Functional ANOVA Decomposition

Juliet Fleischer

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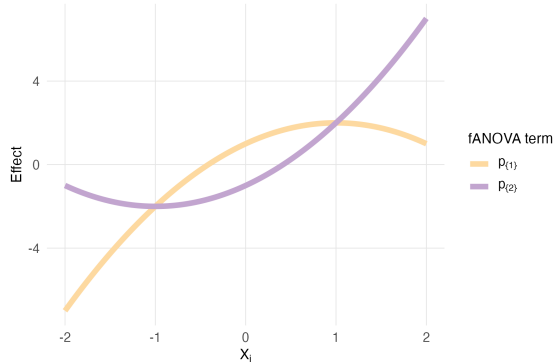
Outline

Foundations

Overview of the fANOVA Research Field

Foundations $\longrightarrow$ (Generalized) fANOVA

Sensitivity Analysis

Foundations → (Generalized) fANOVA

Overview of the fANOVA Research Field

Foundations $\longrightarrow$ (Generalized) fANOVA $\longrightarrow$ Nonparametric Modeling

Sensitivity Analysis

Domain-Specific Modeling

Interpretability

IML

Outline

Decomposition of Model into Interpretable Components

General Form

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

Decomposition of Model into Interpretable Components
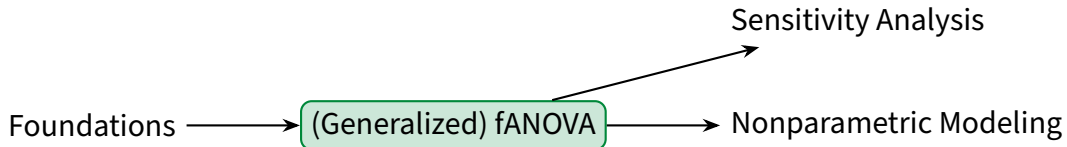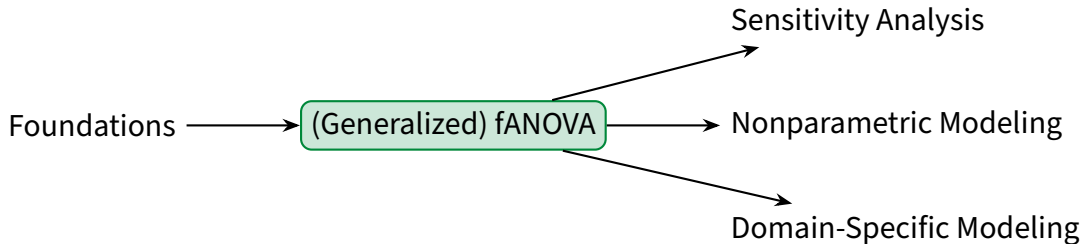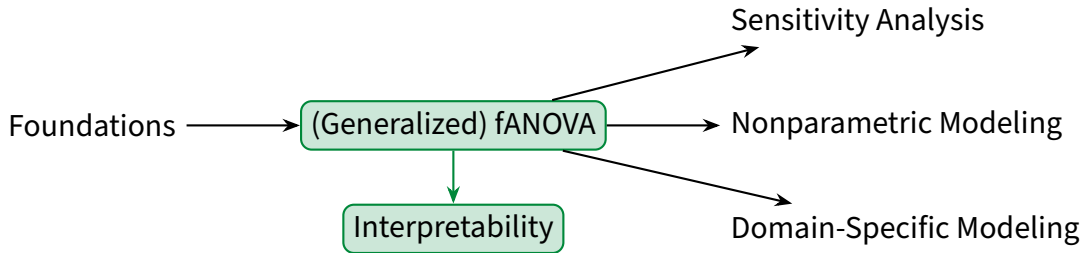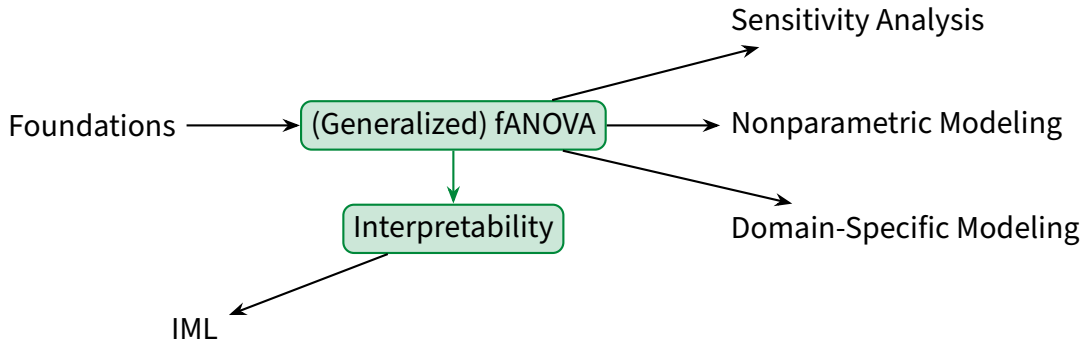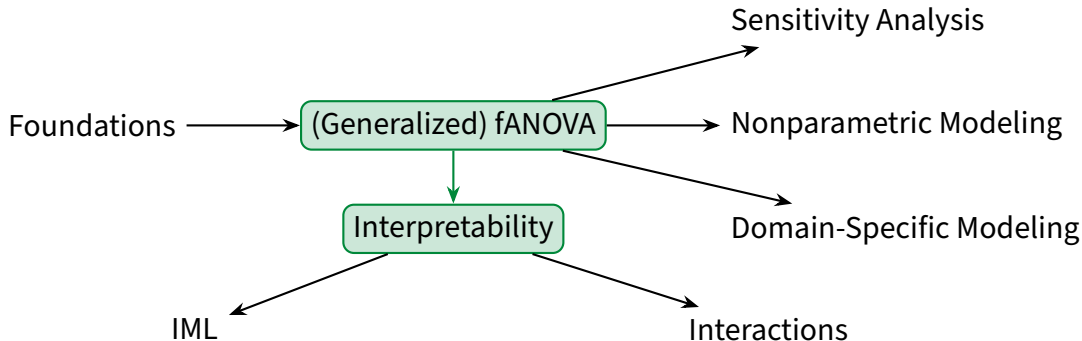
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$$y(\boldsymbol{X}) = \sum_{u \subseteq \{1,\ldots,N\}} y_u(\boldsymbol{X}_u)$$

- y : Model
- y_u : Component functions for subvector $\boldsymbol{X}_u$
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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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Remark: fANOVA components can be seen from lens of orthogonal projections.

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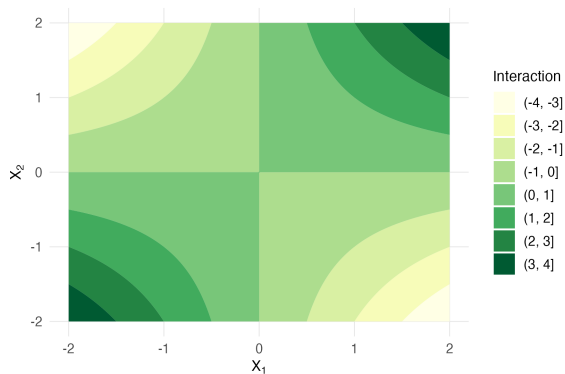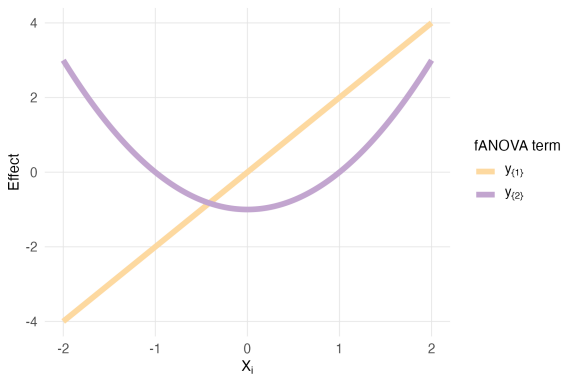
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Components:

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

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

Outline

Visualization offANOVA components under Dependence

$$y(x_1, x_2) = 2x_1 + x_2^2 + x_1 x_2, \qquad \rho = 0.8$$
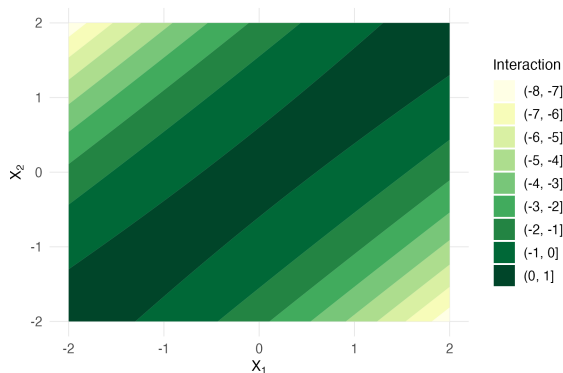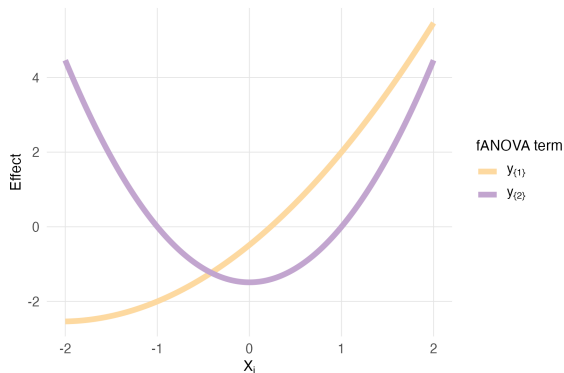
Ensuring Interpretability under Dependent Inputs

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

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

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

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

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

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

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

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

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

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$$= \underbrace{c_0}_{y_0} + \underbrace{\left(c_{1,1}\, \psi_{1,1}(x_1) + c_{1,2}\, \psi_{1,2}(x_1)\right)}_{y_1(x_1)}$$

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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$$+ \underbrace{c_{12,11} \, \psi_{12,11}(x_1, x_2)}_{y_{12}(x_1, x_2)}$$

Choosing Orthogonal Basis Functions

In [2] 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 $d = 2$

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

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

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

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

Decomposition under Weak Correlation

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

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

Figure: Interaction effect for $\rho = 0.3$.
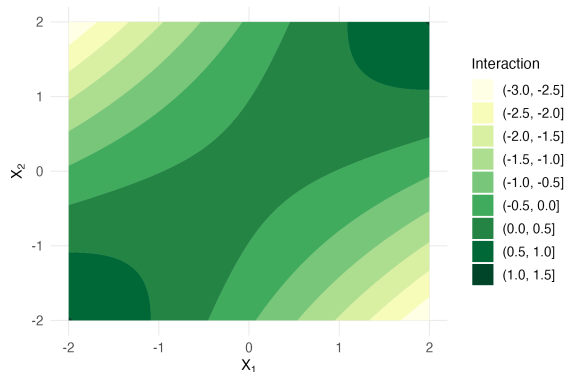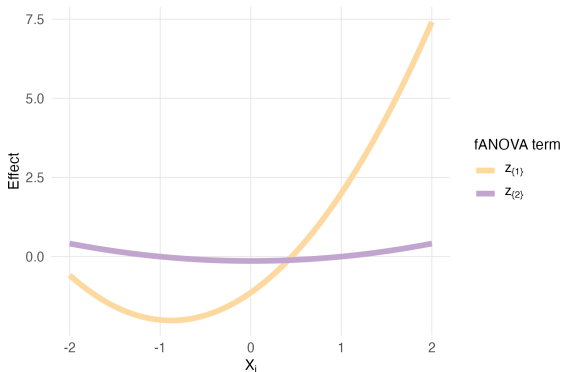
Decomposition under Independence
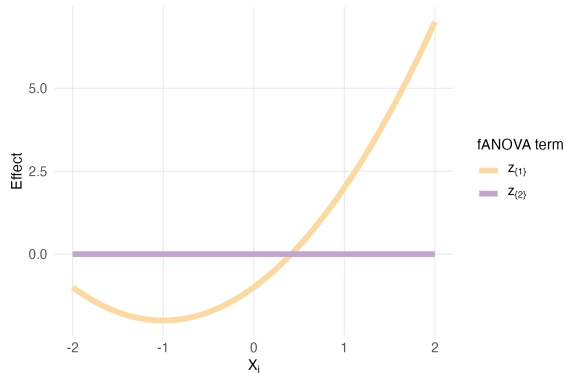
Figure: Main effect for $\rho = 0$.
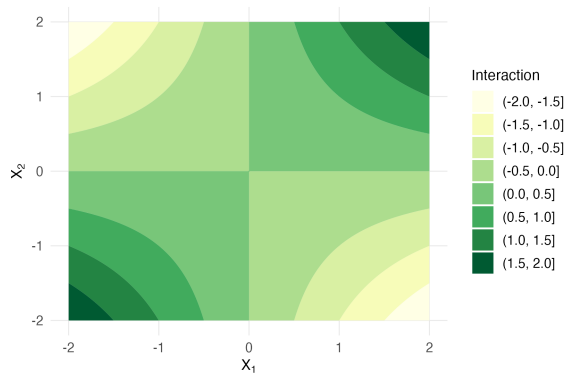
Figure: Interaction effect for $\rho = 0$.

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

Potential Usecase: Variance Decomposition

First proposed by [3], Sobol' indices build on variance decomposition:

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

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

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

Alternative Generalization of fANOVA

In [1] 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

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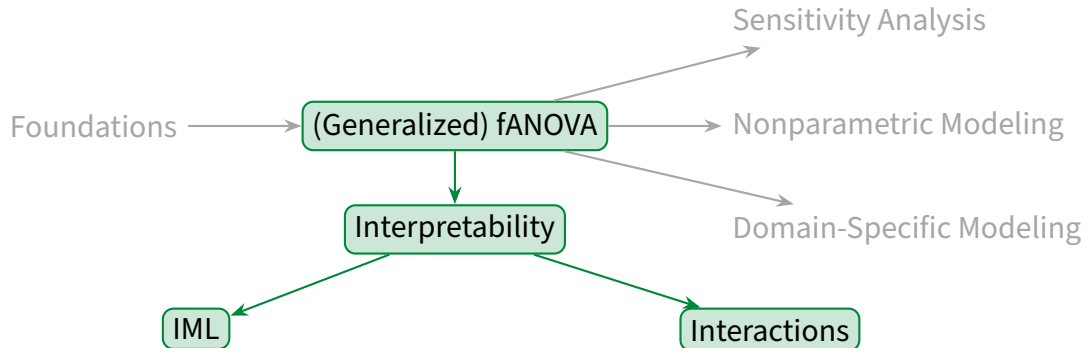
$$\Pi_{\mathcal{G}} y = \arg \min_{g \in \mathcal{G}} \|y - g\|^2 = \arg \min_{g \in \mathcal{G}} \mathbb{E}[(y(\boldsymbol{X}) - g(\boldsymbol{X}))^2].$$

- $\mathcal{G}$: 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

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

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

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

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

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

$$y_{\{1\}}(x_1) = \sum_{B \subseteq \{1\}} (-1)^{1-|B|}\, \mathbb{E}[y(\boldsymbol{X}) \,|\, X_B] = -\mathbb{E}[y] + \mathbb{E}[y | X_1 = x_1]$$

$$= -1 + (2x_1 + \mathbb{E}[X_2^2] + x_1 \mathbb{E}[X_2]) = 2x_1,$$

$$y_{\{2\}}(x_2) = \sum_{B \subseteq \{2\}} (-1)^{1-|B|}\, \mathbb{E}[y(\boldsymbol{X}) \,|\, X_B] - \mathbb{E}[y] + \mathbb{E}[y | X_2 = x_2]$$

$$= -1 + (2\mathbb{E}[X_1] + x_2^2 + x_2 \mathbb{E}[X_1]) = x_2^2 - 1.$$

$$y_{\{1,2\}}(x_1, x_2) = \sum_{B \subseteq \{1,2\}} (-1)^{2-|B|} \, \mathbb{E}[y(\boldsymbol{X}) \mid X_B]$$

$$= (+1) \, \mathbb{E}[y] - \mathbb{E}[y|X_1 = x_1] - \mathbb{E}[y|X_2 = x_2] + y(x_1, x_2)$$

$$= 1 - (2x_1 + 1) - (x_2^2) + (2x_1 + x_2^2 + x_1 x_2)$$

$$= x_1 x_2.$$

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

Substituting the basis functions:

$$y(x_1, x_2) = \underbrace{c_0}_{y_0} + \underbrace{\left(c_{1,1}\, x_1 + c_{1,2}\left(x_1^2 - 1\right)\right)}_{y_1(x_1)}$$

$$+ \underbrace{\left(c_{2,1}\, x_2 + c_{2,2}\left(x_2^2 - 1\right)\right)}_{y_2(x_2)}$$

$$+ \underbrace{c_{12,11}\left(\frac{\rho(x_1^2 + x_2^2)}{1 + \rho^2} - x_1 x_2 + \frac{\rho(\rho^2 - 1)}{1 + \rho^2}\right)}_{y_{12}(x_1, x_2)}.$$

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

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

Coefficient Matching

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

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

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

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

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

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

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

Example: Only Main

$$y(x_1, x_2) = -2x_1 - 2x_2 + x_1^2 + x_2^2 \qquad \rho = 0$$
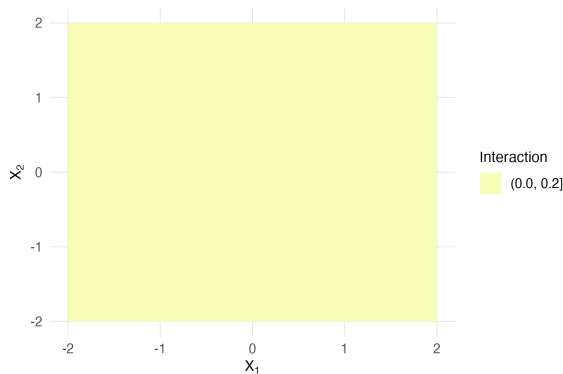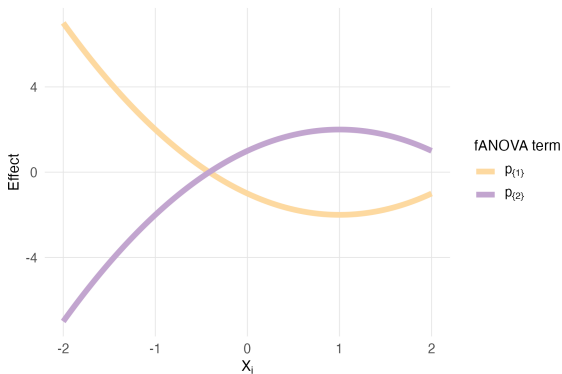
Example: Only Linear Terms
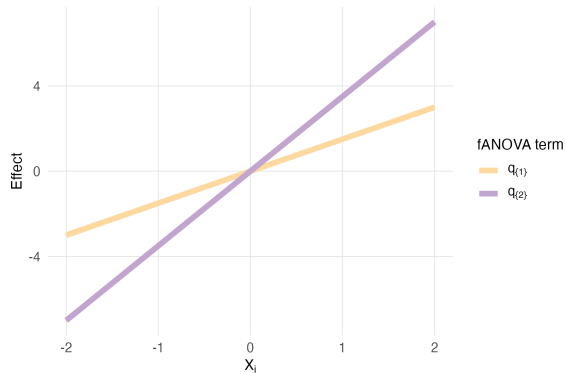
Figure: $q(x_1, x_2) = 1.5x_1 + 3.5x_2$
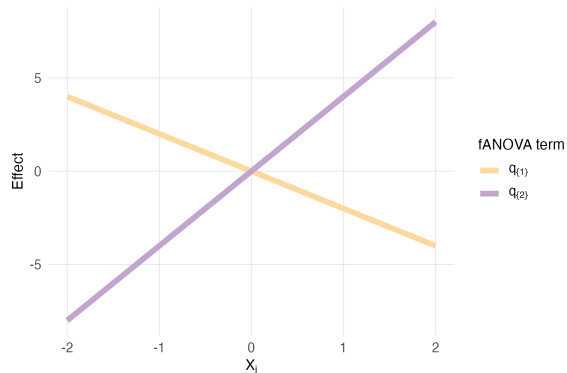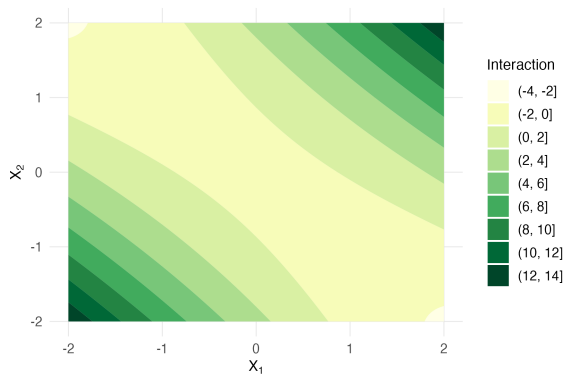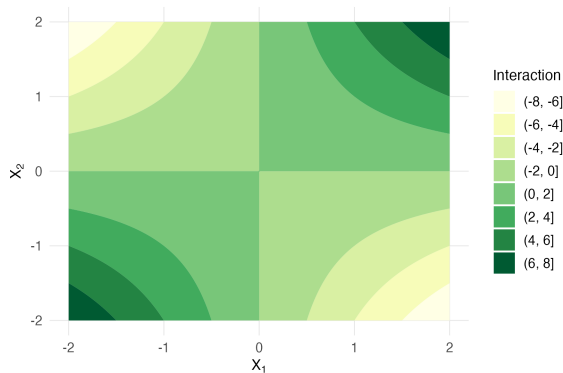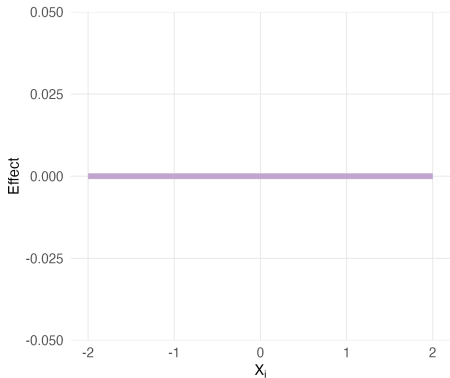

Figure: $q(x_1, x_2) = -2x_1 + 4x_2$

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

Example: Interaction

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

Formula for classical Sobol' indices?
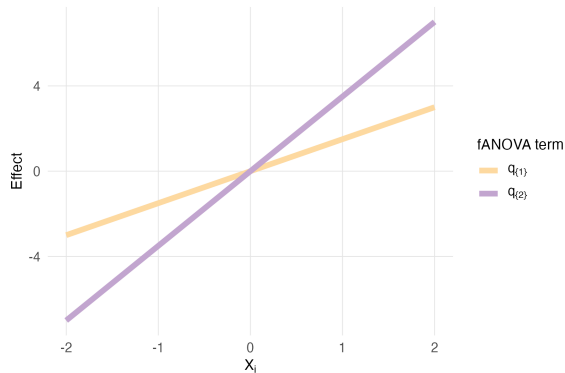
Decomposition of linear functions
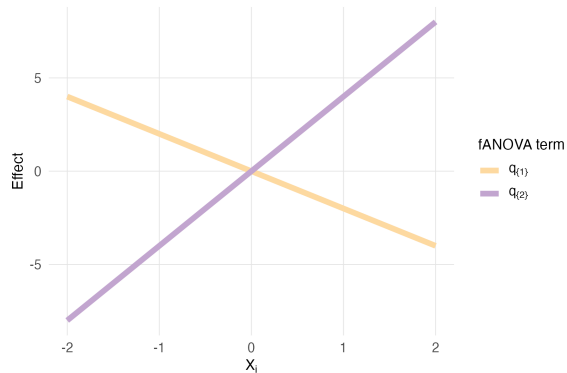

Figure: $q(x_1, x_2) = 1.5x_1 + 3.5x_2$

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

- 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

📄 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.

📄 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.