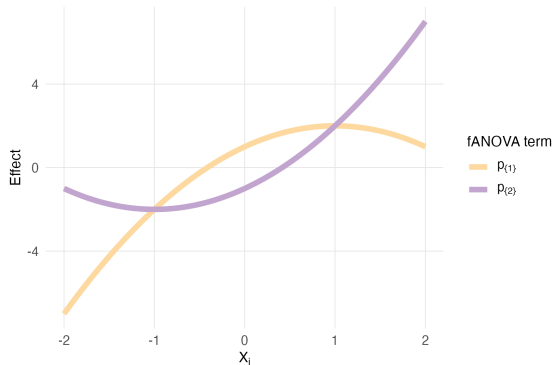


Functional ANOVA Decomposition

Juliet Fleischer
August 10, 2025



Outline

1 Research Context

2 Classical fANOVA

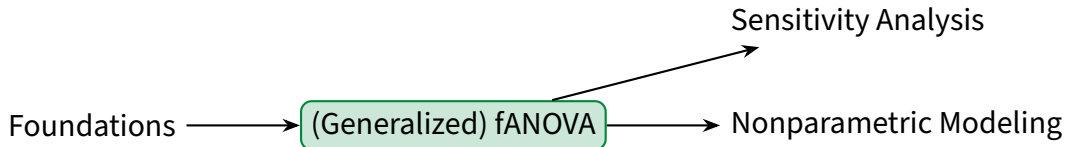
3 Generalized fANOVA

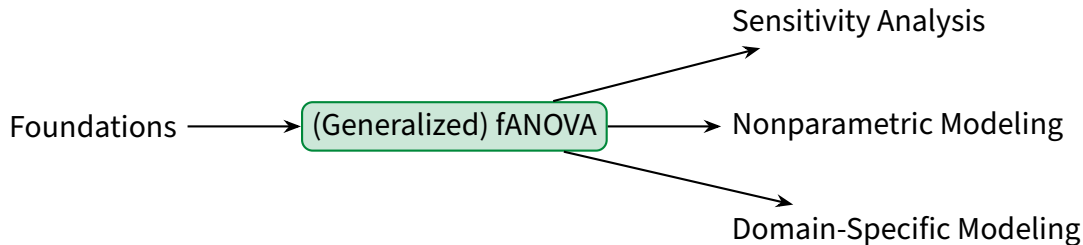
4 Conclusion

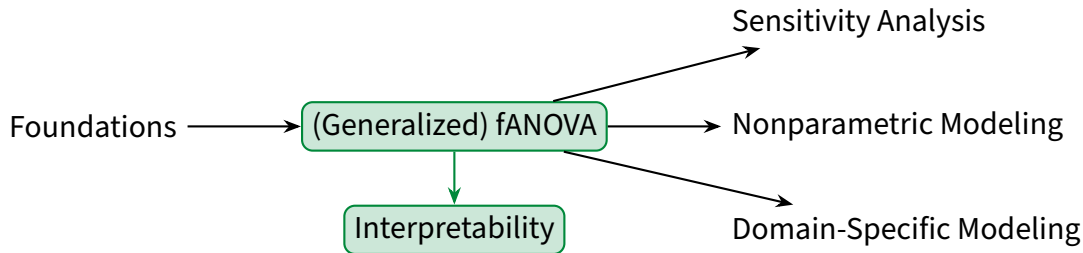
Foundations

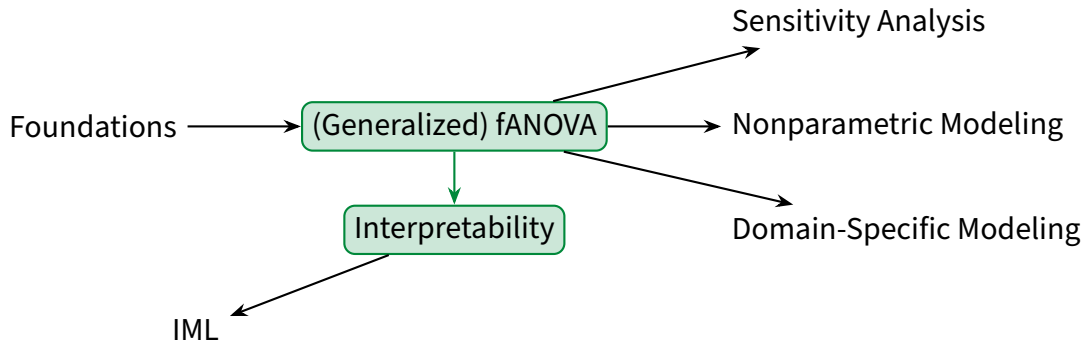
Foundations → (Generalized) fANOVA

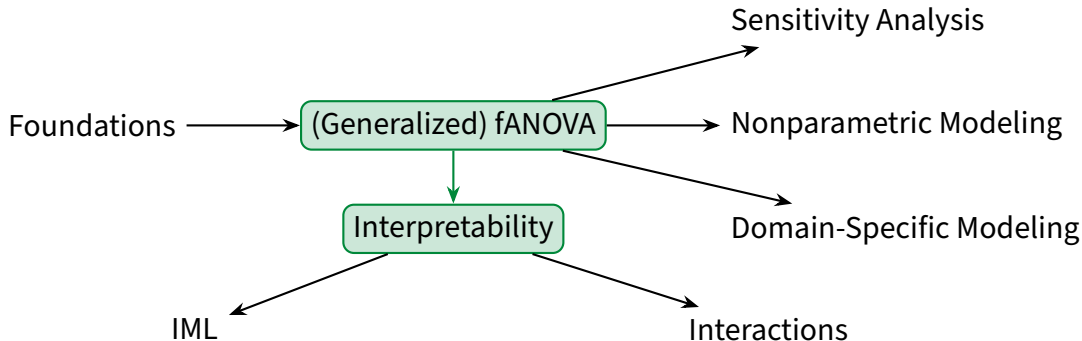












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4 Conclusion

General Form

$$y(\mathbf{x}) = \sum_{u \subseteq \{1, \dots, N\}} y_u(\mathbf{x}_u)$$

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- y_u : Component functions for subvector \mathbf{X}_u
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$$\begin{aligned} y(\mathbf{X}) &= \sum_{u \subseteq \{1, \dots, N\}} y_u(\mathbf{X}_u) \\ &= y_{\emptyset} + (y_{\{1\}}(\mathbf{X}_1) + \dots + y_{\{N\}}(\mathbf{X}_N)) \end{aligned}$$

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

Example with Independent MVN Input

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

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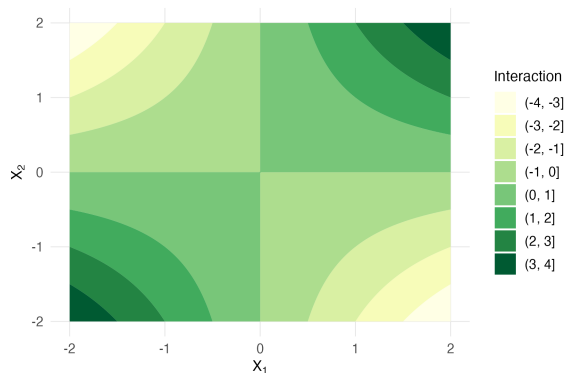
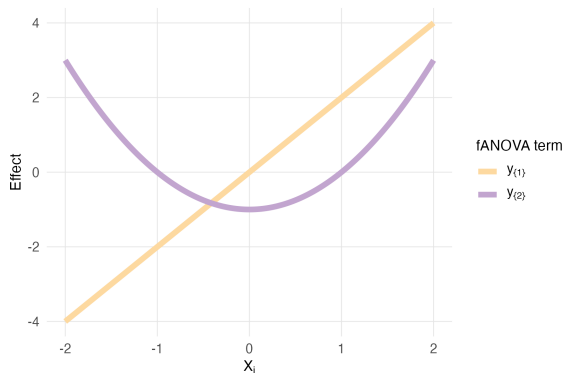
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Components:

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

Visualization of fANOVA components under Independence

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

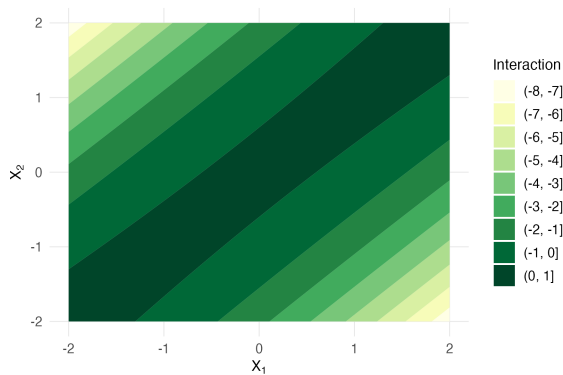
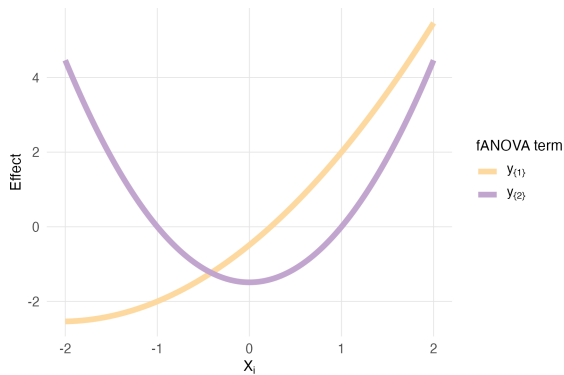


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Visualization of ANOVA components under Dependence

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



Weak Annihilating Conditions

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

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

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

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$$\begin{aligned} y_{\{1,2\},G}(\mathbf{x}_u) &= \int_{\mathbb{R}} y(x_1, x_2, x_3) f_{\{3\}}(x_3) d\nu(x_3) - y_{\emptyset,G} - y_{\{1\},G} - y_{\{2\},G} \\ &\quad - \int_{\mathbb{R}} y_{\{1,2,3\},G}(x_1, x_2, x_3) f_{\{3\}}(x_3) d\nu(x_3) \end{aligned}$$

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 $(\emptyset \neq v \subseteq \{1, \dots, N\}, v \cap u \neq \emptyset, v \not\subseteq u) = \emptyset$

$$y_{\{1,2,3\},G}(\mathbf{X}_u) = y(x_1, x_2, x_3) - y_{\emptyset,G}$$

$$- y_{\{1\},G} - y_{\{2\},G} - y_{\{3\},G}$$

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

$$\begin{aligned}y(x_1, x_2) &= a_0 + a_1x_1 + a_2x_2 + a_{11}x_1^2 + a_{22}x_2^2 + a_{12}x_1x_2 \\ &= c_0 + c_{1,1} \psi_{1,1}(x_1) + c_{2,1} \psi_{2,1}(x_2)\end{aligned}$$

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

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

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

In [7] Hermite polynomial basis functions are proposed

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

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

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

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

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

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

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

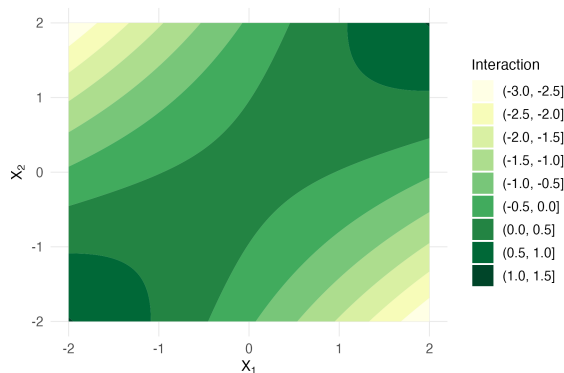
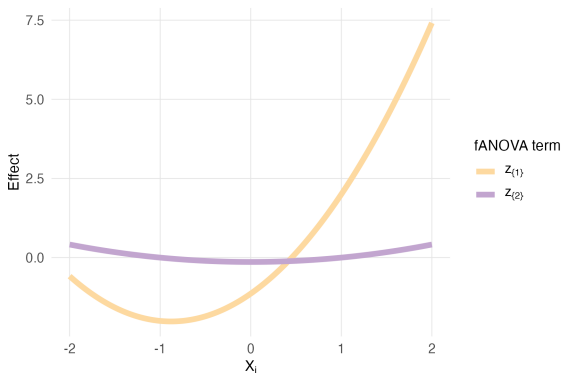
$$y_{\emptyset,G} = a_0 + a_{11} + a_{22} + \rho a_{12},$$

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

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

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

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



Decomposition under Independence

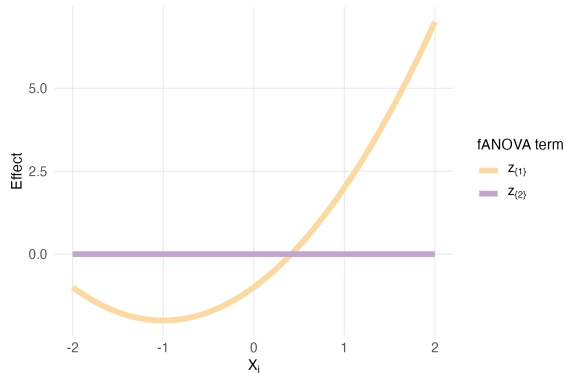


Figure: Main effect for $\rho = 0$.

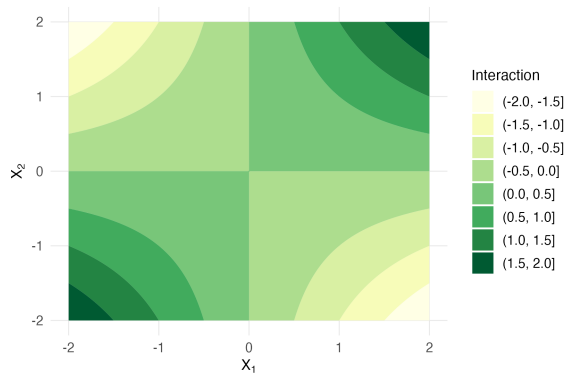


Figure: Interaction effect for $\rho = 0$.

\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:

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

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

$$= \sum_u \mathbb{E} [y_{u, G}^2(\mathbf{x}_u)] + \sum_{u \not\subseteq v, v \not\subseteq u} \mathbb{E} [y_{u, G}(\mathbf{x}_u) y_{v, G}(\mathbf{x}_v)]$$

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

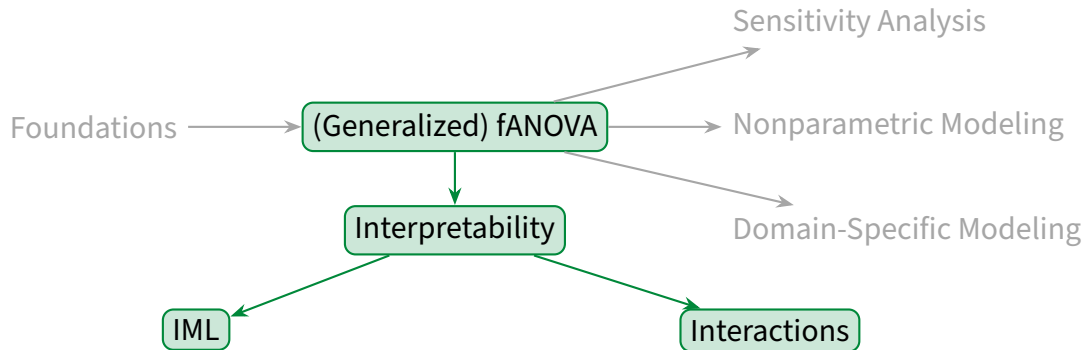
$$\{y_{u,G}(\mathbf{x}_u) \mid u \subseteq d\} = \arg \min_{\{g_u \in \mathcal{L}^2(\mathbb{R}^{|u|})\}} \int_{\mathbb{R}^N} \left(\sum_{u \subseteq d} g_u(\mathbf{x}_u) - y(\mathbf{x}) \right)^2 f_{\mathbf{x}}(\mathbf{x}) d\nu(\mathbf{x}),$$

subject to hierarchical orthogonality conditions:

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

Outline

- 1 Research Context
- 2 Classical fANOVA
- 3 Generalized fANOVA
- 4 Conclusion**



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

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

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

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

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

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

Hoeffding Decomposition

$$y(\mathbf{x}) = \sum_{A \subseteq D} y_A(\mathbf{x}_A), \quad D := \{1, \dots, N\}, \quad (2)$$

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

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

where y_u are orthogonal components.

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

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

$$y_{\emptyset} = \mathbb{E}[y(X_1, X_2)] = 2 \mathbb{E}[X_1] + \mathbb{E}[X_2^2] + \mathbb{E}[X_1X_2] = 1,$$

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

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

$$\begin{aligned}
y_{\{1,2\}}(x_1, x_2) &= \sum_{B \subseteq \{1,2\}} (-1)^{2-|B|} \mathbb{E}[y(\mathbf{x}) | X_B] \\
&= (+1) \mathbb{E}[y] - \mathbb{E}[y | X_1 = x_1] - \mathbb{E}[y | X_2 = x_2] + y(x_1, x_2) \\
&= 1 - (2x_1 + 1) - (x_2^2) + (2x_1 + x_2^2 + x_1x_2) \\
&= x_1x_2.
\end{aligned}$$

$$y(x_1, x_2) = y_{\emptyset} + y_{\{1\}}(x_1) + y_{\{2\}}(x_2) + y_{\{1,2\}}(x_1, x_2) = 1 + 2x_1 + (x_2^2 - 1) + x_1x_2$$

Substituting the basis functions:

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

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

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

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

$$-c_{12,11} = a_{12} \quad \Rightarrow \quad c_{12,11} = -a_{12}$$

$$c_{1,2} + c_{12,11} \frac{\rho}{1+\rho^2} = a_{11} \quad \Rightarrow \quad c_{1,2} = a_{11} + \frac{\rho}{1+\rho^2} a_{12}$$

$$c_{2,2} + c_{12,11} \frac{\rho}{1+\rho^2} = a_{22} \quad \Rightarrow \quad c_{2,2} = a_{22} + \frac{\rho}{1+\rho^2} a_{12}$$

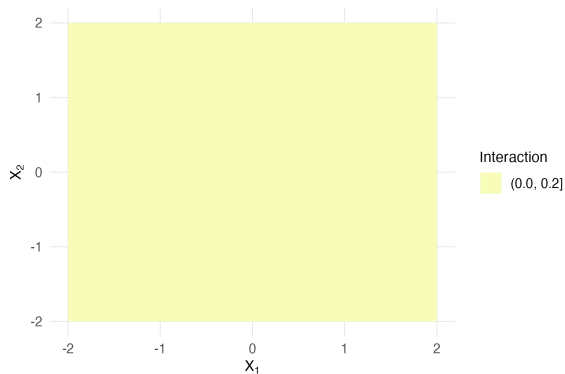
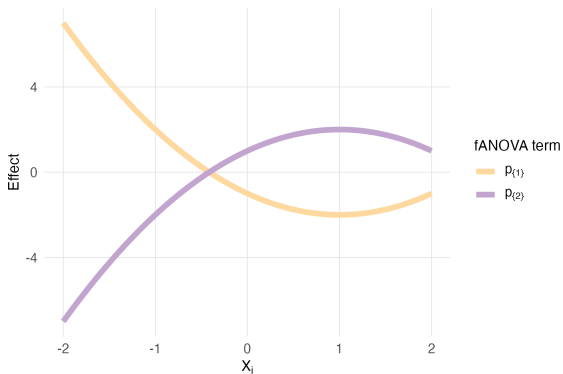
$$c_{1,1} = a_1$$

$$c_{2,1} = a_2$$

$$c_0 - c_{1,2} - c_{2,2} + c_{12,11} \frac{\rho(\rho^2-1)}{1+\rho^2} = a_0 \quad \Rightarrow \quad c_0 = a_0 + a_{11} + a_{22} + \rho a_{12}$$

Example: Only Main

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



Example: Only Linear Terms

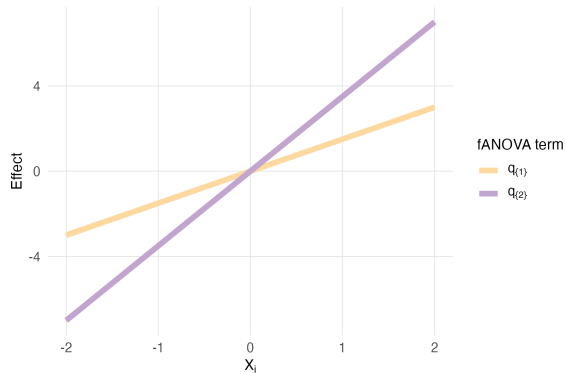


Figure: $q(x_1, x_2) = 1.5x_1 + 3.5x_2$

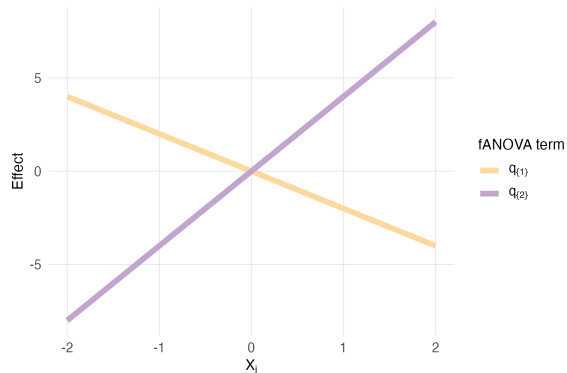
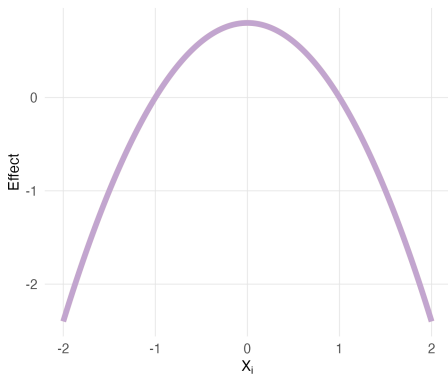


Figure: $q(x_1, x_2) = -2x_1 + 4x_2$

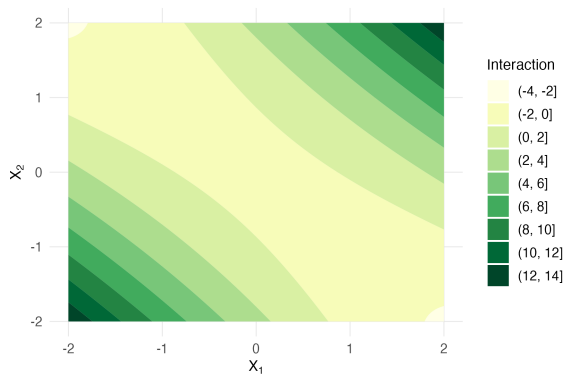
Example: Interaction

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



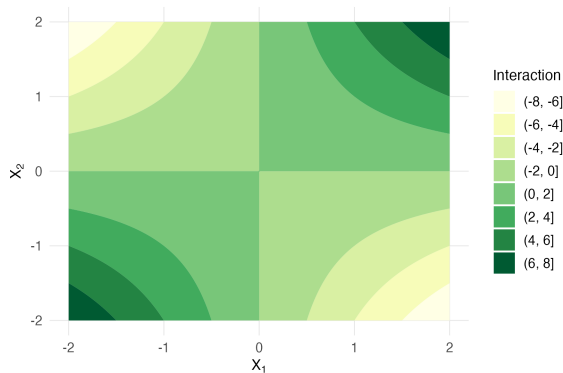
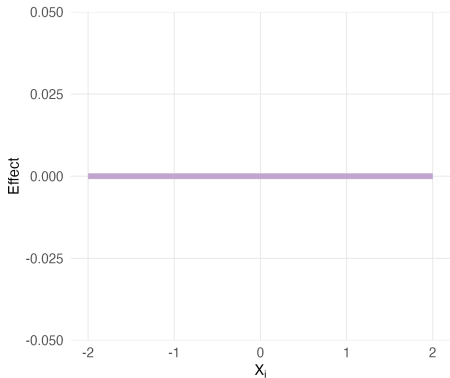
fANOVA term

$w_{(1)}$
 $w_{(2)}$



Example: Interaction

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



Formula for classical Sobol' indices?

Decomposition of linear functions

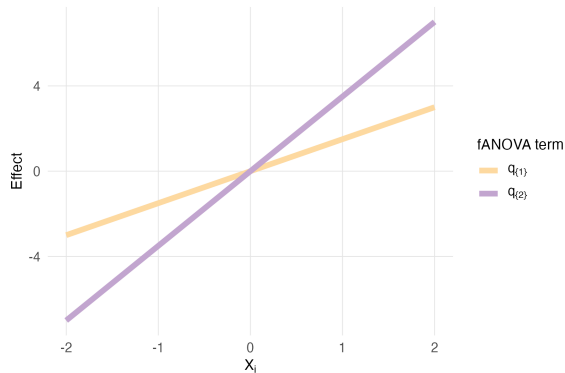


Figure: $q(x_1, x_2) = 1.5x_1 + 3.5x_2$

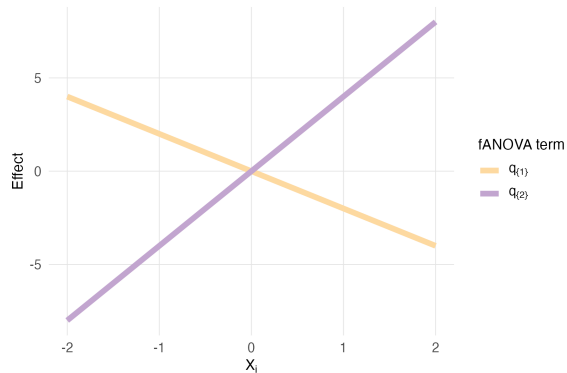


Figure: $q(x_1, x_2) = -2x_1 + 4x_2$

Strong annihilating conditions hold, so:

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

Proof of orthogonality for Classical Components

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

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

Hence,

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

Proof of zero-mean Property for Generalized Components

We assume the weak annihilating conditions hold, then:

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

Proof of hierarchical orthogonality

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

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

- 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

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



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