = \int y(x) f_{-u}(x_{-u}) dx_{-u} - \sum_{v \subsetneq u} y_v(x_v)$$

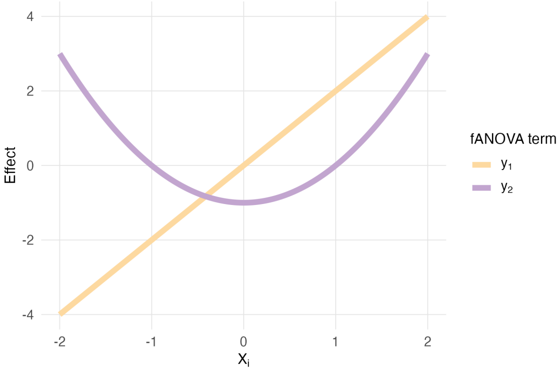
- f_{-u} : marginal density of variables not in u
- Components solved sequentially by increasing order

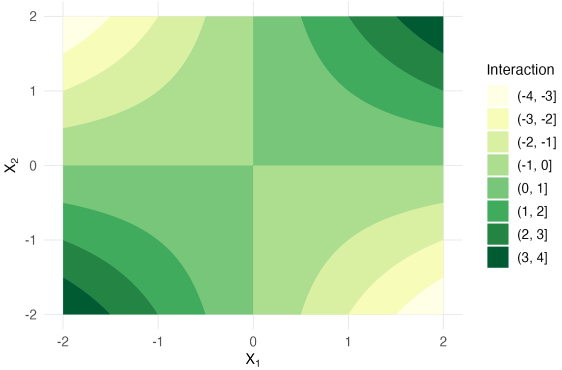
Example: Two degree Polynomial

$$y(x_1, x_2) = 2x_1 + x_2^2 + x_1 x_2 \tag{1}$$

- Coefficients: $a_1 = 20, a_2 = 0, a_{11} = 0, a_{22} = 10, a_{12} = 10$
- Independent variables: $\rho = 0$

Example: 2D Function





Equality to Hoeffding Decomposition

Hoeffding Decomposition

$$y(\boldsymbol{X}) = \sum_{A \subseteq D} y_A(\boldsymbol{X}_A), \qquad D := \{1, \ldots, N\}, \tag{2}$$

where, for each $A \subseteq D$, the component function y_A is defined by:

$$y_A(\boldsymbol{X}_A) = \sum_{B \subseteq A} (-1)^{|A|-|B|} \, \mathbb{E}[y(\boldsymbol{X}) \mid \boldsymbol{X}_B] \,, \tag{3}$$

where y_u are orthogonal components.

- Classical fANOVA and Hoeffding decomposition yield same components under zero-centered inputs
- Both assume independence of input variables

General Definition of Orthogonal Projection

$$\Pi_{\mathcal{G}} y = \arg\min_{g \in \mathcal{G}} \|y - g\|^2 = \arg\min_{g \in \mathcal{G}} \mathbb{E}[(y(\boldsymbol{X}) - g(\boldsymbol{X}))^2]. \tag{4}$$

- $\mathcal{G}$: linear subspace of $\mathcal{L}^2$ we project onto
- g all functions in the subspace

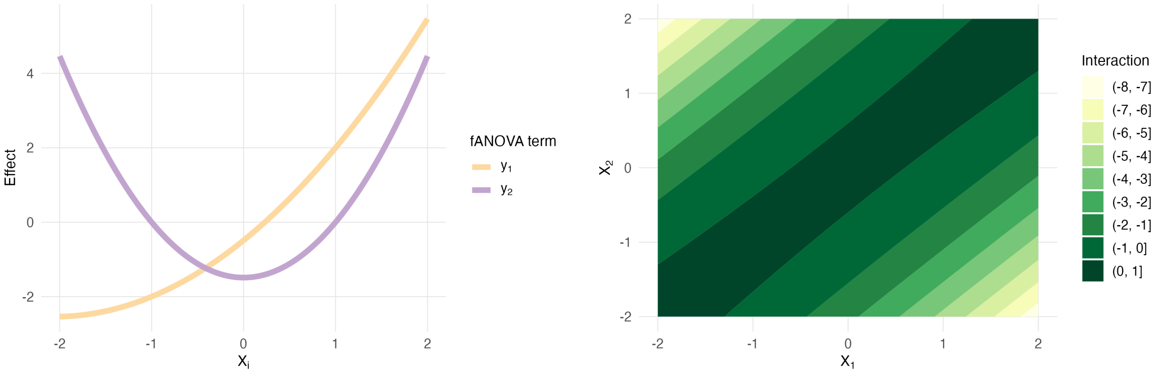
fANOVA as Orthogonal Projection

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

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

Outline

Example with Dependent Inputs ($\rho = 0.8$)



Weaker Annihilating Conditions

Weak Annihilating Conditions

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

- Allows dependent input distributions
- Leads to hierarchical orthogonality

Key Properties (Generalized)

$$\mathbb{E}[y_{u,G}(\boldsymbol{X}_u)] := \int_{\mathbb{R}^N} y_{u,G}(\boldsymbol{x}_u) f_{\boldsymbol{X}}(\boldsymbol{x})\, d\nu(\boldsymbol{x}) = 0.$$

$$\mathbb{E}[y_{u,G}(\boldsymbol{X}_u) y_{v,G}(\boldsymbol{X}_v)] := \int_{\mathbb{R}^N} y_{u,G}(\boldsymbol{x}_u) y_{v,G}(\boldsymbol{x}_v) f_{\boldsymbol{X}}(\boldsymbol{x})\, d\nu(\boldsymbol{x}) = 0.$$

- Zero mean components remain
- Orthogonality is weaker: hierarchical

Component Definition (Coupled System)

$$y_{\emptyset,G} = \int_{\mathbb{R}^N} y(\boldsymbol{x}) f_{\boldsymbol{X}}(\boldsymbol{x}) \, d\nu(\boldsymbol{x}) \tag{5}$$

$$\begin{aligned} y_{u,G}(\boldsymbol{X}_u) &= \int_{\mathbb{R}^{N-|u|}} y(\boldsymbol{X}_u, \boldsymbol{x}_{-u}) f_{-u}(\boldsymbol{x}_{-u}) \, d\nu(\boldsymbol{x}_{-u}) - \sum_{v \subsetneq u} y_{v,G}(\boldsymbol{X}_v) \\ &\quad - \sum_{\substack{\emptyset \neq v \subseteq \{1,\dots,N\} \\ v \cap u \neq \emptyset,\ v \not\subset u}} \int_{\mathbb{R}^{|v \cap -u|}} y_{v,G}(\boldsymbol{X}_{v\cap u}, \boldsymbol{x}_{v\cap -u}) f_{v\cap -u}(\boldsymbol{x}_{v\cap -u}) \, d\nu(\boldsymbol{x}_{v\cap -u}). \end{aligned} \tag{6}$$

- All components solved simultaneously
- Depends on marginal densities and coupling terms

How to Construct the Components

- Coupled system $\rightarrow$ difficult to obtain analytical solutions
- Use alternative method via Fourier Polynomial ([5])
- Building blocks: mutually orthogonal, zero-mean basis functions $\psi_{i,j}$, coefficients $c_{i,j}$

Basis Representation of a Polynomial

$$
\begin{aligned}
y(x_1, x_2) &= a_0 + a_1 x_1 + a_2 x_2 + a_{11} x_1^2 + a_{22} x_2^2 + a_{12} x_1 x_2 \\
&= c_0 + c_{1,1}\, \psi_{1,1}(x_1) + c_{2,1}\, \psi_{2,1}(x_2) \\
&\quad + c_{1,2}\, \psi_{1,2}(x_1) + c_{2,2}\, \psi_{2,2}(x_2) + c_{12,11}\, \psi_{12,11}(x_1, x_2) \\
&= \underbrace{c_0}_{y_0} + \underbrace{\left(c_{1,1}\, \psi_{1,1}(x_1) + c_{1,2}\, \psi_{1,2}(x_1)\right)}_{y_1(x_1)} \\
&\quad + \underbrace{\left(c_{2,1}\, \psi_{2,1}(x_2) + c_{2,2}\, \psi_{2,2}(x_2)\right)}_{y_2(x_2)} \\
&\quad + \underbrace{c_{12,11}\, \psi_{12,11}(x_1, x_2)}_{y_{12}(x_1,x_2)} .
\end{aligned}
$$

Basis Functions proposed by Rahman (2014)[5]

$$
\begin{aligned}
\psi_{\emptyset}(x_1, x_2) &= 1, \\
\psi_{1,1}(x_1) &= x_1, \\
\psi_{2,1}(x_2) &= x_2, \\
\psi_{1,2}(x_1) &= x_1^2 - 1, \\
\psi_{2,2}(x_2) &= x_2^2 - 1, \\
\psi_{12,11}(x_1, x_2) &= \frac{\rho(x_1^2 + x_2^2)}{1 + \rho^2} - x_1 x_2 + \frac{\rho(\rho^2 - 1)}{1 + \rho^2},
\end{aligned}
$$

Alternative Generalization of fANOVA, [2]

$$\{y_{u,G}(\boldsymbol{x}_u) \mid u \subseteq d\} = \arg \min_{\{g_u \in \mathcal{L}^2(\mathbb{R}^{|u|})\}} \int_{\mathbb{R}^N} \left(\sum_{u \subseteq d} g_u(\boldsymbol{x}_u) - y(\boldsymbol{x}) \right)^2 f_{\boldsymbol{X}}(\boldsymbol{x}) \, d\nu(\boldsymbol{x}),$$

subject to hierarchical orthogonality conditions:

$$\forall v \subseteq u, \ \forall g_v : \int_{\mathbb{R}^N} y_u(\boldsymbol{x}_u) g_v(\boldsymbol{x}_v) f_{\boldsymbol{X}}(\boldsymbol{x}) \, d\nu(\boldsymbol{x}) = 0.$$

Variance Decomposition, [6]

$$\mu := \mathbb{E}[y(\boldsymbol{X})] = y_{\emptyset,G}.$$

$$\begin{aligned}
\sigma^2 &:= \mathbb{E}\left[(y(\boldsymbol{X}) - \mu_G)^2\right] \\
&= \mathbb{E}\left[\left(y_{\emptyset,G} + \sum_u y_{u,G}(\boldsymbol{X}_u) - y_{\emptyset,G}\right)^2\right] \\
&= \mathbb{E}\left[\left(\sum_u y_{u,G}(\boldsymbol{X}_u)\right)^2\right] \\
&= \sum_u \mathbb{E}\left[y^2_{u,G}(\boldsymbol{X}_u)\right] + \sum_{u \not\subseteq v,\, v \not\subseteq u} \mathbb{E}\left[y_{u,G}(\boldsymbol{X}_u) y_{v,G}(\boldsymbol{X}_v)\right],
\end{aligned}$$

Outline

Limitations

Future Research

- Estimation schemes and software implementation
- Extension of Fourier polynomial expansion to other distributions

Outline

Classical fANOVA Proofs

- Zero mean property: factorized density, Fubinis Theorem, strong annihilating conditions
- Mutual orthogonality: factorized density, Fubinis Theorem, strong annihilating conditions

Generalized fANOVA Proofs

- Zero mean property: separating x into subvectors, marginal density, Fubinis Theorem, weak annihilating conditions
- Hierarchical orthogonality: set the scene, u is a proper subset of v $u \subsetneq v$, so there is an index in u which is not in v; divide x_u into subvectors, marginal density, Fubini and weak annihilating conditions
- Weak annihilating becomes strong under independence: assume the weak ones, product density, factor out
- Three integration cases: distinguish between different relationships u and v, depending on the relationship the integral w.r.t. to marginal density simplifies
- Generalized fANOVA components by Rahman: first build constant term; for nonconstant terms use integration cases
- Integration constraint Hooker: show that hierarchical orthogonality is fulfilled if the conditions hold, show that it is not fulfilled if they do not hold; but why exactly these conditions a bit unclear
- Take a look at Sobols proof again

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