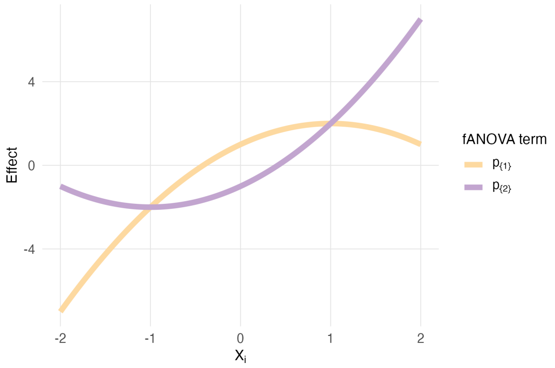
Functional ANOVA Decomposition

Juliet Fleischer

August 9, 2025



Outline

Overview of the fANOVA Research Field

Foundations

Overview of the fANOVA Research Field

Foundations $\longrightarrow$ (Generalized) fANOVA

Overview of the fANOVA Research Field

Sensitivity Analysis

Foundations → (Generalized) fANOVA → Sensitivity Analysis

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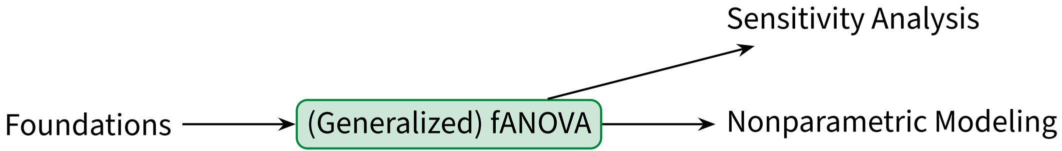

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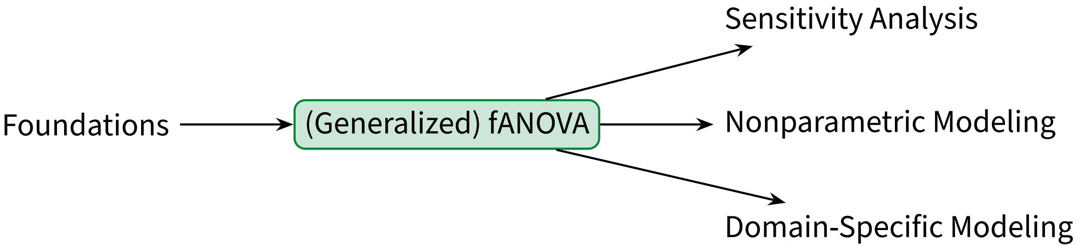

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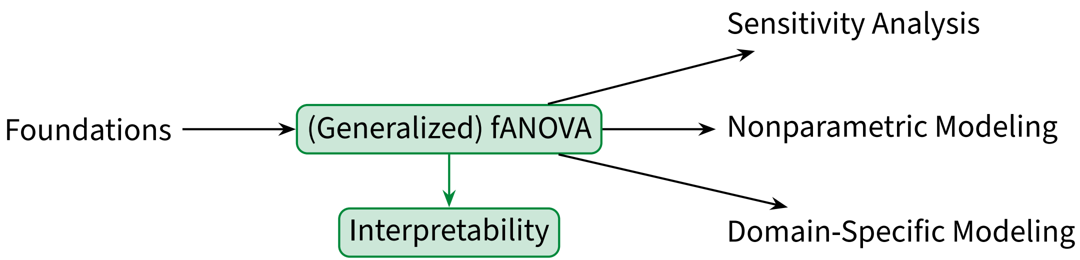

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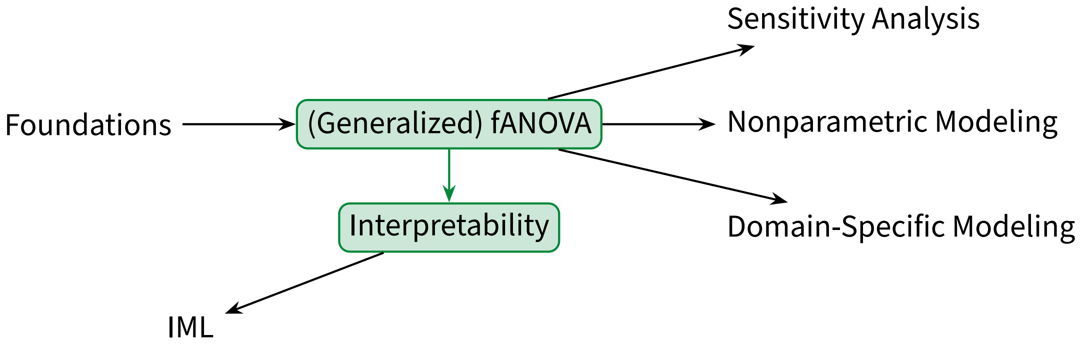

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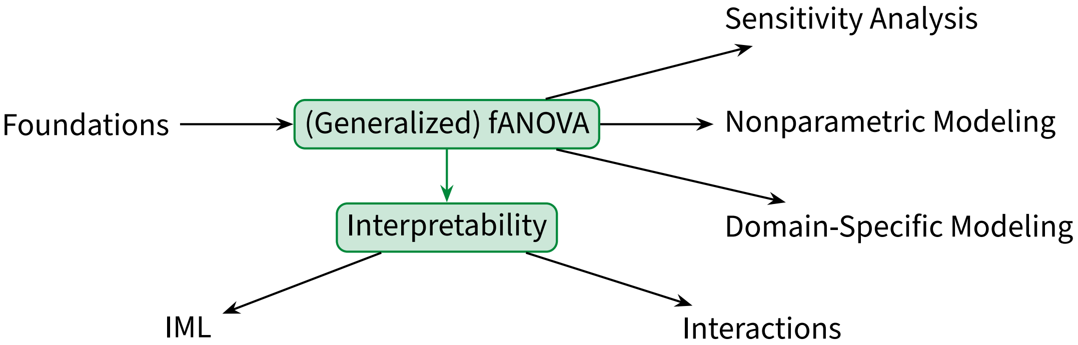

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Decomposition of Model into Interpretable Components

General Form

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

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Ensure Uniqueness and Interpretability of the Components

Strong Annihilating Conditions

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

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Recursive Form of the Components

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Remark: fANOVA components can be seen from lens of orthogonal projections.

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

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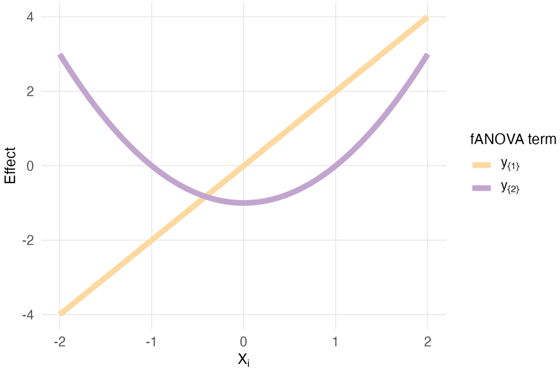
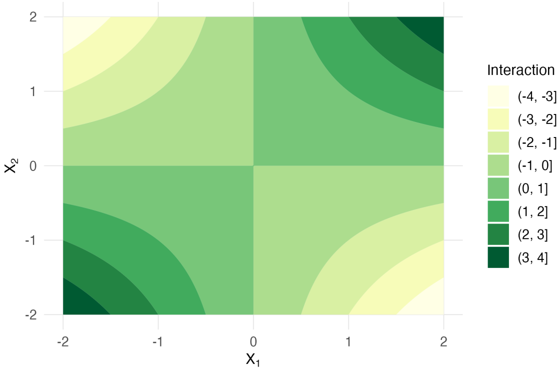
Components:

$$y_\emptyset = 1, \qquad y_{\{1\}}(x_1) = 2x_1, \qquad y_{\{2\}}(x_2) = x_2^2 - 1, \qquad y_{\{1,2\}}(x_1, x_2) = x_1 x_2.$$

Visualization of fANOVA components under Independence

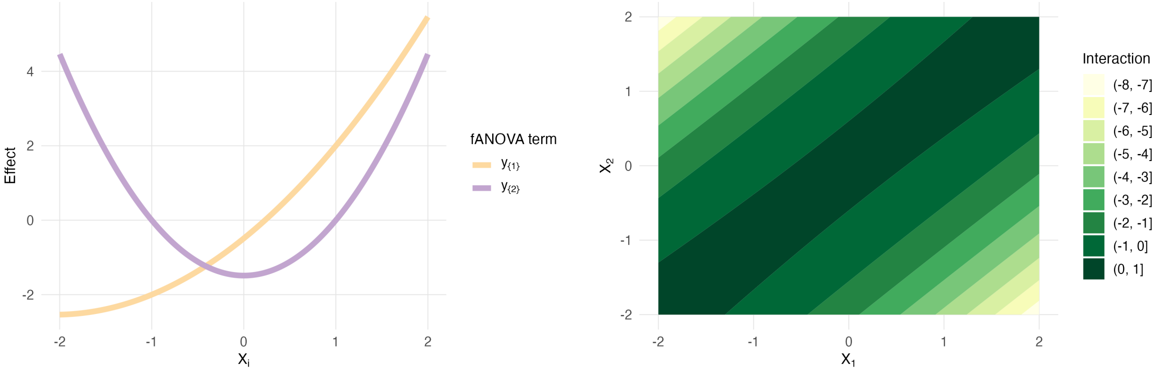
$$y(x_1, x_2) = 2x_1 + x_2^2 + x_1 x_2$$





Outline

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



Ensuring Interpretability under Dependent Inputs

Weak Annihilating Conditions

$$\int_{\mathbb{R}} y_{u,G}(\boldsymbol{x}_u) f_{\boldsymbol{u}}(\boldsymbol{x}_u) d\nu(x_i) = 0 \quad \text{for} \quad i \in u \neq \emptyset. \tag{1}$$

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

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Building the Generalized Components as Coupled System

- $N = 3, u = \emptyset$

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

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$(\emptyset \neq v \subseteq \{1, \dots, N\},\ v \cap u \neq \emptyset,\ v \not\subset u) \in \{\{1,2\}, \{1,3\}, \{1,2,3\}\}$

$$y_{\{1\},G}(\boldsymbol{X}_u) = \int_{\mathbb{R}^2} y(x_1, x_2, x_3) f_{\{2,3\}}(x_2, x_3)\, d\nu(x_2, x_3) - y_{\emptyset,G}$$

$$- \int_{\mathbb{R}} y_{\{1,2\},G}(x_1, x_2) f_{\{2\}}(x_2)\, d\nu(x_2) - \int_{\mathbb{R}} y_{\{1,3\},G}(x_1, x_3) f_{\{3\}}(x_3)\, d\nu(x_3)$$

$$- \int_{\mathbb{R}^2} y_{\{1,2,3\},G}(x_1, x_2, x_3) f_{\{2,3\}}(x_2, x_3)\, d\nu(x_2, x_3)$$

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$$y_{\{1,2\},G}(\boldsymbol{X}_u) = \int_{\mathbb{R}} y(x_1,x_2,x_3) f_{\{3\}}(x_3)\, d\nu(x_3) - y_{\emptyset,G} - y_{\{1\},G} - y_{\{2\},G}$$

$$- \int_{\mathbb{R}} y_{\{1,2,3\},G}(x_1,x_2,x_3) f_{\{3\}}(x_3)\, d\nu(x_3)$$

Building the Generalized Components as Coupled System

- $u = \{1,2,3\} \rightarrow v \subsetneq u \in \{\emptyset, \{1\}, \{2\}, \{3\}, \{1,2\}, \{1,3\}, \{2,3\}\}$ and $(\emptyset \neq v \subseteq \{1,\ldots,N\},\ v \cap u \neq \emptyset,\ v \not\subset u) \in \{\emptyset\}$

$$
\begin{aligned}
y_{\{1,2,3\},G}(\boldsymbol{X}_u) &= y(x_1, x_2, x_3) - y_{\emptyset,G} \\
&\quad - y_{\{1\},G} - y_{\{2\},G} - y_{\{3\},G} \\
&\quad - y_{\{1,2\},G} - y_{\{1,3\},G} - y_{\{2,3\},G}
\end{aligned}
$$

Construction of Components via Fourier-polynomial Expansion

$$y(x_1, x_2) = a_0 + a_1 x_1 + a_2 x_2 + a_{11} x_1^2 + a_{22} x_2^2 + a_{12} x_1 x_2$$

Construction of Components via Fourier-polynomial Expansion

$$
\begin{aligned}
y(x_1, x_2) &= a_0 + a_1 x_1 + a_2 x_2 + a_{11} x_1^2 + a_{22} x_2^2 + a_{12} x_1 x_2 \\
&= c_0 + c_{1,1}\,\psi_{1,1}(x_1) + c_{2,1}\,\psi_{2,1}(x_2)
\end{aligned}
$$

Construction of Components via Fourier-polynomial Expansion

$$
\begin{aligned}
y(x_1, x_2) &= a_0 + a_1 x_1 + a_2 x_2 + a_{11} x_1^2 + a_{22} x_2^2 + a_{12} x_1 x_2 \\
&= c_0 + c_{1,1}\, \psi_{1,1}(x_1) + c_{2,1}\, \psi_{2,1}(x_2) \\
&\quad + c_{1,2}\, \psi_{1,2}(x_1) + c_{2,2}\, \psi_{2,2}(x_2) + c_{12,11}\, \psi_{12,11}(x_1, x_2)
\end{aligned}
$$

Construction of Components via Fourier-polynomial Expansion

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

Construction of Components via Fourier-polynomial Expansion

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

Construction of Components via Fourier-polynomial Expansion

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

Choosing Orthogonal Basis Functions

In [7] Hermite polynomial basis functions are proposed

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

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

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

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

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

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

fANOVA Components of a two-degree Polynomial

- Yields fANOVA components for MVN Inputs
- Works for polynomials of degree up to $d = 2$

$$y_{\emptyset,G} = a_0 + a_{11} + a_{22} + \rho\, a_{12},$$

$$y_{\{1\},G}(x_1) = a_1\, x_1 + \left(a_{11} + \frac{\rho}{1+\rho^2} a_{12}\right)\left(x_1^2 - 1\right),$$

$$y_{\{2\},G}(x_2) = a_2\, x_2 + \left(a_{22} + \frac{\rho}{1+\rho^2} a_{12}\right)\left(x_2^2 - 1\right),$$

$$y_{\{1,2\},G}(x_1, x_2) = -a_{12}\left(\frac{\rho(x_1^2 + x_2^2)}{1+\rho^2} - x_1 x_2 + \frac{\rho(\rho^2 - 1)}{1+\rho^2}\right).$$

Decomposition under Weak Correlation

$$z(x_1, x_2) = 2x_1 + x_1^2 + 0.5x_1x_2$$

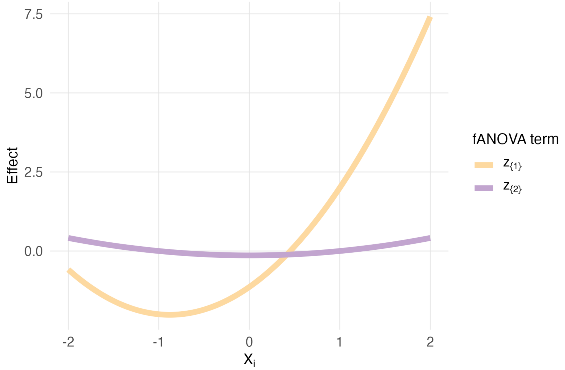

Figure: Main effect for $\rho = 0.3$.

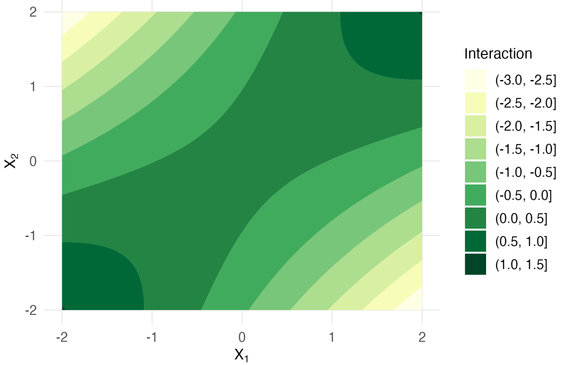

Figure: Interaction effect for $\rho = 0.3$.

Decomposition under Independence

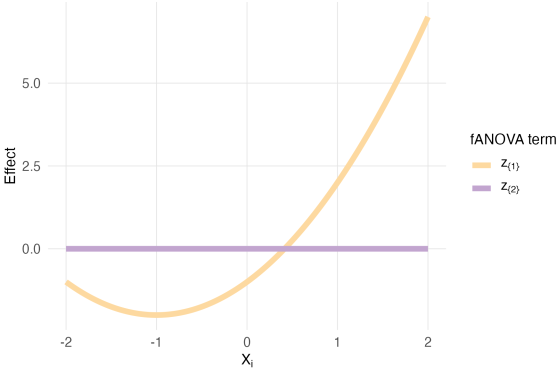

Figure: Main effect for $\rho = 0$.

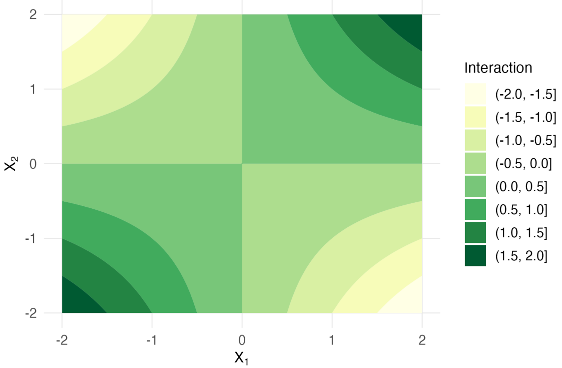

Figure: Interaction effect for $\rho = 0$.

$\Rightarrow$ nonzero main effect of X_2 only present under correlation.

Potential Usecase: Variance Decomposition

First proposed by [8], Sobol' indices build on variance decomposition:

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

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$$= \mathbb{E}\left[\left(\sum_u y_{u,G}(\boldsymbol{X}_u)\right)^2\right]$$

Potential Usecase: Variance Decomposition

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

Alternative Generalization of fANOVA

In [3] Hooker originally proposed different formulation of generalized fANOVA components:

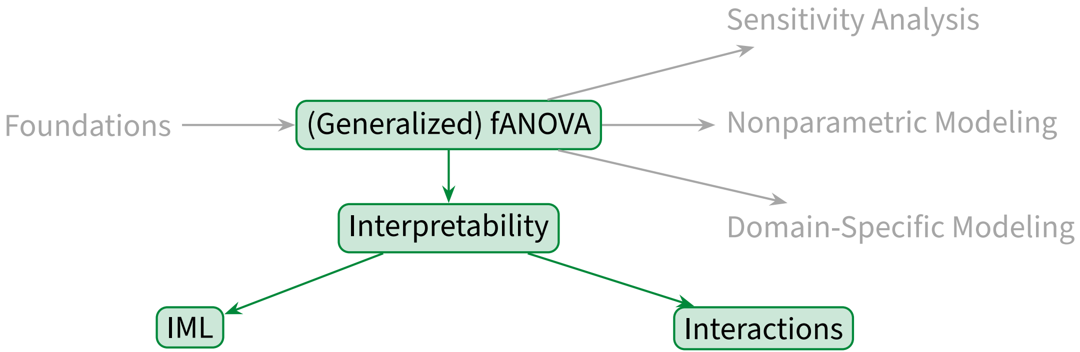
$$\{y_{u,G}(\boldsymbol{x}_u) \mid u \subseteq d\} = \arg \min_{\{g_u \in \mathcal{L}^2(\mathbb{R}^{|u|})\}} \int_{\mathbb{R}^N} \left(\sum_{u \subseteq d} g_u(\boldsymbol{x}_u) - y(\boldsymbol{x}) \right)^2 f_{\boldsymbol{X}}(\boldsymbol{x}) \, d\nu(\boldsymbol{x}),$$

subject to hierarchical orthogonality conditions:

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

Outline

Summary and Future Research



- For IML, see e.g. [2, 3, 4, 1]
- For interactions, see e.g. [6, 5]

Reminder: Definition of Orthogonal Projection

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

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

fANOVA as Orthogonal Projection

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

fANOVA as Orthogonal Projection

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

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

Equality to Hoeffding Decomposition

Hoeffding Decomposition

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

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

Hoeffding Decomposition Example

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

$$y_\emptyset = \mathbb{E}[y(X_1, X_2)] = 2\,\mathbb{E}[X_1] + \mathbb{E}[X_2^2] + \mathbb{E}[X_1 X_2] = 1,$$

$$\begin{aligned} y_{\{1\}}(x_1) &= \sum_{B \subseteq \{1\}} (-1)^{1-|B|}\,\mathbb{E}[y(\boldsymbol{X}) \mid X_B] = -\,\mathbb{E}[y] + \mathbb{E}[y|X_1 = x_1] \\ &= -1 + (2x_1 + \mathbb{E}[X_2^2] + x_1\mathbb{E}[X_2]) = 2x_1, \end{aligned}$$

$$\begin{aligned} y_{\{2\}}(x_2) &= \sum_{B \subseteq \{2\}} (-1)^{1-|B|}\,\mathbb{E}[y(\boldsymbol{X}) \mid X_B] - \;\mathbb{E}[y] + \mathbb{E}[y|X_2 = x_2] \\ &= -1 + (2\mathbb{E}[X_1] + x_2^2 + x_2\mathbb{E}[X_1]) = x_2^2 - 1. \end{aligned}$$

$$
\begin{aligned}
y_{\{1,2\}}(x_1, x_2) &= \sum_{B \subseteq \{1,2\}} (-1)^{2-|B|}\, \mathbb{E}[y(\boldsymbol{X}) \mid X_B] \\
&= (+1)\, \mathbb{E}[y] - \mathbb{E}[y|X_1 = x_1] - \mathbb{E}[y|X_2 = x_2] + y(x_1, x_2) \\
&= 1 - (2x_1 + 1) - (x_2^2) + (2x_1 + x_2^2 + x_1 x_2) \\
&= x_1 x_2.
\end{aligned}
$$

$$
y(x_1, x_2) = y_\emptyset + y_{\{1\}}(x_1) + y_{\{2\}}(x_2) + y_{\{1,2\}}(x_1, x_2) = 1 + 2x_1 + (x_2^2 - 1) + x_1 x_2
$$

Substituting the basis functions:

$$
\begin{aligned}
y(x_1, x_2) = \underbrace{c_0}_{y_0} &+ \underbrace{\left(c_{1,1}\, x_1 + c_{1,2}\left(x_1^2 - 1\right)\right)}_{y_1(x_1)} \\
&+ \underbrace{\left(c_{2,1}\, x_2 + c_{2,2}\left(x_2^2 - 1\right)\right)}_{y_2(x_2)} \\
&+ \underbrace{c_{12,11}\left(\frac{\rho(x_1^2 + x_2^2)}{1+\rho^2} - x_1x_2 + \frac{\rho(\rho^2 - 1)}{1+\rho^2}\right)}_{y_{12}(x_1,x_2)}.
\end{aligned}
$$

Find weights to recover original polynomial while fulfilling zero-mean and hierarchical orthogonality:

$$y(x_1, x_2) = a_0 + a_1x_1 + a_2x_2 + a_{11}x_1^2 + a_{22}x_2^2 + a_{12}x_1x_2$$

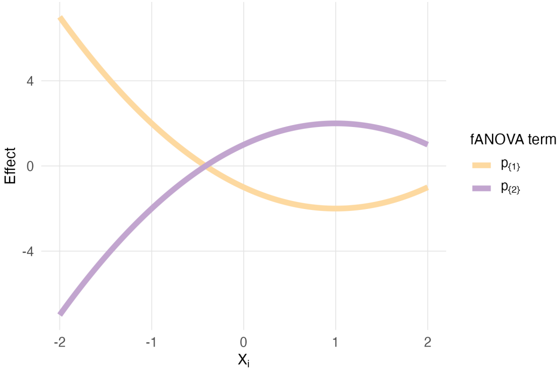
Coefficient Matching

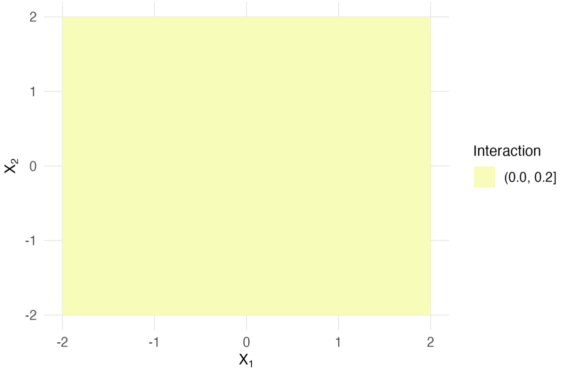
The corresponding weights can be found via coefficient matching. Start from the interaction term:

$$
\begin{aligned}
-c_{12,11} &= a_{12} & \Rightarrow \quad c_{12,11} &= -a_{12} \\
c_{1,2} + c_{12,11}\tfrac{\rho}{1+\rho^2} &= a_{11} & \Rightarrow \quad c_{1,2} &= a_{11} + \tfrac{\rho}{1+\rho^2} a_{12} \\
c_{2,2} + c_{12,11}\tfrac{\rho}{1+\rho^2} &= a_{22} & \Rightarrow \quad c_{2,2} &= a_{22} + \tfrac{\rho}{1+\rho^2} a_{12} \\
c_{1,1} &= a_1 & & \\
c_{2,1} &= a_2 & & \\
c_0 - c_{1,2} - c_{2,2} + c_{12,11}\tfrac{\rho(\rho^2-1)}{1+\rho^2} &= a_0 & \Rightarrow \quad c_0 &= a_0 + a_{11} + a_{22} + \rho\, a_{12}
\end{aligned}
$$

Example: Only Main

$$y(x_1, x_2) = -2x_1 - 2x_2 + x_1^2 + x_2^2 \qquad \rho = 0$$





Example: Only Linear Terms

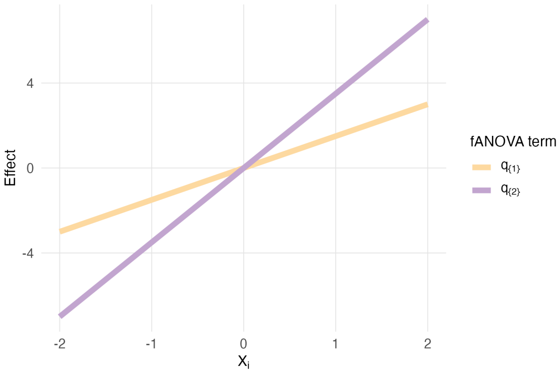


Figure: $q(x_1, x_2) = 1.5x_1 + 3.5x_2$

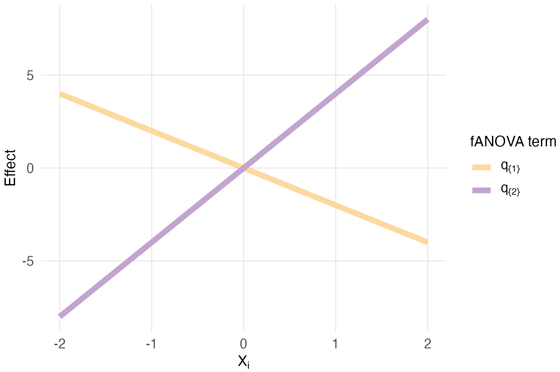
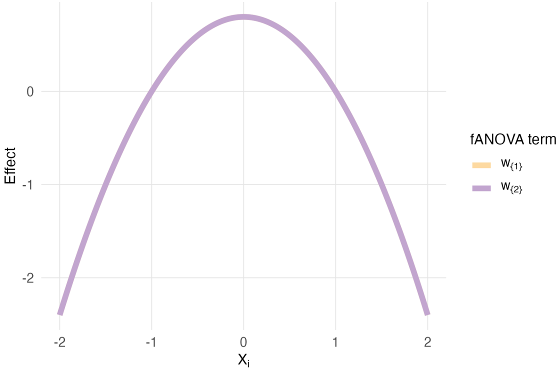
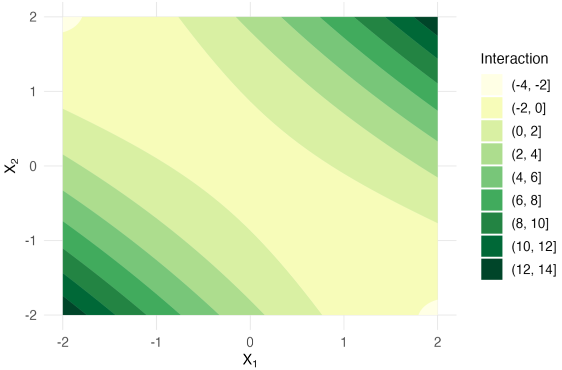


Figure: $q(x_1, x_2) = -2x_1 + 4x_2$

Example: Interaction

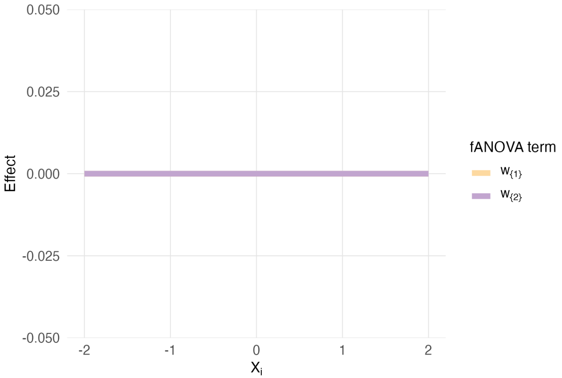
$$y(x_1, x_2) = x_1 x_2 \qquad \rho = -0.5$$

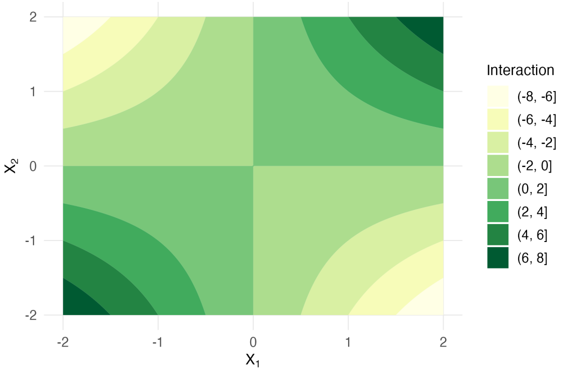




Example: Interaction

$$y(x_1, x_2) = x_1 x_2 \qquad \rho = 0$$





Sobol Indices

Formula for classical Sobol’ indices?

Decomposition of linear functions

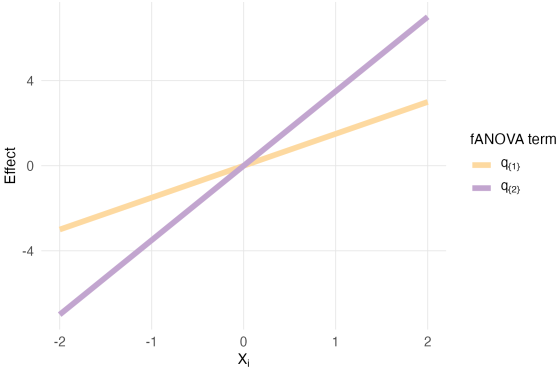


Figure: $q(x_1, x_2) = 1.5x_1 + 3.5x_2$

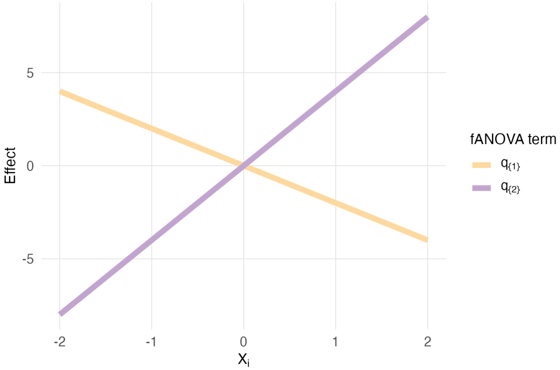


Figure: $q(x_1, x_2) = -2x_1 + 4x_2$

Proof of zero-mean Property for Classical Components

Strong annihilating conditions hold, so:

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

Proof of orthogonality for Classical Components

- $u \neq v$, so pick $i \in u \setminus v$
- $y_v(\boldsymbol{x_v})$ is independent of x_i
- strong annihilating conditions hold by assumption

$$\int_{\mathbb{R}} y_u(\boldsymbol{x}_u) f_{\{i\}}(x_i)\, d\nu(x_i) = 0 \quad \text{for all fixed } \boldsymbol{x}_{u\setminus\{i\}}.$$

Hence,

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

Proof of zero-mean Property for Generalized Components

We assume the weak annihilating conditions hold, then:

$$
\begin{aligned}
\mathbb{E}[y_{u,G}(\boldsymbol{X}_u)] :=& \int_{\mathbb{R}^N} y_{u,G}(\boldsymbol{x}_u) f_{\boldsymbol{X}}(\boldsymbol{x})\, d\nu(\boldsymbol{x}) \\
=& \int_{\mathbb{R}^{|u|}} y_{u,G}(\boldsymbol{x}_u) \left(\int_{\mathbb{R}^{N-|u|}} f_{\boldsymbol{X}}(\boldsymbol{x})\, d\nu(\boldsymbol{x}_{-u}) \right) d\nu(\boldsymbol{x}_u) \\
=& \int_{\mathbb{R}^{|u|}} y_{u,G}(\boldsymbol{x}_u) f_u(\boldsymbol{x}_u)\, d\nu(\boldsymbol{x}_u) \\
=& \int_{\mathbb{R}^{|u|-1}} \left(\int_{\mathbb{R}} y_{u,G}(\boldsymbol{x}_u) f_u(\boldsymbol{x}_u)\, d\nu(x_i) \right) \prod_{j \in u, j \neq i} d\nu(\boldsymbol{x}_j) \\
=& \, 0.
\end{aligned}
$$

Proof of hierarchical orthogonality

For any two subsets $\emptyset \neq u \subseteq \{1, \ldots, N\}$ and $\emptyset \neq v \subseteq \{1, \ldots, N\}$, where $v \subsetneq u$, the subset $u = v \cup (u \setminus v)$. Let $i \in (u \setminus v) \subseteq u$. Then we obtain:

$$\begin{aligned}
\mathbb{E}[y_{u,G}(\boldsymbol{X}_u)\, y_{v,G}(\boldsymbol{X}_v)] &:= \int_{\mathbb{R}^N} y_{u,G}(\boldsymbol{x}_u) y_{v,G}(\boldsymbol{x}_v) f_{\boldsymbol{X}}(\boldsymbol{x})\, d\nu(\boldsymbol{x}) \\
&= \int_{\mathbb{R}^{|u|}} y_{u,G}(\boldsymbol{x}_u) y_{v,G}(\boldsymbol{x}_v) \left(\int_{\mathbb{R}^{N-|u|}} f_{\boldsymbol{X}}(\boldsymbol{x})\, d\nu(\boldsymbol{x}_{-u}) \right) d\nu(\boldsymbol{x}_u) \\
&= \int_{\mathbb{R}^{|u|}} y_{u,G}(\boldsymbol{x}_u) y_{v,G}(\boldsymbol{x}_v) f_u(\boldsymbol{x}_u)\, d\nu(\boldsymbol{x}_u) \\
&= \int_{\mathbb{R}^{|v|}} y_{v,G}(\boldsymbol{x}_v) \int_{\mathbb{R}^{|u \setminus v|}} y_{u,G}(\boldsymbol{x}_u) f_u(\boldsymbol{x}_u)\, d\nu(\boldsymbol{x}_{u \setminus v})\, d\nu(\boldsymbol{x}_v) \\
&= \int_{\mathbb{R}^{|v|}} y_{v,G}(\boldsymbol{x}_v) \int_{\mathbb{R}^{|u \setminus v|-1}} \left(\int_{\mathbb{R}} y_{u,G}(\boldsymbol{x}_u) f_u(\boldsymbol{x}_u)\, d\nu(\boldsymbol{x}_i) \right) \\
&\times \prod d\nu(x_j)\, d\nu(\boldsymbol{x}_v) = 0.
\end{aligned}$$

Generalized fANOVA Proofs

- 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

Relevant External Links

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

References I

Fabian Fumagalli, Maximilian Muschalik, Eyke Hüllermeier, Barbara Hammer, and Julia Herbinger.
Unifying Feature-Based Explanations with Functional ANOVA and Cooperative Game Theory, April 2025.
arXiv:2412.17152 [cs].

Giles Hooker.
Discovering additive structure in black box functions.
In *Proceedings of the tenth ACM SIGKDD international conference on Knowledge discovery and data mining*, pages 575–580, Seattle WA USA, August 2004. ACM.

Giles Hooker.
Generalized Functional ANOVA Diagnostics for High-Dimensional Functions of Dependent Variables.
Journal of Computational and Graphical Statistics, 16(3):709–732, September 2007.

References II

Linwei Hu, Vijayan N. Nair, Agus Sudjianto, Aijun Zhang, Jie Chen, and Zebin Yang.
Interpretable Machine Learning Based on Functional ANOVA Framework: Algorithms and Comparisons.
Applied Stochastic Models in Business and Industry, 41(1):e2916, January 2025.

Gunnar König, Eric Günther, and Ulrike von Luxburg.
Disentangling Interactions and Dependencies in Feature Attribution, October 2024.
arXiv:2410.23772.

Benjamin Lengerich, Sarah Tan, Chun-Hao Chang, Giles Hooker, and Rich Caruana.
Purifying Interaction Effects with the Functional ANOVA: An Efficient Algorithm for Recovering Identifiable Additive Models.
In *Proceedings of the Twenty Third International Conference on Artificial Intelligence and Statistics*, pages 2402–2412. PMLR, June 2020.
ISSN: 2640-3498.

References III

Sharif Rahman.
A Generalized ANOVA Dimensional Decomposition for Dependent Probability Measures.
SIAM/ASA Journal on Uncertainty Quantification, 2(1):670–697, 2014.

I. M. Sobol.
Sensitivity Estimates for Nonlinear Mathematical Models.
Mathematical Modelling and Computational Experiments, 1:407–414, 1993.