

LUDWIG-MAXIMILIANS UNIVERSITÄT MÜNCHEN



## **Your Title**

Your Name July 31, 2025

# Showcase Figure

## Outline

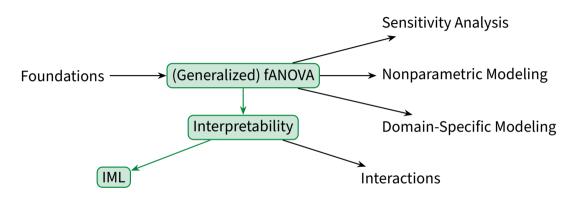


Research Context

- 2 Classical fANOVA
- Generalized fANOVA
- 4 Conclusion

### Overview of the fANOVA Research Field





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

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# Classical fANOVA Decomposition



#### **General Form**

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

- y: Model output
- $y_u$ : Component functions for subset u

#### Conditions for Classical fANOVA



#### **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

## **Key Properties**



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

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

- Zero mean components
- Mutual orthogonality

# **Component Construction**



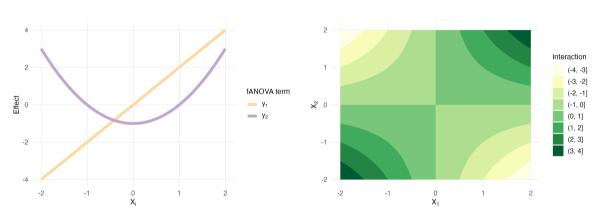
$$y_{\emptyset} = \int_{\mathbb{R}^N} y(\boldsymbol{x}) \prod_{i=1}^N f_{\{i\}}(x_i) \, d\nu(x_i) = \mathbb{E}[y(\boldsymbol{x})].$$

$$y_u(x_u) = \int y(x)f_{-u}(x_{-u})dx_{-u} - \sum_{v \subset u} y_v(x_v)$$

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

## Example: 2D Function





## Outline

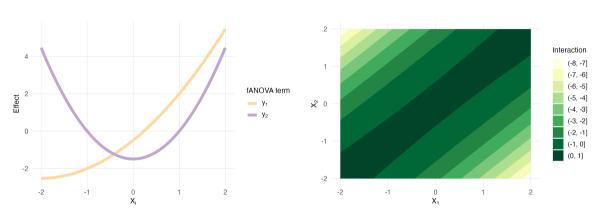


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# Example with Dependent Inputs (ho = 0.8)





# Weaker Annihilating Conditions



#### **Weak Annihilating Conditions**

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

- Allows dependent input distributions
- Leads to hierarchical orthogonality

# Key Properties (Generalized)



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

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

- Zero mean components remain
- Orthogonality is weaker: hierarchical

# Component Definition (Coupled System)



$$y_{\emptyset,G} = \int_{\mathbb{R}^N} y(\mathbf{x}) f_{\mathbf{X}}(\mathbf{x}) \, d\nu(\mathbf{x}) \tag{1}$$

$$y_{u,G}(\mathbf{X}_{u}) = \int_{\mathbb{R}^{N-|u|}} y(\mathbf{X}_{u}, \mathbf{x}_{-u}) f_{-u}(\mathbf{x}_{-u}) d\nu(\mathbf{x}_{-u}) - \sum_{v \subsetneq u} y_{v,G}(\mathbf{X}_{v})$$

$$- \sum_{\substack{\emptyset \neq v \subseteq \{1, \dots, N\} \\ v \cap u \neq \emptyset, \ v \not\subset u}} \int_{\mathbb{R}^{|v \cap -u|}} y_{v,G}(\mathbf{X}_{v \cap u}, \mathbf{x}_{v \cap -u}) f_{v \cap -u}(\mathbf{x}_{v \cap -u}) d\nu(\mathbf{x}_{v \cap -u}). \tag{2}$$

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

## How to Construct the Components



- ullet Coupled system o difficult to obtain analytical solutions
- Use alternative method via Fourier Polynomial ([5])
- ullet Building blocks: mutually orthogonal, zero-mean basis functions  $\psi_{i,j}$ , coefficients  $c_{i,j}$

# Basis Representation of a Polynomial



$$y(x_{1},x_{2}) = a_{0} + a_{1}x_{1} + a_{2}x_{2} + a_{11}x_{1}^{2} + a_{22}x_{2}^{2} + a_{12}x_{1}x_{2}$$

$$= c_{0} + c_{1,1} \psi_{1,1}(x_{1}) + c_{2,1} \psi_{2,1}(x_{2})$$

$$+ c_{1,2} \psi_{1,2}(x_{1}) + c_{2,2} \psi_{2,2}(x_{2}) + c_{12,11} \psi_{12,11}(x_{1},x_{2})$$

$$= \underbrace{c_{0}}_{y_{0}} + \underbrace{\left(c_{1,1} \psi_{1,1}(x_{1}) + c_{1,2} \psi_{1,2}(x_{1})\right)}_{y_{1}(x_{1})}$$

$$+ \underbrace{\left(c_{2,1} \psi_{2,1}(x_{2}) + c_{2,2} \psi_{2,2}(x_{2})\right)}_{y_{2}(x_{2})}$$

$$+ \underbrace{c_{12,11} \psi_{12,11}(x_{1},x_{2})}_{y_{12}(x_{1},x_{2})}.$$

# Basis Functions proposed by Rahman (2014)[5]



$$egin{aligned} \psi_\emptyset(x_1,x_2)&=1,\ \psi_{1,1}(x_1)&=x_1,\ \psi_{2,1}(x_2)&=x_2,\ \psi_{1,2}(x_1)&=x_1^2-1,\ \psi_{2,2}(x_2)&=x_2^2-1,\ \end{pmatrix} \ \psi_{12,11}(x_1,x_2)&=rac{
ho(x_1^2+x_2^2)}{1+
ho^2}-x_1x_2+rac{
ho(
ho^2-1)}{1+
ho^2}, \end{aligned}$$

# Alternative Generalization of fANOVA, [2]



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

subject to hierarchical orthogonality conditions:

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

# Variance Decomposition, [6]



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

$$\sigma^{2} := \mathbb{E}\left[\left(y(\mathbf{X}) - \mu_{G}\right)^{2}\right]$$

$$= \mathbb{E}\left[\left(y_{\emptyset,G} + \sum_{u} y_{u,G}(\mathbf{X}_{u}) - y_{\emptyset,G}\right)^{2}\right]$$

$$= \mathbb{E}\left[\left(\sum_{u} y_{u,G}(\mathbf{X}_{u})\right)^{2}\right]$$

$$= \sum_{u} \mathbb{E}\left[y_{u,G}^{2}(\mathbf{X}_{u})\right] + \sum_{u \subseteq v, v \subseteq u} \mathbb{E}\left[y_{u,G}(\mathbf{X}_{u})y_{v,G}(\mathbf{X}_{v})\right],$$

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#### References I





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.



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

#### References II





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.



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.

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#### References III





Charles J. Stone.

The Use of Polynomial Splines and Their Tensor Products in Multivariate Function Estimation.

The Annals of Statistics, 22(1):118–171, 1994.

Publisher: Institute of Mathematical Statistics.