Functional ANOVA and Variance Decomposition of Functions

May 12, 2025 // Damar Wicaksono

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Functional Decomposition

Functional decomposition is a method that:

- **breaks down** complex multidimensional functions, and
- **represents** them as the sum of **individual effects** (also called **main effects**) of the inputs and the **interaction effects** between them.

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It provides a way to look and succinctly describe complex multidimensional functions.

Let $f : \mathbb{R}^m \rightarrow \mathbb{R}$, then functional decomposition of f yields:

$$f(\boldsymbol{x}) = \underbrace{f_0}_{\text{baseline effect}} + \underbrace{f_1(x_1) + f_2(x_2) + \ldots}_{\text{main effects}} + \underbrace{f_{1,2}(x_1, x_2) + f_{1,3}(x_1, x_3) + \ldots}_{\text{2-way interaction effects}} + \ldots + \underbrace{f_{1,\ldots,m}(x_1, \ldots, x_m)}_{m\text{-way interaction effect}}$$

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Observations:

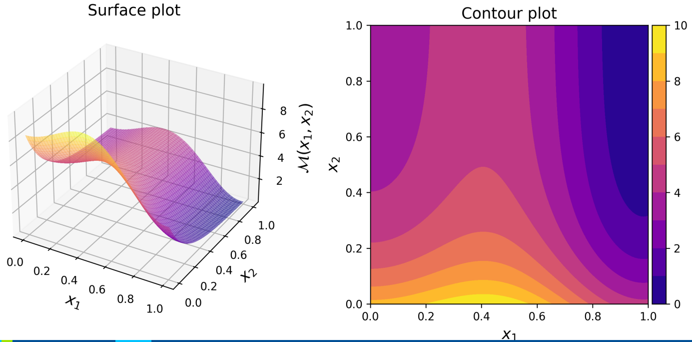
- There are 2^m components in the summation
- The summation recovers the original function

Example

Consider a two-dimensional function:

$$f(x_1, x_2) = \frac{1}{6}\left[120 + 20x_1 \sin(5x_1) + 30e^{-5x_2} + 20x_1 \sin(5x_1)e^{-5x_2} - 100\right], \quad x_1, x_2 \in [0, 1].$$

(Lim et al., 2002)



Example: Functional Decomposition

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So, by **inspection**:

$$f(x_1, x_2) = \frac{1}{6}\left[120 + 20x_1 \sin(5x_1) + 30e^{-5x_2} + 20x_1 \sin(5x_1)e^{-5x_2} - 100\right],$$

$$f_0 = \frac{20}{6};\; f_1(x_1) = \frac{20}{6}x_1 \sin(5x_1);\; f_2(x_2) = 5e^{-5x_2};\; f_{1,2}(x_1, x_2) = x_1 \sin(5x_1)e^{-5x_2}.$$

There are $2^2 = 4$ components by just looking and the sum indeed recovers the original function.

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Are we done?

Problems

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- **Uniqueness**: You can come with different decompositions as long as the sum recovers the function by adjusting the last term.

  Example:

$$f_1(x_1) = \frac{20}{6}\left(x_1 \sin\left(5x_1\right) + x_1 \cos\left(5x_1\right)\right); \; f_{1,2}(x_1, x_2) = x_1 \left(\sin\left(5x_1\right) - \frac{20}{6}\cos\left(5x_1\right)\right) e^{-5x_2}.$$

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- **Input effect**: *Shouldn't the decomposition take into account the inputs?*

  Example:

$$x_2 \in [3, 4] \rightarrow f_2 \approx 0, f_{1,2} \approx 0.$$

The effect of x_2 on f depends how it is specified.

Problems

Our way of decomposing the function by inspection is unsatisfying:

Our decomposition is neither unique nor meaningful.

Outline

Assumption: Space of square-integrable functions

We assume that our function of interest belongs to $L^2(\mathcal{D}_{\boldsymbol{X}}, \rho_{\boldsymbol{X}})$, i.e., the space of square-integrable functions over domain $\mathcal{D}_{\boldsymbol{X}} \subseteq \mathbb{R}^m$ with respect to the weight function $\rho_{\boldsymbol{X}}$.

- A function f is square integrable over the domain $\mathcal{D}_{\boldsymbol{X}}$ with respect to the weight function $\rho_{\boldsymbol{X}}$ if:
$$\int_{\mathcal{D}_{\boldsymbol{X}}} f^2(\boldsymbol{x}) \rho_{\boldsymbol{X}}(\boldsymbol{x}) \; d\boldsymbol{x} < \infty.$$
- The space is equipped with inner product (it's a Hilbert space). That is, for $f, g \in L^2(\mathcal{D}_{\boldsymbol{X}}, \rho_{\boldsymbol{X}})$,
$$\langle f, g \rangle_{\rho_{\boldsymbol{X}}} \equiv \int_{\mathcal{D}_{\boldsymbol{X}}} f(\boldsymbol{x}) g(\boldsymbol{x}) \rho_{\boldsymbol{X}}(\boldsymbol{x}) d\boldsymbol{x}.$$
- The function norm is defined as:
$$\| f \|^2_{\rho_{\boldsymbol{X}}} \equiv \langle f, f \rangle_{\rho_{\boldsymbol{X}}} < \infty.$$

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In practice, we are interested in selecting the weight function $\rho_{\boldsymbol{X}}$ to be a **(joint) probability density function**.

$L^2(\mathcal{D}_{\boldsymbol{X}}, \rho_{\boldsymbol{X}})$ is then equivalent to the space of random variables with **finite variance**, where the elements are functions of random vectors.

Uncertainty Quantification Framework

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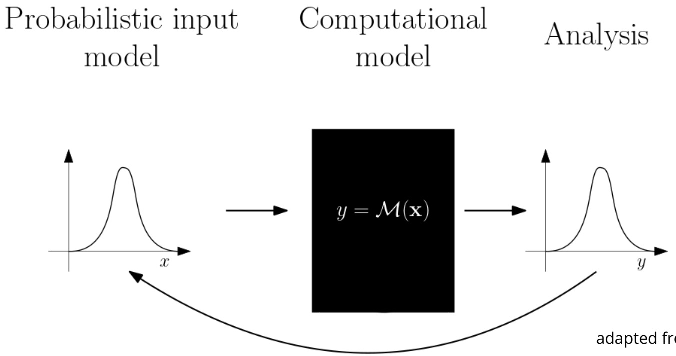

adapted from (Marelli and Sudret, 2014)

Assumption: Mutually Independent $\boldsymbol{X}$

We further assume that $\boldsymbol{X}$ is a mutually independent random vector such that its joint probability density function (PDF) reads:

$$\rho_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{j=1}^{m} \rho_{X_j}(x_j),$$

where ρ_{X_j} is the univariate PDF of X_j.

Multi-Index Notation

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Through decomposition, we write an m-dimensional function f as a sum of functions:

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{u} \subseteq [1:m]} f_{\boldsymbol{u}}(\boldsymbol{x}_{\boldsymbol{u}}),$$

where:

- $[1:m]$ is a short-hand for the set $\{1, \ldots, m\}$
- $\boldsymbol{x}_{\boldsymbol{u}}$ is the vector of inputs in the index set $\boldsymbol{u}$, i.e., $\boldsymbol{u} = \{i_1, \ldots, i_{|\boldsymbol{u}|}\}$ means $(x_i)_{i \in \boldsymbol{u}}$
- $f_{\boldsymbol{u}}$ is the component function that depends only on $\boldsymbol{x}_{\boldsymbol{u}}$

Multi-Index Notation

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Example: For $m = 3$, the full decomposition of f consists of $2^3 = 8$ terms and it reads:

$$\begin{aligned} f(\boldsymbol{x}) = f_\emptyset & \qquad \text{baseline effect} \\ + f_{\{1\}}(x_1) + f_{\{2\}}(x_2) + f_{\{3\}}(x_3) & \qquad \text{main effects} \\ + f_{\{1,2\}}(x_1, x_2) + f_{\{1,3\}}(x_1, x_3) + f_{\{2,3\}}(x_2, x_3) & \qquad \text{2-way interactions} \\ + f_{\{1,2,3\}}(x_1, x_2, x_3). & \qquad \text{3-way interactions} \end{aligned}$$

Functional ANOVA: Constructive Definition

We seek to obtain a unique functional decomposition of f using the following **summands**:

- **Baseline effect** for $\boldsymbol{u} = \emptyset$ (global mean)

$$f_{\emptyset} = \int_{\mathcal{D}_{\boldsymbol{X}}} f(\boldsymbol{x}) \rho_{\boldsymbol{X}}(\boldsymbol{x}) \, d\boldsymbol{x}.$$

where $\sim \boldsymbol{u}$ is the set complement of $\boldsymbol{u}$.

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- **Main effect** for $\boldsymbol{u} = \{j\}, j = 1, \ldots, m$ (singletons)

$$f_{\{j\}}(x_j) = \int_{\mathcal{D}_{\boldsymbol{X}_{\sim\{j\}}}} f(\boldsymbol{x}) \rho_{\boldsymbol{X}_{\sim\{j\}}}(\boldsymbol{x}_{\sim\{j\}}) \, d\boldsymbol{x}_{\sim\{j\}} - f_{\emptyset}$$

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- **Interaction effect** for $\boldsymbol{u} \subseteq [1:m]$, $\boldsymbol{u} \neq \emptyset, |\boldsymbol{u}| > 1$

$$f_{\boldsymbol{u}}(x_{\boldsymbol{u}}) = \int_{\mathcal{D}_{\boldsymbol{X}_{\sim\boldsymbol{u}}}} f(\boldsymbol{x}) \rho_{\boldsymbol{X}_{\sim\boldsymbol{u}}}(\boldsymbol{x}_{\sim\boldsymbol{u}}) \, d\boldsymbol{x}_{\sim\boldsymbol{u}} - \sum_{\boldsymbol{v} \subset \boldsymbol{u}} f_{\boldsymbol{v}}(\boldsymbol{x}_{\boldsymbol{v}})$$

where $\sim \boldsymbol{u}$ is the set complement of $\boldsymbol{u}$.

Functional ANOVA: Intuition

Consider the **interaction effect** for $\boldsymbol{u} \subseteq [1:m]$, $\boldsymbol{u} \neq \emptyset, |\boldsymbol{u}| > 1$

$$f_{\boldsymbol{u}}(x_{\boldsymbol{u}}) = \int_{\mathcal{D}_{\boldsymbol{X}_{\sim \boldsymbol{u}}}} f(\boldsymbol{x}) \rho_{\boldsymbol{X}_{\sim \boldsymbol{u}}}(\boldsymbol{x}_{\sim \boldsymbol{u}}) \, d\boldsymbol{x}_{\sim \boldsymbol{u}} - \sum_{\boldsymbol{v} \subset \boldsymbol{u}} f_{\boldsymbol{v}}(\boldsymbol{x}_{\boldsymbol{v}})$$

Intuition

When we compute $f_{\boldsymbol{u}}$:

- We don't want to attribute anything to it that can be explained by $\boldsymbol{x}_{\boldsymbol{v}}$ for $\boldsymbol{v} \subset \boldsymbol{u}$
- $f_{\boldsymbol{u}}$ must be strictly only due to $\boldsymbol{x}_{\boldsymbol{u}}$; **not** $\boldsymbol{x}_{\sim \boldsymbol{u}}$ **nor** subsets of $\boldsymbol{x}_{\boldsymbol{u}}$ (lower order terms)
- Therefore, we integrate f over all $\boldsymbol{x}_{\sim \boldsymbol{u}}$ then substract all the lower order terms

Functional ANOVA: Example

Consider $f \in L^2(\mathcal{D}_{\boldsymbol{X}}, \rho_{\boldsymbol{X}})$ with mutually independent $\boldsymbol{X}$ for $m = 3$:

- **Baseline effect** (global mean)

$$f_{\emptyset} = \int_{\mathcal{D}_{X_1}} \int_{\mathcal{D}_{X_2}} \int_{\mathcal{D}_{X_3}} f(\boldsymbol{x}) \rho_{X_1}(x_1) \rho_{X_2}(x_2) \rho_{X_3}(x_3) \, dx_1 dx_2 dx_3.$$

- **Main effects**

$$f_{\{1\}}(x_1) = \int_{\mathcal{D}_{X_2}} \int_{\mathcal{D}_{X_3}} f(\boldsymbol{x}) \rho_{X_2}(x_2) \rho_{X_3}(x_3) \, dx_2 dx_3 - f_{\emptyset}$$

$$f_{\{2\}}(x_2) = \int_{\mathcal{D}_{X_1}} \int_{\mathcal{D}_{X_3}} f(\boldsymbol{x}) \rho_{X_1}(x_1) \rho_{X_3}(x_3) \, dx_1 dx_3 - f_{\emptyset}$$

$$f_{\{3\}}(x_3) = \int_{\mathcal{D}_{X_1}} \int_{\mathcal{D}_{X_2}} f(\boldsymbol{x}) \rho_{X_1}(x_1) \rho_{X_2}(x_2) \, dx_1 dx_2 - f_{\emptyset}.$$

Functional ANOVA: Example

Consider $f \in L^2(\mathcal{D}_{\boldsymbol{X}}, \rho_{\boldsymbol{X}})$ for $m = 3$:

- Two-way interaction effects

$$f_{\{1,2\}}(x_1, x_2) = \int_{\mathcal{D}_{X_3}} f(\boldsymbol{x}) \rho_{X_3}(x_3)\, dx_3 - f_{\{1\}}(x_1) - f_{\{2\}}(x_2) - f_{\emptyset}$$

$$f_{\{1,3\}}(x_1, x_3) = \int_{\mathcal{D}_{X_2}} f(\boldsymbol{x}) \rho_{X_2}(x_2)\, dx_2 - f_{\{1\}}(x_1) - f_{\{3\}}(x_2) - f_{\emptyset}$$

$$f_{\{2,3\}}(x_2, x_3) = \int_{\mathcal{D}_{X_1}} f(\boldsymbol{x}) \rho_{X_1}(x_1)\, dx_1 - f_{\{2\}}(x_2) - f_{\{3\}}(x_2) - f_{\emptyset}$$

- Three-way interaction effect

$$\begin{aligned} f_{\{1,2,3\}}(x_1, x_2, x_3) = f(\boldsymbol{x}) &- f_{\{1,2\}}(x_1, x_2) - f_{\{1,3\}}(x_1, x_3) - f_{\{2,3\}}(x_2, x_3) \\ &- f_{\{1\}}(x_1) - f_{\{2\}}(x_2) - f_{\{3\}}(x_3) - f_{\emptyset} \end{aligned}$$

Functional ANOVA: Important Properties

Let $f \in L^2(\mathcal{D}_{\boldsymbol{X}} \subseteq \mathbb{R}^m, \rho_{\boldsymbol{X}})$ with mutually independent $\boldsymbol{X}$ such that its functional ANOVA decomposition:

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{u} \subseteq [1:m]} f_{\boldsymbol{u}}(\boldsymbol{x}_{\boldsymbol{u}})$$

Then for $\boldsymbol{u}, \boldsymbol{v} \subseteq [1:m] \setminus \emptyset$:

- **Lemma**: Functional ANOVA summands average to zero w.r.t any of its indices

$$\int_{\mathcal{D}_{X_j}} f_{\boldsymbol{u}}(\boldsymbol{x}_{\boldsymbol{u}}) \rho_{X_j}(x_j) \, dx_j = 0, \quad \forall j \in \boldsymbol{u}.$$

- **Lemma**: Functional ANOVA summands are orthogonal

$$\int_{\mathcal{D}_{\boldsymbol{X}}} f_{\boldsymbol{u}}(\boldsymbol{x}_{\boldsymbol{u}}) \, f_{\boldsymbol{v}}(\boldsymbol{x}_{\boldsymbol{v}}) \, \rho_{\boldsymbol{X}}(\boldsymbol{x}) \, d\boldsymbol{x} = 0, \boldsymbol{u} \neq \boldsymbol{v}.$$

Functional ANOVA: Variance Decomposition

ANOVA stands for Analysis of Variance; so taking it one step further.

- Total variance of f

$$\sigma^2 \equiv \int_{\mathcal{D}_{\boldsymbol{X}}} \left(f_{\boldsymbol{x}}(\boldsymbol{x}) - f_{\emptyset}\right)^2 \rho_{\boldsymbol{X}}(\boldsymbol{x}) \, d\boldsymbol{x}.$$

- Partial variances of $f_{\boldsymbol{u}}$

$$\sigma^2_{\boldsymbol{u}} \equiv \begin{cases} \int_{\mathcal{D}_{\boldsymbol{X}_{\boldsymbol{u}}}} f^2_{\boldsymbol{u}}(\boldsymbol{x}_{\boldsymbol{u}}) \rho_{\boldsymbol{X}_{\boldsymbol{u}}}(\boldsymbol{x}_{\boldsymbol{u}}) \, d\boldsymbol{x}_{\boldsymbol{u}}, & |\boldsymbol{u}| > 0 \\ 0, & |\boldsymbol{u}| = 0. \end{cases}$$

Functional ANOVA: Variance Decomposition

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$$\sigma^2 \equiv \int_{\mathcal{D}_{\boldsymbol{X}}} \left(f_{\boldsymbol{x}}(\boldsymbol{x}) - f_{\emptyset} \right)^2 \rho_{\boldsymbol{X}}(\boldsymbol{x}) \, d\boldsymbol{x}.$$

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$$\sigma_{\boldsymbol{u}}^2 \equiv \begin{cases} \int_{\mathcal{D}_{\boldsymbol{X}_{\boldsymbol{u}}}} f_{\boldsymbol{u}}^2(\boldsymbol{x}_{\boldsymbol{u}}) \rho_{\boldsymbol{X}_{\boldsymbol{u}}}(\boldsymbol{x}_{\boldsymbol{u}}) \, d\boldsymbol{x}_{\boldsymbol{u}}, & |\boldsymbol{u}| > 0 \\ 0, & |\boldsymbol{u}| = 0. \end{cases}$$

Theorem: Variance decomposition of f (Sobol' decomposition)

The total variance of f is decomposed into a sum of variances of the summands:

$$\sigma^2 = \sum_{|\boldsymbol{u}|>0} \sigma_{\boldsymbol{u}}^2.$$

Functional ANOVA: Historical Perspective

(Functional) ANOVA has a long history rooted in statistics and applied mathematics:

- ANOVA for tabular data developed by Fisher
  (Fisher, 1919)
- generalized for $[0,1]^m$ as U-statistics
  (Hoeffding, 1948)
- generalized for $[0,1]^m$ as Sobol' decomposition for Quasi Monte Carlo integration
  (Sobol', 1969)
- popularized for practical sensitivity analysis in applied science and engineering
  (Saltelli et al., 2000)
- revisited in the context of Monte Carlo integration and effective dimensions
  (Caflisch et al., 1997; Liu and Owen, 2006)


R.A. Fisher
(1890–1962)


W. Hoeffding
(1914–1991)


I.M. Sobol'
(1926–)


A. Saltelli
(1953–)


A. Owen
(1958–)

Outline

Applications and Interpretations

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Given the variance decomposition of f into a sum of partial variances:

$$\sigma^2 = \sum_{|\boldsymbol{u}|>0} \sigma^2_{\boldsymbol{u}},$$

We gain insight into f (with respect to its inputs) by aggregating partial variances into few interpretable numbers.

Outline

Functional Decomposition

Functional ANOVA

Applications

Application: Global Sensitivity Analysis

Application: Effective Dimensions

Notes on Computation

Notes on Computation: Direct Computation

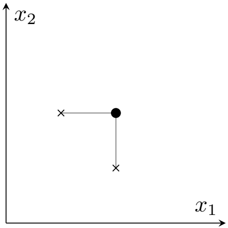
Notes on Computation: Function Approximations

Summary

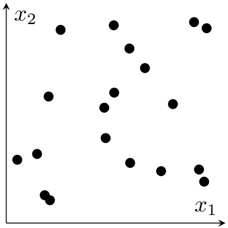
Sensitivity Analysis: Local vs Global

How variation in the inputs affect the variation in the output of a complex model

We often distinguish **local analysis** (effects of perturbations around a particular instance) from **global analysis** (variations over all possible instances in the domain).



Local analysis



Global analysis

Sobol' Sensitivity Indices: Main Effect

The **Sobol' main-effect index** is defined as the **main-effect partial variance** of x_j normalized by the total variance:

$$S_j \equiv \frac{\sigma^2_{\{j\}}}{\sigma^2}.$$

(Sobol', 1993)

This index measures the proportion of the total variance of f that can be explained **only by** x_j without any interactions with any other variables.

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Additive function: Function with

$$\sum_{j=1}^{m} S_j = 1.0$$

is called additive function, i.e.,

$$f(\boldsymbol{x}) = f_{\emptyset} + \sum_{j=1}^{m} f_{\{j\}}(x_j).$$

Sobol' Sensitivity Indices: Total Effect

The **Sobol' total-effect index** is defined as the **total-effect partial variance** of x_j normalized by the total variance:

$$ST_j \equiv \frac{\bar{\tau}^2_{\{j\}}}{\sigma^2}; \quad \bar{\tau}^2_{\{j\}} \equiv \sum_{\boldsymbol{v}:\boldsymbol{v}\cap\{j\}\neq\emptyset} \sigma^2_{\boldsymbol{v}}.$$

(Homma and Saltelli, 1996)

This index measures the proportion of the total variance of f that can be explained by x_j **and** its interaction with any other variables.

Example: For $\{j\} = \{1\}$ with $m = 3$:

$$\bar{\tau}^2_{\{1\}} = \sum_{\boldsymbol{v}:\boldsymbol{v}\cap\{j\}\neq\emptyset} \sigma^2_{\boldsymbol{v}} = \sigma^2_{\{1\}} + \sigma^2_{\{1,2\}} + \sigma^2_{\{1,3\}} + \sigma^2_{\{1,2,3\}}.$$

Sobol' Sensitivity Indices: Some Interpretations

Consider the following two cases:

- S_j is large $\rightarrow x_j$ is important: S_j is a measure of a variable **importance**

Setting x_j to a particular value (thus reducing its variance to zero) will on average reduce the variance of f significantly.

- ST_j is small $\leftrightarrow x_j$ is not important: ST_j is a measure of a variable **non-importance**

Setting x_j to a particular value (thus reducing its variance to zero) will on average do nothing to the variance of f. x_j doesn't matter.

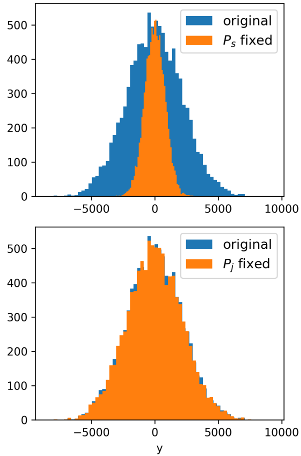
Example: Simple Portfolio Model

Consider the following 3-dimensional function:

$$f(\boldsymbol{x}) = $$ [redacted]

Input	ρ_X	S_j	ST_j
X_1	$\mathcal{N}(0.0, 4.0)$	0.861	0.861
X_2	$\mathcal{N}(0.0, 2.0)$	0.1376	0.1376
X_3	$\mathcal{N}(0.0, 1.0)$	0.0021	0.0021

X_1 is the most influential input; X_3 is the non-influential input; f is additive.



Example: Simple Portfolio Model

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Consider the following 3-dimensional function:

$$f(\boldsymbol{x}) = 500x_1 + 400x_2 + 100x_3$$

(Saltelli et al., 2004)

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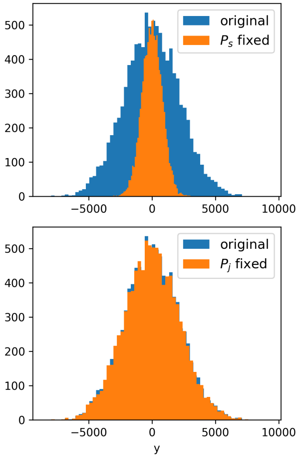


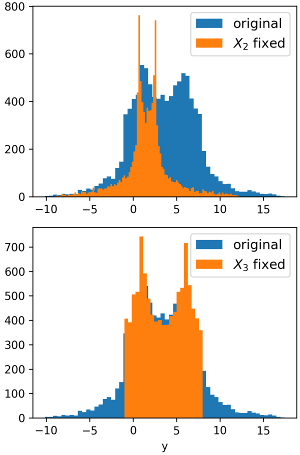
Example: Ishigami Function

Consider the following 3-dimensional function:

$$f(\boldsymbol{x}) = \blacksquare$$

Input	ρ_X	S_j	ST_j
X_1	$\mathcal{U}(-\pi, \pi)$	0.314	0.558
X_2	$\mathcal{U}(-\pi, \pi)$	0.442	0.442
X_3	$\mathcal{U}(-\pi, \pi)$	0.000	0.244

X_2 is the most influential input; no input is non-influential; f is not additive.



Example: Ishigami Function

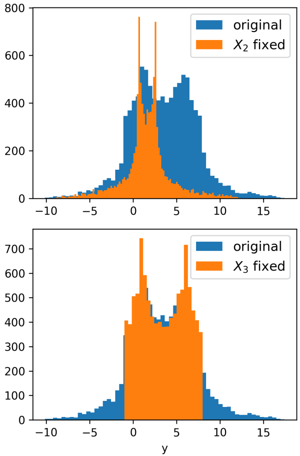
Consider the following 3-dimensional function:

$$f(\boldsymbol{x}) = \sin(x_1) + 7\sin(x_2)^2 + 0.1 x_3^4 \sin(x_1)$$

(Ishigami and Homma, 1991)

Input	ρ_X	S_j	ST_j
X_1	$\mathcal{U}(-\pi,\pi)$	0.314	0.558
X_2	$\mathcal{U}(-\pi,\pi)$	0.442	0.442
X_3	$\mathcal{U}(-\pi,\pi)$	0.000	0.244

X_2 is the most influential input; no input is non-influential; f is not additive.



Outline

Functional Decomposition

Functional ANOVA

Applications

Application: Global Sensitivity Analysis

Application: Effective Dimensions

Notes on Computation

Notes on Computation: Direct Computation

Notes on Computation: Function Approximations

Summary

Dimensions of Functions: Nominal vs Effective

Sobol' indices describe function in few numbers; we can go one step further to characterize functions…

The **nominal dimension** of a function is usually known in advance, but functions often have a lower **effective dimension** than their nominal value.

Effective Dimension: Superposition Sense

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The effective dimension of f in the **superposition sense** is the smallest integer m_s such that

$$\sum_{|\boldsymbol{u}| \leq m_s} \sigma_{\boldsymbol{u}}^2 \geq p\, \sigma^2,$$

(Caflisch et al., 1997)

where $0 < p < 1$. The choice of p is arbitrary, but a common choice for p is 0.99.

The effective dimension in superposition sense is the **maximum order of interactions** one must include in the sum in order to reach the target variance.

For $m_s = 1$, the function is purely **additive**.

Effective Dimension: Truncation Sense

The effective dimension of f in the **truncation sense** is the smallest integer m_t such that

$$\sum_{\boldsymbol{u} \subseteq [1:m_t]} \sigma_{\boldsymbol{u}}^2 \geq p\, \sigma^2.$$

(Caflisch et al., 1997)

where $0 < p < 1$. The choice of p is arbitrary, but a common choice for p is 0.99. Here we assumed that we order the first m_t variables with respect to their importance.

The effective dimension in truncation sense is the number of **active input variables** of the function.

Example: Simple Portfolio Model

Consider the following 3-dimensional function:

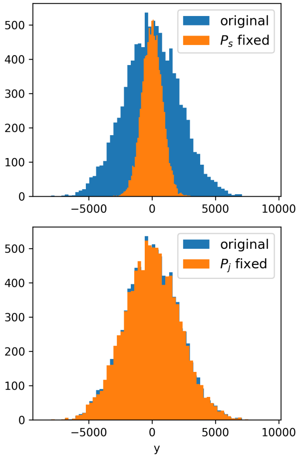
$$f(\boldsymbol{x}) = 500P_s + 400P_t + 100P_j$$

(Saltelli et al., 2004)

Input	ρ_X	S_j	ST_j
X_1	$\mathcal{N}(0.0, 4.0)$	0.861	0.861
X_2	$\mathcal{N}(0.0, 2.0)$	0.1376	0.1376
X_3	$\mathcal{N}(0.0, 1.0)$	0.0021	0.0021

The effective dimensionalities of this nominally 3D function:

- $m_s = 1$: Additive function, no interaction
- $m_t = 2$: One fewer than the nominal dimension



Example: Ishigami Function

Consider the following 3-dimensional function:

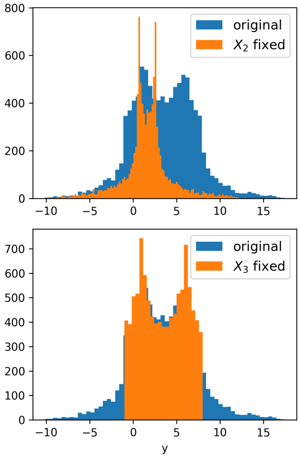
$$f(\boldsymbol{x}) = \sin(x_1) + 7\sin(x_2)^2 + 0.1 x_3^4 \sin(x_1)$$

(Ishigami and Homma, 1991)

Input	ρ_X	S_j	ST_j
X_1	$\mathcal{U}(-\pi,\pi)$	0.314	0.558
X_2	$\mathcal{U}(-\pi,\pi)$	0.442	0.442
X_3	$\mathcal{U}(-\pi,\pi)$	0.000	0.244

The effective dimensionalities of this nominally 3D function:

- $m_s = 2$: Max two-way interaction is required
- $m_t = 3$: All inputs are influential



Outline

Partial Variances: Integration Problems

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- To compute the Sobol' main-effect indices, we focus on the following partial variances:

$$\sigma^2_{\{j\}} = \int_{\mathcal{D}_{X_j}} f^2_{\{j\}}(x_j) \rho_{X_j}(x_j) \, dx_j, \quad j = 1, \ldots, m.$$

Partial Variances: Integration Problems

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$$\sigma^2_{\{j\}} = \int_{\mathcal{D}_{X_j}} f^2_{\{j\}}(x_j)\rho_{X_j}(x_j)\, dx_j, \quad j = 1, \ldots, m.$$

- The following "**trick**" often used in probability calculation is useful:

$$\left(\int_{\mathcal{D}_{\boldsymbol{X}}} f(\boldsymbol{x})\, d\boldsymbol{x} \right)^2 = \int_{\mathcal{D}_{\boldsymbol{X}}} f(\boldsymbol{x})\, d\boldsymbol{x} \int_{\mathcal{D}_{\boldsymbol{X}}} f(\boldsymbol{z})\, d\boldsymbol{z},$$

  where we use a dummy variable $\boldsymbol{z}$ to cast the square integrals as a double integral of two independent variables.

Partial Variances: Integration Problems

- To compute the Sobol' main-effect indices, we focus on the following partial variances:

$$\sigma^2_{\{j\}} = \int_{\mathcal{D}_{X_j}} f^2_{\{j\}}(x_j)\rho_{X_j}(x_j)\,dx_j, \quad j = 1, \ldots, m.$$

- The following identity can be proven:

$$\sigma^2_{\{j\}} = \int\limits_{\mathcal{D}_{\boldsymbol{X}_{\sim\{j\}}}} \int\limits_{\mathcal{D}_{\boldsymbol{X}}} f(\boldsymbol{x})\, f(x_j, \boldsymbol{z}_{\sim\{j\}})\, \rho_{\boldsymbol{X}}(\boldsymbol{x})\, \rho_{\boldsymbol{X}_{\sim\{j\}}}(\boldsymbol{z}_{\sim\{j\}})\, d\boldsymbol{x}\, d\boldsymbol{z}_{\sim\{j\}} - f^2_{\emptyset}$$

  where $(x_j, \boldsymbol{z}_{\sim\{j\}})$ takes the value of input variables that corresponds to the index j from $\boldsymbol{x}$ and in $\sim\{j\}$ from $\boldsymbol{z}$; $f_{\emptyset}$ is the mean of f (also an integral).

Partial Variances: Integration Problems

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- The following identity can be proven:

$$\sigma^2_{\{j\}} = \int\limits_{\mathcal{D}_{\boldsymbol{X}_{\sim\{j\}}}} \int\limits_{\mathcal{D}_{\boldsymbol{X}}} f(\boldsymbol{x}) \, f(x_j, \boldsymbol{z}_{\sim\{j\}}) \, \rho_{\boldsymbol{X}}(\boldsymbol{x}) \, \rho_{\boldsymbol{X}_{\sim\{j\}}}(\boldsymbol{z}_{\sim\{j\}}) \, d\boldsymbol{x} \, d\boldsymbol{z}_{\sim\{j\}} - f^2_{\emptyset}$$

where $(x_j, \boldsymbol{z}_{\sim\{j\}})$ takes the value of input variables that corresponds to the index j from $\boldsymbol{x}$ and in $\sim \{j\}$ from $\boldsymbol{z}$; $f_{\emptyset}$ is the mean of f (also an integral).

This is a $(2m-1)$-fold integral!

Partial Variances: Integration Problems

- To compute the Sobol' total-effect indices, we focus on the following partial variances:

$$\bar{\tau}^2_{\{j\}} = \sum_{\boldsymbol{v}:\boldsymbol{v}\cap\{j\}\neq\emptyset} \sigma^2_{\boldsymbol{v}}.$$

- The following identity can be proven:

$$\bar{\tau}^2_{\{j\}} = \frac{1}{2} \int_{\mathcal{D}_{X_j}} \int_{\mathcal{D}_{\boldsymbol{X}}} \left(f(\boldsymbol{x}) - f(z_j, \boldsymbol{x}_{\sim\{j\}}) \right) \, \rho_{\boldsymbol{X}}(\boldsymbol{x}) \, \rho_{X_j}(z_j) \, d\boldsymbol{x} \, dz_j,$$

where $(z_j, \boldsymbol{x}_{\sim\{j\}})$ takes the value of input variables that corresponds to the index j from $\boldsymbol{z}$ and in $\sim \{j\}$ from $\boldsymbol{x}$.

Partial Variances: Integration Problems

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This is an $(m-1)$-fold integral!

Sobol' Indices: Monte Carlo Simulation

- To compute the Sobol' main-effect indices, we cast the integral as expectation:

$$
\begin{aligned}
\sigma^2_{\{j\}} &= \int_{\mathcal{D}_{\boldsymbol{X}_{\sim\{j\}}}} \int_{\mathcal{D}_{\boldsymbol{X}}} f(\boldsymbol{x})\, f(x_j, \boldsymbol{z}_{\sim\{j\}})\, \rho_{\boldsymbol{X}}(\boldsymbol{x})\, \rho_{\boldsymbol{X}_{\sim\{j\}}}(\boldsymbol{z}_{\sim\{j\}})\, d\boldsymbol{x}\, d\boldsymbol{z}_{\sim\{j\}} - f_{\emptyset}^2 \\
&= \mathbb{E}_{\boldsymbol{X}, \boldsymbol{Z}_{\sim\{j\}}} \left[f(\boldsymbol{X})\, f(X_j, \boldsymbol{Z}_{\sim\{j\}}) \right] - \mathbb{E}^2_{\boldsymbol{X}} [f(\boldsymbol{X})]
\end{aligned}
$$

  where $\mathbb{E}_{.}[\cdot]$ is the expectation operator; the subscript indicates the random variable with respect to which the expectation is taken.
- Similarly for the Sobol' total-effect indices:

$$
\begin{aligned}
\tau^2_{\{j\}} &= \frac{1}{2} \int_{\mathcal{D}_{X_j}} \int_{\mathcal{D}_{\boldsymbol{X}}} \left(f(\boldsymbol{x}) - f(z_j, \boldsymbol{x}_{\sim\{j\}}) \right)\, \rho_{\boldsymbol{X}}(\boldsymbol{x})\, \rho_{X_j}(z_j)\, d\boldsymbol{x}\, dz_j \\
&= \frac{1}{2} \mathbb{E}_{\boldsymbol{X}, Z_j} \left[\left(f(\boldsymbol{X}) - f(Z_j, \boldsymbol{X}_{\sim\{j\}}) \right)^2 \right]
\end{aligned}
$$

Sobol' Indices: Monte Carlo Simulation

Replacing the expectations with sample average:

$$\sigma^2_{\{j\}} = \mathbb{E}_{\boldsymbol{X},\boldsymbol{Z}_{\sim\{j\}}}\left[f(\boldsymbol{X})\, f(X_j, \boldsymbol{Z}_{\sim\{j\}})\right] - \mathbb{E}^2_{\boldsymbol{X}}[f(\boldsymbol{X})]$$

$$\approx \frac{1}{N}\sum_{i=1}^{N} f(x_j^{(i)}, \boldsymbol{x}^{(i)}_{\sim\{j\}})\, f(x_j^{(i)}, \boldsymbol{z}^{(i)}_{\sim\{j\}}) - \left(\frac{1}{N}\sum_{i=1}^{N} f(\boldsymbol{x}^{(i)})\right)^2$$

$$\bar{\tau}^2_{\{j\}} = \frac{1}{2}\mathbb{E}_{\boldsymbol{X},Z_j}\left[\left(f(\boldsymbol{X}) - f(Z_j, \boldsymbol{X}_{\sim\{j\}})\right)^2\right]$$

$$\approx \frac{1}{2N}\sum_{i=1}^{N}\left(f(x_j^{(i)}, \boldsymbol{x}^{(i)}_{\sim\{j\}}) - f(z_j^{(i)}, \boldsymbol{x}^{(i)}_{\sim\{u\}})\right)^2$$

(Saltelli, 2002; Saltelli et al., 2010)

where $\{\boldsymbol{x}^{(i)}\}_{i=1}^{N}$ and $\{\boldsymbol{z}^{(i)}\}_{i=1}^{N}$ are two independent sets of sample points generated from $\boldsymbol{X}$. The sample variance for normalization can be computed using the same samples.

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Both Sobol' main-effect and total-effect indices for all m variables can be computed using $N(m+2)$ sample points, $N \sim 10^3 - 10^6$.

Outline

Polynomial Chaos Expansions

Alternatively, we can obtain the full functional ANOVA by expanding the random variable $Y = f(\boldsymbol{X})$ using orthogonal polynomial basis:

$$Y = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^m} c_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{X}), \quad \Psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) = \prod_{j=1}^{m} \psi_j^{(\alpha_j)}(x_j),$$

where:

- $\boldsymbol{\alpha}$: a multi-index indicating the degree of the polynomial basis in each dimension
- $c_{\boldsymbol{\alpha}}$: coefficients
- $\Psi_{\boldsymbol{\alpha}}(\boldsymbol{X})$: (multivariate) orthogonal polynomial basis

From orthogonalities:

$$\mathbb{E}[\Psi_{\boldsymbol{\alpha}}(\boldsymbol{X})] = 0; \quad \mathbb{E}[\Psi_{\boldsymbol{\alpha}}(\boldsymbol{X})\Psi_{\boldsymbol{\beta}}(\boldsymbol{X})] = \delta_{\boldsymbol{\alpha},\boldsymbol{\beta}}$$

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These properties satisfies all what we need from a functional ANOVA decomposition.

Classical orthogonal polynomials

- Two functions g and h are orthogonal w.r.t ρ_X iff: $\langle g, h \rangle_{\rho_X} = 0$
- Several classical orthogonal polynomials are known (orthogonality w.r.t classical probability density functions (PDFs))

Name	Symbol	ρ_X	Support	Distribution
Legendre	$P^{(p)}(x)$	$\frac{1}{2}$	$[-1, 1]$	Uniform
Hermite	$He^{(p)}(x)$	$\frac{1}{\sqrt{2\pi}} e^{-x^2/2}$	$(-\infty, \infty)$	Gaussian
Laguerre	$La_a^{(p)}(x)$	$x^a e^{-x}$	$[0, \infty)$	Gamma
Jacobi	$J_{a,b}^{(p)}(x)$	$\frac{(1-x)^\alpha (1+x)^\beta}{B(\alpha+1, \beta+1)}$	$[-1, 1]$	Beta

(Xiu and Karniadakis, 2002)

Orthonormal polynomials are created by dividing them by the square root of their norm

A.-M. Legendre

C. Hermite

E.N. Laguerre

C.G. Jacobi

Polynomial Chaos Expansions: Moments and Partial Variances

Given PCE, the moments and partial variances of f can be obtained analytically:

- **Mean**

$$\mathbb{E}[f(\boldsymbol{X})] = c_{\boldsymbol{0}}$$

- **Variance**

$$\mathbb{V}[f(\boldsymbol{X})] = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^M \setminus \{\boldsymbol{0}\}} c_{\boldsymbol{\alpha}}^2$$

- **Partial variances**

$$\sigma_{\boldsymbol{u}}^2 = \sum_{\boldsymbol{\alpha} \in A_{\boldsymbol{u}}} c_{\boldsymbol{\alpha}}^2; \quad A_{\boldsymbol{u}} = \{\boldsymbol{\alpha} \in \mathbb{N}^M \setminus \{\boldsymbol{0}\} : \alpha_{j \in \boldsymbol{u}} \neq 0, \alpha_{j \notin \boldsymbol{u}} = 0\}$$

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Moments and partial variances are combinations of the coefficients of the expansions.

Polynomial Chaos Expansions: Sobol' Indices

Sobol' indices can therefore be obtained analytically:

- **Sobol' main-effect indices**

$$\sigma^2_{\boldsymbol{u}} = \frac{\sum_{\boldsymbol{\alpha} \in A_{\{j\}}} c^2_{\boldsymbol{\alpha}}}{\mathbb{V}[f(\boldsymbol{X})]}; \quad A_{\{j\}} = \{\boldsymbol{\alpha} \in \mathbb{N}^M \setminus \{\mathbf{0}\} : \alpha_j \neq 0, \alpha_{i \neq j} = 0\}$$

- **Sobol' total-effect indices**

$$\sigma^2_{\boldsymbol{u}} = \frac{\sum_{\boldsymbol{\alpha} \in \bar{A}_{\{j\}}} c^2_{\boldsymbol{\alpha}}}{\mathbb{V}[f(\boldsymbol{X})]}; \quad \bar{A}_{\{j\}} = \{\boldsymbol{\alpha} \in \mathbb{N}^M \setminus \{\mathbf{0}\} : \alpha_j \neq 0\}$$

(Sudret, 2008)

Outline

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Summary

- Functional ANOVA is a valuable tool for the **exploratory analysis** of functions.
- Sensitivity measures, such as Sobol' indices, provide concise insights into the **importance of input variables**.
- Effective dimensions offer an even **more compact characterization** of function complexity through a single (or two) numerical value(s).
- Monte Carlo estimation and function approximations are two sides of the same coin.

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Thank you very much for your attention!

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