

Your Title

Your Name

August 2, 2025

Showcase
Figure

Outline

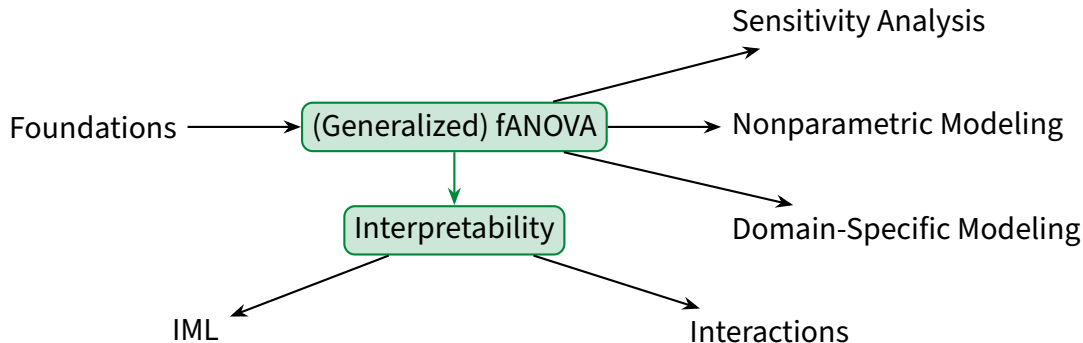
1 Research Context

2 Classical fANOVA

3 Generalized fANOVA

4 Conclusion

5 Extra Slides



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

Outline

1 Research Context

2 Classical fANOVA

3 Generalized fANOVA

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5 Extra Slides

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

General Form

$$\begin{aligned} y(\mathbf{X}) &= \sum_{u \subseteq \{1, \dots, N\}} y_u(\mathbf{X}_u) \\ &= y_{\emptyset} + (y_{\{1\}}(\mathbf{X}_1) + \dots + y_{\{N\}}(\mathbf{X}_N)) \\ &\quad + (y_{\{1,2\}}(\mathbf{X}_1, \mathbf{X}_2) + y_{\{1,3\}}(\mathbf{X}_1, \mathbf{X}_3) + \dots) \\ &\quad + (y_{\{1,2,3\}}(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3) + \dots) + \dots + y_{\{1, \dots, N\}}(\mathbf{X}_1, \dots, \mathbf{X}_N) \end{aligned}$$

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

Strong Annihilating Conditions

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

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

$$\mathbb{E}[y_u(\mathbf{x}_u)] = 0$$

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

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

$$y_u(\mathbf{x}_u) = \int_{\mathbb{R}^{N-|u|}} y(\mathbf{x}_u, \mathbf{x}_{-u}) \prod_{i=1, i \notin u}^N f_{\{i\}}(x_i) d\nu(x_i) - \sum_{v \subsetneq u} y_v(\mathbf{x}_v). \quad (1)$$

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

- $N = 3$

$$y_{\emptyset} = \int_{\mathbb{R}^3} y(\mathbf{x}) \prod_{i=1}^3 f_{\{i\}}(x_i) d\nu(x_i) = \mathbb{E}[y(\mathbf{x})].$$

- $u = \{1\} \rightarrow v = \emptyset$

$$y_{\{1\}}(X_1) = \int_{\mathbb{R}^2} y(X_1, x_2, x_3) \prod_{i=2}^3 f_{\{i\}}(x_i) d\nu(x_i) - y_{\emptyset} = \mathbb{E}[y(X_1, X_2, X_3) | X_1 = x_1] - y_{\emptyset}.$$

- $u = \{1, 2\} \rightarrow v = \{1\}, \{2\}, \emptyset$

$$\begin{aligned} y_{\{1,2\}}(X_1, X_2) &= \int_{\mathbb{R}} y(X_1, X_2, x_3) f_{\{3\}}(x_3) d\nu(x_3) - y_{\{1\}}(X_1) - y_{\{2\}}(X_2) - y_{\emptyset} \\ &= \mathbb{E}[y(X_1, X_2, X_3) | X_1 = x_1, X_2 = x_2] - y_{\{1\}}(X_1) - y_{\{2\}}(X_2) - y_{\emptyset}. \end{aligned}$$

$$y(x_1, x_2) = 2x_1 + x_2^2 + x_1x_2$$

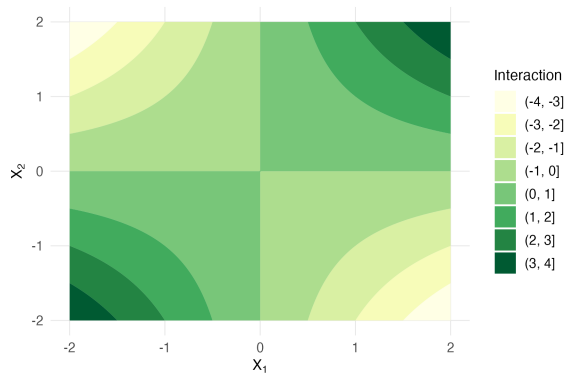
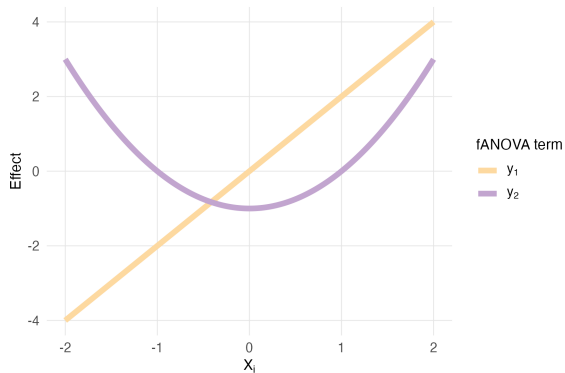
$$(X_1, X_2)^T \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}\right),$$

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

Components:

$$y_{\emptyset} = 0, \quad y_{\{1\}}(x_1) = 2x_1, \quad y_{\{2\}}(x_2) = x_2^2, \quad y_{\{1,2\}}(x_1, x_2) = x_1x_2.$$

Example: 2D Function



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

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

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

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

Hoeffding Decomposition

$$y(\mathbf{x}) = \sum_{A \subseteq D} y_A(\mathbf{x}_A), \quad D := \{1, \dots, N\}, \quad (3)$$

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

$$y_A(\mathbf{x}_A) = \sum_{B \subseteq A} (-1)^{|A|-|B|} \mathbb{E}[y(\mathbf{x}) \mid \mathbf{x}_B], \quad (4)$$

where y_u are orthogonal components.

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

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1 Research Context

2 Classical fANOVA

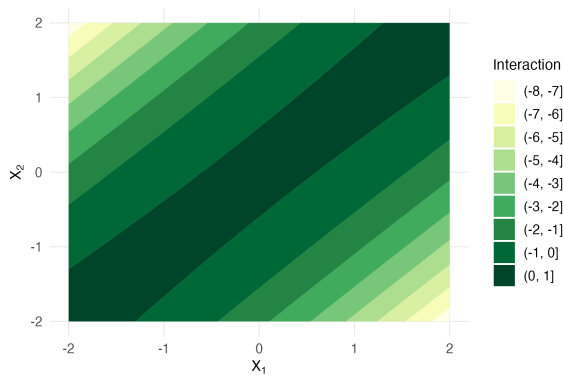
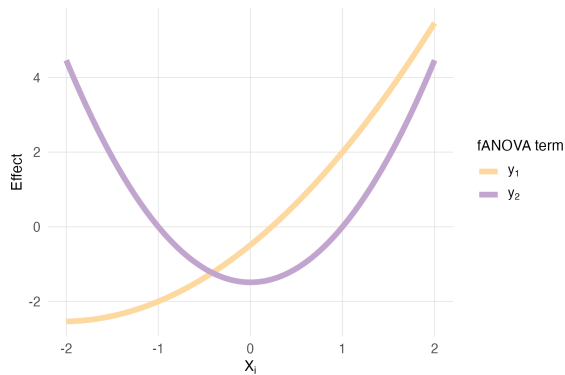
3 Generalized fANOVA

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Example with Dependent Inputs

$$y(x_1, x_2) = 2x_1 + x_2^2 + x_1x_2, \quad \rho = 0.8$$



Weak Annihilating Conditions

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

- Allows dependent input distributions
- Leads to hierarchical orthogonality

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

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

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

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

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

- $N = 3$

$$y_{\emptyset, G} = \int_{\mathbb{R}^3} y(\mathbf{x}) f_{\mathbf{X}}(\mathbf{x}) d\nu(\mathbf{x}) = \mathbb{E}[y(\mathbf{X})]$$

- $u = \{1\}$

- ▶ $v \subsetneq u \rightarrow \emptyset$
- ▶ $(\emptyset \neq v \subseteq \{1, \dots, N\}, v \cap u \neq \emptyset, v \not\subseteq u) \rightarrow \{1, 2\}, \{1, 2, 3\}$

- 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 $c_{i,j}$

$$\begin{aligned}y(x_1, x_2) &= a_0 + a_1x_1 + a_2x_2 + a_{11}x_1^2 + a_{22}x_2^2 + a_{12}x_1x_2 \\&= c_0 + c_{1,1} \psi_{1,1}(x_1) + c_{2,1} \psi_{2,1}(x_2) \\&\quad + c_{1,2} \psi_{1,2}(x_1) + c_{2,2} \psi_{2,2}(x_2) + c_{12,11} \psi_{12,11}(x_1, x_2) \\&= \underbrace{c_0}_{y_0} + \underbrace{(c_{1,1} \psi_{1,1}(x_1) + c_{1,2} \psi_{1,2}(x_1))}_{y_1(x_1)} \\&\quad + \underbrace{(c_{2,1} \psi_{2,1}(x_2) + c_{2,2} \psi_{2,2}(x_2))}_{y_2(x_2)} \\&\quad + \underbrace{c_{12,11} \psi_{12,11}(x_1, x_2)}_{y_{12}(x_1, x_2)}.\end{aligned}$$

$$\psi_{\emptyset}(x_1, x_2) = 1,$$

$$\psi_{1,1}(x_1) = x_1,$$

$$\psi_{2,1}(x_2) = x_2,$$

$$\psi_{1,2}(x_1) = x_1^2 - 1,$$

$$\psi_{2,2}(x_2) = x_2^2 - 1,$$

$$\psi_{12,11}(x_1, x_2) = \frac{\rho(x_1^2 + x_2^2)}{1 + \rho^2} - x_1x_2 + \frac{\rho(\rho^2 - 1)}{1 + \rho^2},$$

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

subject to hierarchical orthogonality conditions:

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

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

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

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

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- Zero mean property: factorized density, Fubini's Theorem, strong annihilating conditions
- Mutual orthogonality: factorized density, Fubini's Theorem, strong annihilating conditions

- Zero mean property: separating x into subvectors, marginal density, Fubini's 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 Sobol's proof again

- https://docs.google.com/spreadsheets/d/1K5ECL6hDPDnHwM_k342xa29H-vHWzdk27PTgDHUwfFE/edit?usp=sharing - Table with fANOVA-related literature



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