Functional ANOVA Decomposition

Juliet Fleischer

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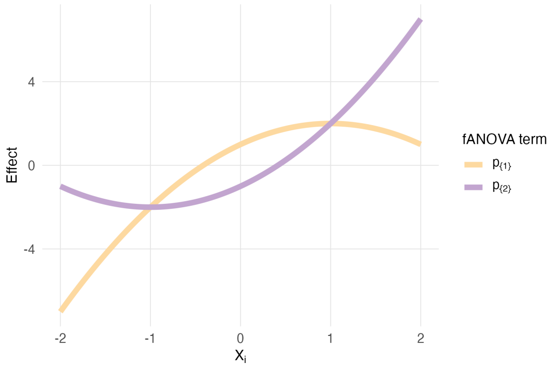
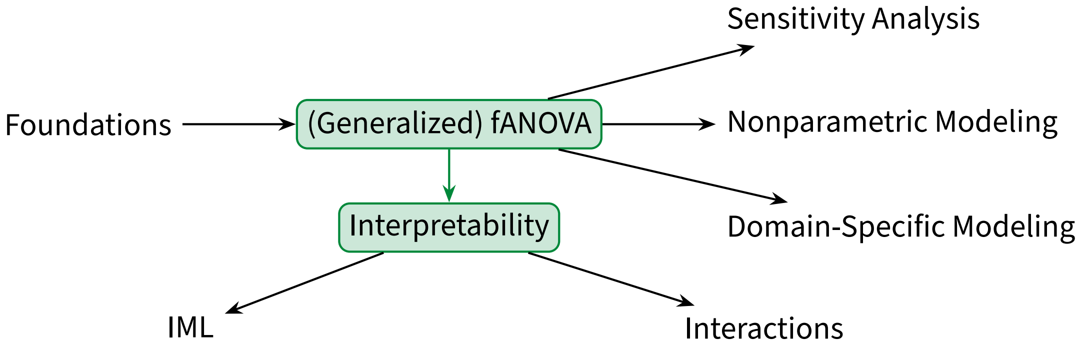


Outline

Overview of the fANOVA Research Field



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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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- $\boldsymbol{X} = (X_1, \ldots, X_N)$: independent input variables

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$$= y_\emptyset + \left(y_{\{1\}}(\boldsymbol{X}_1) + \cdots + y_{\{N\}}(\boldsymbol{X}_N)\right)$$

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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

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

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

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&= \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.
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$$

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

fANOVA as Orthogonal Projection

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

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$$
\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}
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Example with Independent MVN Input

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

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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 MVN Example under Independence

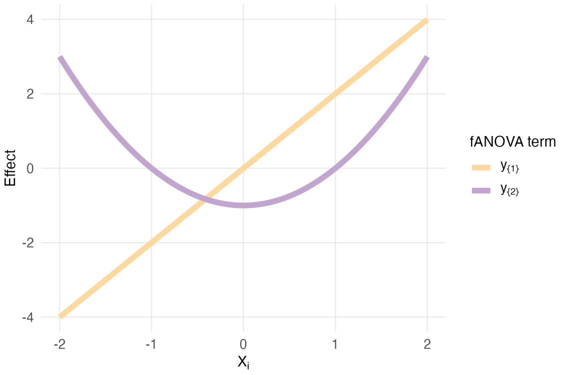


Figure: Main effects

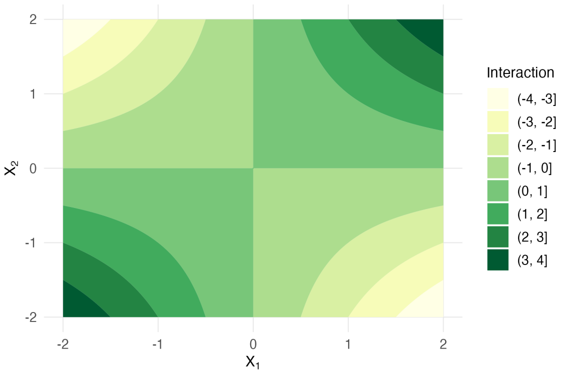
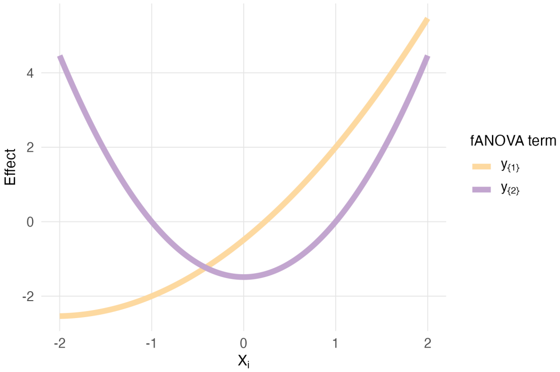


Figure: Interaction

Outline

Visualization of MVN Example under Dependence

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



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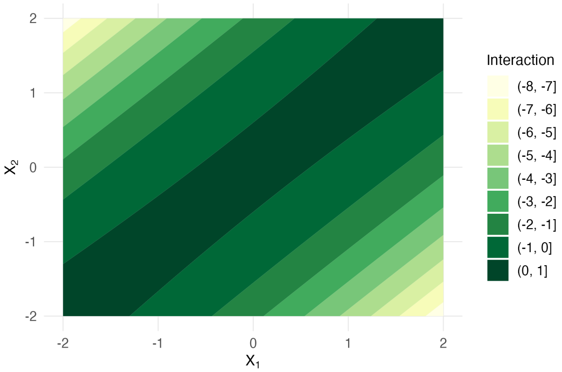

Figure: Interaction

Ensuring Interpretability under Dependent Inputs

Weak Annihilating Conditions

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

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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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$$- \sum_{\substack{\emptyset \neq v \subseteq \{1,\ldots,N\} \\ v \cap u \neq \emptyset, \; v \not\subset u}} \int_{\mathbb{R}^{|v \cap -u|}} y_{v,G}(\boldsymbol{X}_{v \cap u}, \boldsymbol{x}_{v \cap -u}) f_{v \cap -u}(\boldsymbol{x}_{v \cap -u}) \, d\nu(\boldsymbol{x}_{v \cap -u})$$

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Building the Generalized Components as Coupled System

- $N = 3, u = \emptyset$

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

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

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

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

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

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

Construction of Components via Fourier-polynomial Expansion

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

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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)
\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 [6] Hermite polynomial basis functions are proposed

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

fANOVA Components of a two-degree Polynomial

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

$$
\begin{aligned}
y_{\emptyset,G} &= a_0 + a_{11} + a_{22} + \rho\, a_{12}, \\
y_{\{1\},G}(x_1) &= a_1\, x_1 + \left(a_{11} + \frac{\rho}{1+\rho^2} a_{12}\right)\left(x_1^2 - 1\right), \\
y_{\{2\},G}(x_2) &= a_2\, x_2 + \left(a_{22} + \frac{\rho}{1+\rho^2} a_{12}\right)\left(x_2^2 - 1\right), \\
y_{\{1,2\},G}(x_1, x_2) &= -a_{12}\left(\frac{\rho(x_1^2 + x_2^2)}{1+\rho^2} - x_1 x_2 + \frac{\rho(\rho^2 - 1)}{1+\rho^2}\right).
\end{aligned} \tag{1}
$$

Decomposition under Weak Correlation

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

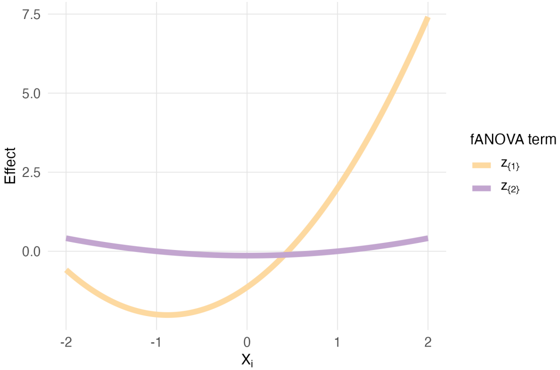


Figure: Main effect for $\rho = 0.3$.

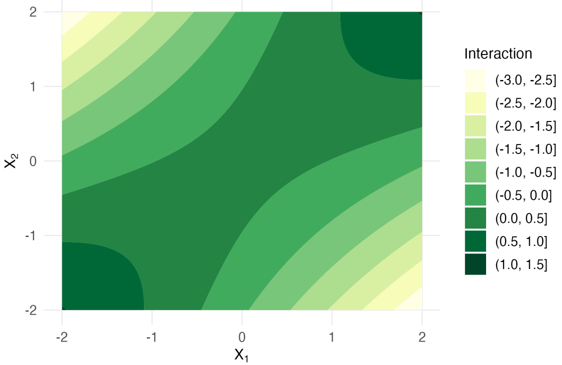


Figure: Interaction effect for $\rho = 0.3$.

Decomposition under Independence

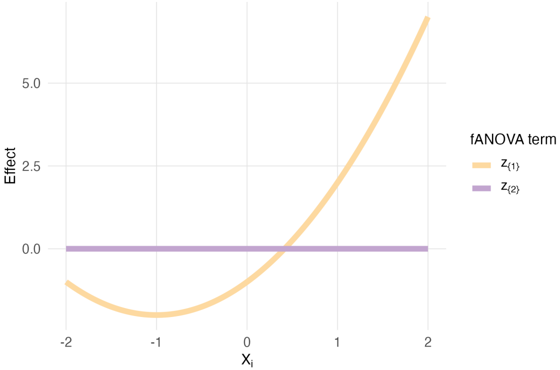


Figure: Main effect for $\rho = 0$.

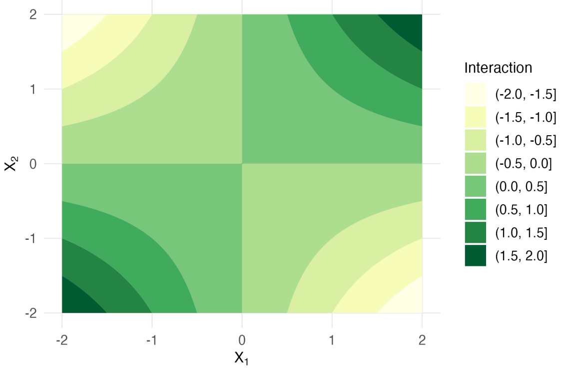


Figure: Interaction effect for $\rho = 0$.

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

Variance Decomposition

First proposed by [7], Sobol' indices build on variance decomposition:

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

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

Alternative Generalization of fANOVA

In [2] Hooker originally proposed different formulation of generalized fANOVA components:

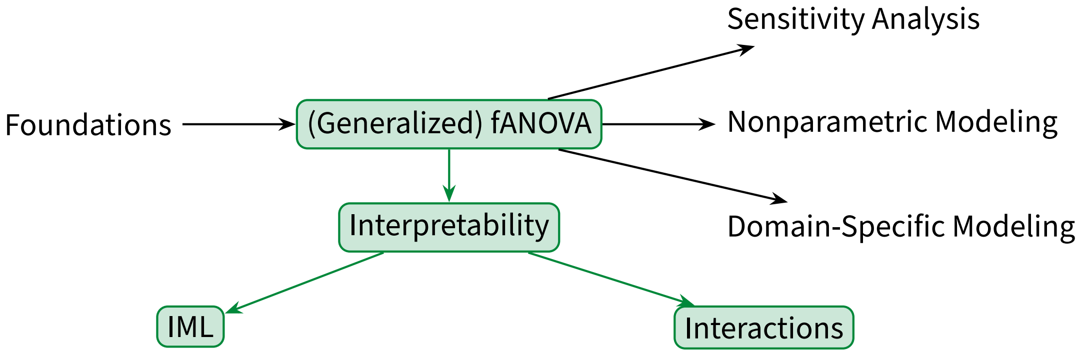
$$\{y_{u,G}(\boldsymbol{x}_u) \mid u \subseteq d\} = \arg \min_{\{g_u \in \mathcal{L}^2(\mathbb{R}^{|u|})\}} \int_{\mathbb{R}^N} \left(\sum_{u \subseteq d} g_u(\boldsymbol{x}_u) - y(\boldsymbol{x}) \right)^2 f_{\boldsymbol{X}}(\boldsymbol{x}) \, d\nu(\boldsymbol{x}),$$

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



- Purify Interactions [5, 4]
- Model-agnostic tool for effect quantification and visualization [1, 2, 3]
- HPO based on fANOVA components estimated by surrogate models

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

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

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:

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

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

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

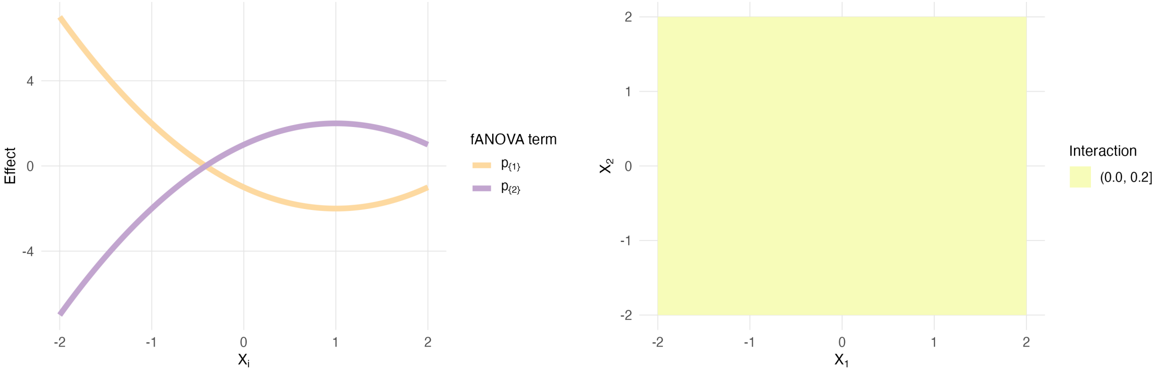
Coefficient Matching

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

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

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

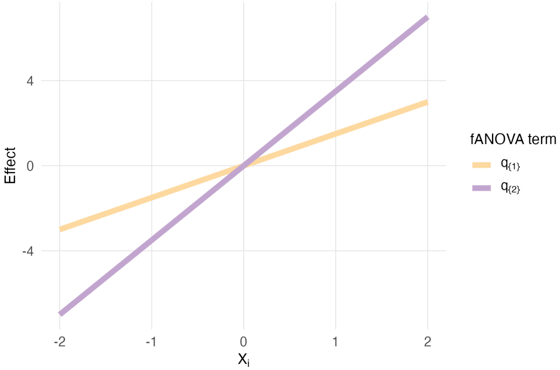


Figure: $q(x_1, x_2) = 1.5x_1 + 3.5x_2$

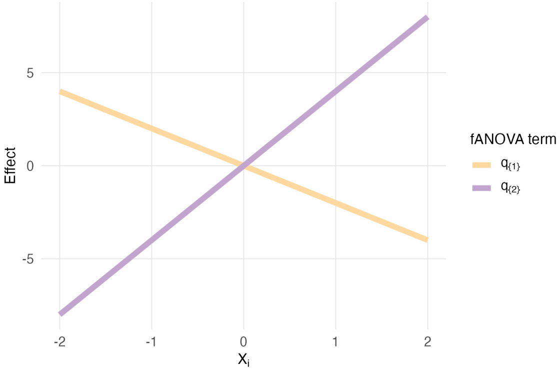
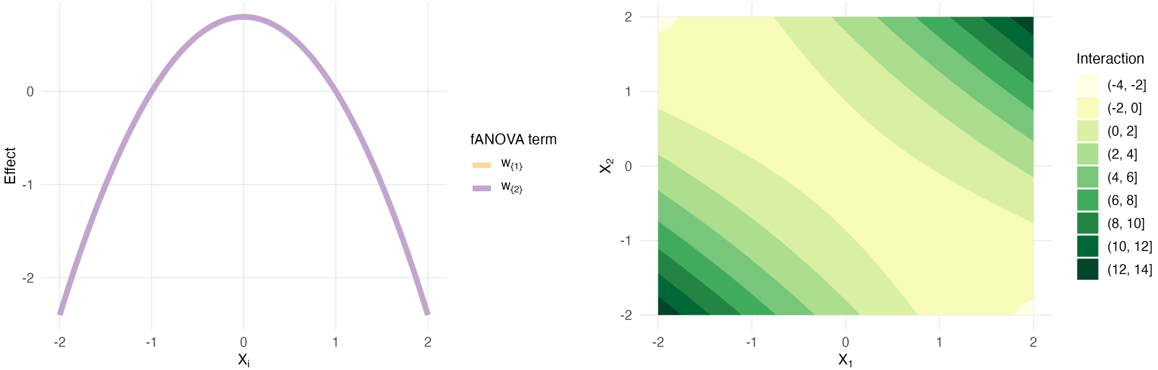


Figure: $q(x_1, x_2) = -2x_1 + 4x_2$

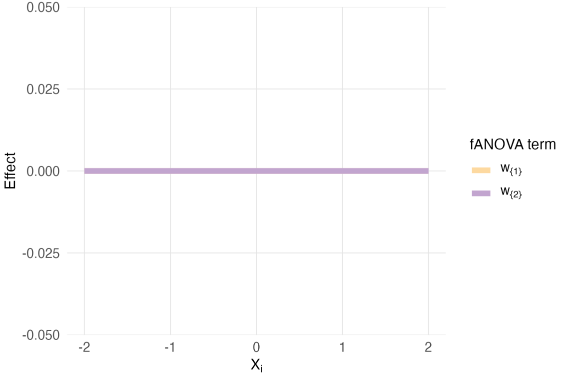
Example: Interaction

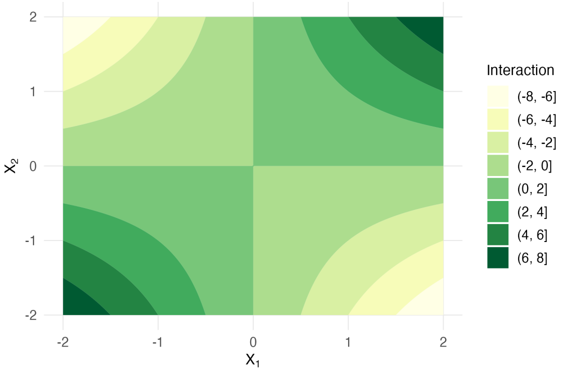
$$y(x_1, x_2) = x_1 x_2 \qquad \rho = -0.5$$



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

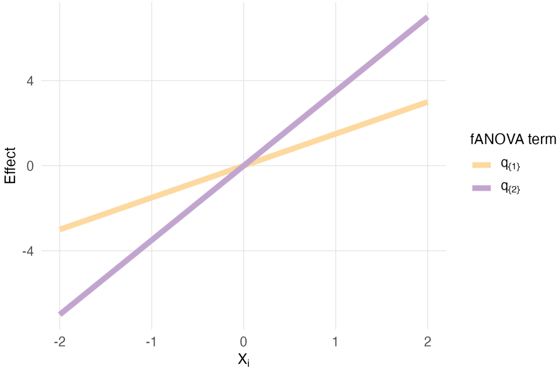


Figure: $q(x_1, x_2) = 1.5x_1 + 3.5x_2$

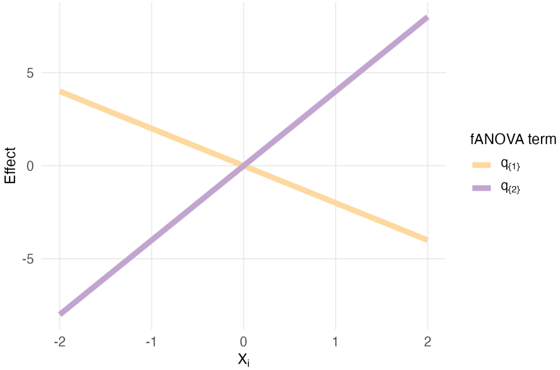


Figure: $q(x_1, x_2) = -2x_1 + 4x_2$

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

Relevant External Links

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

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