A new paradigm for global sensitivity analysis

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Abstract

Current theory of global sensitivity analysis, based on a nonlinear functional ANOVA decomposition of the random output, is limited in scope—for instance, the analysis is limited to the output's variance and the inputs have to be mutually independent—and leads to sensitivity indices the interpretation of which is not fully clear, especially interaction effects. Alternatively, sensitivity indices built for arbitrary user-defined importance measures have been proposed but a theory to define interactions in a systematic fashion and/or establish a decomposition of the total importance measure is still missing. It is shown that these important problems are solved all at once by adopting a new paradigm. By partitioning the inputs into those causing the change in the output and those which do not, arbitrary user-defined variability measures are identified with the outcomes of a factorial experiment at two levels, leading to all factorial effects without assuming any functional decomposition. To link various well-known sensitivity indices of the literature (Sobol indices and Shapley effects), weighted factorial effects are studied and utilized.

Keywords: interactions; main effects; Sobol indices; factorial experiment; global sensitivity analysis.

1 Introduction

Global sensitivity analysis is an important step in model checking, understanding, and calibration [29]. To do the global sensitivity analysis of a given model f, the main task is to calculate *sensitivity indices*. With each input or combination of inputs one associates a value supposed to represent how sensitive the output of the model is with respect to that input or combination of inputs. What "sensitive" means depends on the mathematical definition of the index used, but the idea is that the output is sensitive to some input if a change in the input's value leads to a change in the output's value; the bigger the change in the output's value the more sensitive.

Let $f : \mathbf{R}^d \to \mathbf{R}$ be mathematical function representing a numerical or machine learning model or algorithm, or any system that takes inputs and returns outputs. These are assumed real for simplicity and clarity. In classical global sensitivity analysis, the uncertainty about the inputs is represented by a distribution P on the input space. Since they are uncertain, the inputs are represented by a random vector $X = (X_1, \ldots, X_d)$ with distribution P; the output $f(X)$ is, therefore, a random variable with distribution $P \circ f^{-1}$.

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Current theory of global sensitivity analysis is based on a nonlinear functional ANOVA decomposition of the output [9, 28, 25], namely

$$f(X) - \mathbf{E}\, f(X) = f_1(X_1) + \cdots + f_d(X_d) + f_{12}(X_1, X_2) + \cdots ,$$

where, by construction, all the 2^{d-1} terms in the right-hand side are statistically independent. This decomposition, known as the Sobol or Sobol-Hoeffding decomposition, is attributed to Hoeffding [13] (see [35]), although it was Sobol [32] who, after rediscovering it, applied it to calculate sensitivity indices.

By independence of the terms in the right-hand side, the variance of the sum is the sum of the variances, yielding

$$\operatorname{Var} f(X) = \operatorname{Var} f_1(X_1) + \cdots + \operatorname{Var} f_d(X_d) + \operatorname{Var} f_{12}(X_1, X_2) + \cdots$$

The variance of the output has been broken into a sum of smaller variances, called the *Sobol indices*. Sobol indices associated with singletons are called *main* or *first-order effects*, and the others *interaction* or *higher-order effects*. In applications, a sensitivity analysis mainly consists of reporting estimated Sobol indices. The functional decomposition that led to these indices seems to be there solely to justify the existence of the indices themselves.

That the Sobol indices arise from the functional decomposition has limitations. First, the inputs have to be mutually independent, *de facto* excluding interesting applications [6, 16, 27]. Second, the interpretation of the higher-order Sobol indices lacks clarity, and, as a matter of fact, these are rarely studied [20]. Finally, the sensitivity analysis is necessarily restricted to the analysis of the variance, which may be insufficient to give a complete account of uncertainty [3, 7, 8, 10, 11, 31].

The problem we propose to address, therefore, runs thus: can we construct sensitivity indices such that

- any arbitrary distribution can be assumed for the inputs;
- sensitivity analysis is not restricted to the analysis of the variance and can be performed for arbitrary measures of variability;
- main and interaction effects are well-defined and interpretable;
- decompositions of the total output variability can still be obtained?

It is shown that the above issues can be solved all at once by considering a new paradigm for global sensitivity analysis. The key is to notice that sensitivity indices, because they can be seen as maps defined on the set of all subsets of the input combinations, can be identified with a factorial experiment at two levels where each input combination is a point in a factorial design and the outcome is the variability of the output given that some inputs are fixed and some are not. Main and interaction effects are then naturally defined, with no resort to any functional decomposition. Arbitrary measures of variability are permitted, as long as they satisfy three posited axioms.

The rest of the manuscript is organized as follows. The sensitivity maps are defined in Section 2. Here two large classes of sensitivity maps are given. The correspondence between sensitivity maps and factorial experiments is made in Section 3. In Section 4, factorial effects are extended to weighted factorial effects, allowing us to recover known sensitivity indices. Some properties of weighted factorial effects are derived in Section 5. It is shown in this section how decompositions of the total output variability can be obtained by choosing appropriate weights. Known sensitivity indices of the literature are recovered as examples in Section 7. A Discussion section closes the paper. All proofs are available in the Appendix.

Throughout, we shall assume that the distribution P is a probability distribution on the measurable space $(\mathbf{R}^d, \mathscr{B}^d)$, where $\mathscr{B}^d$ is the σ-field comprising the d-dimensional Borel sets. The function f is of course assumed to be Borel measurable, as shall be every function in the present manuscript. All random variables are defined on the same arbitrary probability space endowed with probability measure $\mathbf{P}$ and are assumed to have a sufficiently large number of finite moments. Recall that X has distribution P, denoted by $X \sim P$. (That is, $P = \mathbf{P} \circ X^{-1}$.) All equality statements between random variables are meant with probability one, that is, *almost surely* (a. s.).

2 Sensitivity maps

To define sensitivity maps, three axioms are posited in Section 2.1. Two general classes of sensitivity maps are given in Section 2.2.

2.1 General sensitivity maps

Let us introduce some notations. If A is some subset of $\{1, \dots, d\} =: D$ then we let X_A denote the subvector with components indexed by A. For instance if $d = 3$ and $A = \{3, 1\}$ then $X_A = (X_1, X_3)$. By convention $X_\emptyset$ is some arbitrary constant. We denote the set of all subsets of D by $\mathbf{2}^D$. We use "$\subset$" in the weak sense so that $A \subset A$. (Remember that the empty set is a subset of every set, including a subset of itself.) Singletons $\{i\}$ are sometimes simply written i.

It is a tautology to say that sensitivity of a function f to its arguments is the extent to which it depends on them. Thus if f is unsensitive to its arguments indexed by some subset A of D then, whatever the value of the other arguments, the value of f must be constant with respect to a change in the arguments in A. In other words, f is a function of its arguments in $D \setminus A$ only. This leads to Definition 1.

Definition 1. *A map $\tau : \mathbf{2}^D \to \mathbf{R}$ is a* sensitivity map *for f with respect to P if, for each $A \subset D$,*

- *(i)* $\tau(A) \geq 0$
- *(ii)* $\tau(\emptyset) = 0$
- *(iii)* $\tau(A) = 0$ *if and only if there is a map $g_A : \mathbf{R}^{|D \setminus A|} \to \mathbf{R}$ such that $X \sim P$ implies $f(X) = g(X_{D \setminus A})$ almost surely.*

Remark 1. *Without loss of generality we can take $g_A(X_{D \setminus A}) = \mathbf{E}(f(X) | X_{D \setminus A})$ in Definition 1.*

Definition 1 agrees with common sense: (i) sensitivity cannot be negative; (ii) if there are no arguments then f must be unsensitive; (iii) a function is unsensitive to some of its arguments A if it does not depend on them The phrase "for f with respect to P" in Definition 1 is important. Indeed, a map τ can be a sensitivity map for some choice of f and P but not for some other. For instance, let $f(X) = \sum_{i=1}^{d} c_i X_i$, where $X_1, \ldots, X_d$ are independent random variables with mean zero and variance one. Define $\tau(A) = \|c_A\|_2$, where c_A denotes the subvector of c with components indexed by A. If $\tau(A) = 0$ then $c_i = 0$ for all $i \in A$ and hence $f(X) = \sum_{i \notin A} c_i X_i =: g_A(X_{D\setminus A})$. Conversely, if $f(X) = \mathbf{E}(f(X)|X_{D\setminus A})$ then $\sum_{i \in A} c_i X_i = 0$ and hence $\|c_A\|_2^2 = 0$. Therefore, τ is a sensitivity map for f but it is clear that τ fails to be a sensitivity map in general. Similarly, if $f(X) = X_1^2 + X_2$; $\mathbf{P}(X_1 = -1) = \mathbf{P}(X_1 = 1) = 1/2$; $X_2 \sim \mathrm{N}(0,1)$ independent of X_1; $\tau(A) = \mathbf{E}\,\mathrm{Var}(f(X)|X_{\{1\}\cup(D\setminus A)})$, then τ is a sensitivity map for the above mentioned f and P but is not a sensitivity map with respect to $X_1 \sim \mathrm{N}(0,1)$.

In what follows we shall not impose anything on f and P and hence fix them to some arbitrary Borel measurable function and arbitrary probability distribution.

2.2 Sensitivity maps based on divergences between outputs

Definition 1 is arguably the widest possible but does not lead to any useful theory. We specialize slightly. Let $\psi : \mathbf{R}^2 \to \mathbf{R}$ be a function such that

(a) $\psi(x, y) \geq 0$,

(b) $\psi(x, y) = 0$ if and only if $x = y$,

for every $x \in \mathbf{R}$ and $y \in \mathbf{R}$. Such a function ψ is called a *divergence*. Define

$$\tau(A) = \mathbf{E}\,\psi(f(X), f(X^{\setminus A})), \tag{1}$$

where above X and $X^{\setminus A}$ are two random vectors such that $X \sim P$ and

(i) X and $X^{\setminus A}$ are independent and identically distributed conditionally on $X_{D\setminus A}$;

(ii) $X^{\setminus A}_{D\setminus A} = X_{D\setminus A}$ almost surely.

The generation of two random vectors X and $X^{\setminus A}$ obeying the two conditions above can be done as follows: first, sample X from P; then, independently of X, sample Z from the conditional law of X given $X_{D\setminus A}$ and define $X^{\setminus A}$ by putting $X^{\setminus A}_A = Z$ and $X^{\setminus A}_{D\setminus A} = X_{D\setminus A}$. If P is a product measure, that is, if the components of X are mutually independent, then we can sample $X' \sim P$ independently of X and put $X^{\setminus A}_A = X'_A$.

Proposition 1. *The map τ defined in (1) is a sensitivity map.*

The quantity (1) is interpreted as *the expected variability of the output caused by a change in the inputs indexed by A while the others are fixed to some random values.* For instance if $d = 3$ and $A = \{1, 3\}$ then $\tau(\{1, 3\}) = \mathbf{E}\,\psi(f(X_1, X_2, X_3), f(X_1^{\setminus\{1,3\}}, X_2, X_3^{\setminus\{1,3\}}))$. We see that the first and third inputs fluctuate, while the second input is randomly fixed.

Variability is represented by the divergence function. For instance if $\psi(x, y) = (x - y)^2/2$ then "variability" literally means "variance", see Example 1.

Example 1. *Put* $\psi(x,y) = (x-y)^2/2$*. Then* $\tau(A) = \mathbf{E}(f(X) - f(X^{\setminus A}))^2/2 = \mathbf{E}\,\mathbf{E}(f(X) - f(X^{\setminus A}))^2/2|X_{D\setminus A})$*. Conditionally on* $X_{D\setminus A}$*, the random variables* $f(X)$ *and* $f(X^{\setminus A})$ *are independent and identically distributed, and hence* $\mathbf{E}(f(X) - f(X^{\setminus A}))^2/2|X_{D\setminus A}) = \mathrm{Var}(f(X)|X_{D\setminus A})$*.*

If ψ is furthermore a *contrast* function [10] then there is another method for constructing sensitivity maps. A contrast function $\psi : \mathbf{R}^2 \to \mathbf{R}$ with respect to the conditional probability $\mathbf{P}(f(X) \in \cdot|X_{D\setminus A})$ and some set $\Theta \subset \mathbf{R}$ satisfies, by definition,

$$\min_{\theta\in\Theta} \mathbf{E}(\psi(f(X),\theta)|X_{D\setminus A}) = \mathbf{E}(\psi(f(X), g(X_{D\setminus A}))|X_{D\setminus A})$$

for some almost surely unique $g(X_{D\setminus A}) \in \Theta$. Let us assume that Θ contains the support of the law of $f(X)$ and define

$$\widetilde{\tau}(A) := \mathbf{E}\min_{\theta\in\Theta} \mathbf{E}(\psi(f(X),\theta)|X_{D\setminus A}) = \mathbf{E}\,\psi(f(X), g(X_{D\setminus A})). \tag{2}$$

Then it is immediate to see that $\tilde{\tau}$ is a sensitivity map such that $\tilde{\tau}(A) \leq \tau(A)$.

Some possible choices of contrast functions are given in Table 1, drawn from [10]. To construct sensitivity maps from this table and formula (2), replace Y by $f(X)$ and replace the expectation by the conditional expectation given $X_{D\setminus A}$. For instance with the median, we get $\widetilde{\tau}(A) = \mathbf{E}\min_\theta \mathbf{E}(|f(X)-\theta||X_{D\setminus A})$. If $g(t) = t^2/2$ then formulas (1) and (2) coincide [10].

Remark 2. *The definition given in [10] encompasses contrast functions that are not divergences. One such an example is given by* $\psi(y,\theta) = |\mathbf{1}_{\{y\geq t\}} - \theta|^2$*, which corresponds to the probability of exceeding* t*, that is,* $\arg\min_\theta \mathbf{E}\,|\mathbf{1}_{\{Y\geq t\}} - \theta|^2 = \mathbf{P}(Y \geq t)$*. We deliberately avoided these cases because they do not lead to sensitivity maps in general.*

$\psi(y,\theta)$	$\arg\min_\theta \mathbf{E}\,\psi(Y,\theta)$
$(y-\theta)^2$	mean
$\|y-\theta\|$	median
$(y-\theta)(\alpha - \mathbf{1}_{\{y\leq\theta\}})$	quantile of level α

Table 1: Some contrast functions given in [10].

3 An implicit factorial experiment

A *factorial experiment* is a map that associates *outcomes* with *factor levels*. For instance if there are d factors each with two levels then there are 2^d possible combinations of factor levels and hence 2^d possible outcomes. The set of all possible combinations is called a *factorial design* and its cardinal is called the *size* of the factorial experiment. The mathematical study of factorial experiments started between the two world wars with the objective of improving crop yields with various fertilizers and studying their effects by taking into account possible interactions between them [37]. See [2, 4, 21, 22, 36] for more about factorial experiments.

The formula in the right-hand side of (1) induces a partition of the inputs. Indeed, the two arguments $f(X)$ and $f(X^{\setminus A})$ of the divergence ψ differ because the input vectors X and $X^{\setminus A}$ differ, and, because of (ii), this difference cannot be attributed to the inputs indexed by $D \setminus A$. Thus D is partitioned into A and $D \setminus A$, that is, the inputs are partitioned into those that are allowed to change and those that are not. The former category is called the category of *fluctuating* inputs. This is because, conditionally on $X_{D\setminus A}$, the input vectors X and $X^{\setminus A}$ can be written, up to a permutation of their components, $(X_A, X_{D\setminus A})$ and $(X'_A, X_{D\setminus A})$, where X_A and X'_A are independent and identically distributed (still conditionally on $X_{D\setminus A}$); in other words, the inputs indexed by A fluctuate while those indexed by $D\setminus A$ are kept fixed. By a similar reasoning, formula (2) also induces a partition of the inputs.

We can identify the sensitivity map τ in (1) with a factorial experiment at two levels of size 2^d. The values of the sensitivity map are the outcomes, the subsets of D are the treatment combinations or runs, and the presence or absence of the inputs in the set of fluctuating variables are the factors. An example with $d = 3$ is given in Table 2.

Does the input fluctuate?			
X_1	X_2	X_3	outcome
0	0	0	$\tau(\emptyset)$
0	0	1	$\tau(\{3\})$
0	1	0	$\tau(\{2\})$
0	1	1	$\tau(\{2,3\})$
1	0	0	$\tau(\{1\})$
1	0	1	$\tau(\{1,3\})$
1	1	0	$\tau(\{1,2\})$
1	1	1	$\tau(\{1,2,3\})$

Table 2: The factorial experiment induced by the sensitivity map τ.

Identifying a sensitivity map with a factorial experiment allows us to define main and interaction effects, collectively refered to as *factorial effects*, in a natural way. In experimental design, main effects are defined as averages of differences of outcomes, second order interaction effects as averages of differences of differences of outcomes, and so on. More precisely, the *main effect* of input i is given by

$$\frac{1}{2^{d-1}} \sum_{A\subset D\setminus i} \tau(A \cup \{i\}) - \tau(A) \tag{3}$$

For instance, the main effect of the second input in Table 2 is given by the mean of the terms

$$\tau(\{2\}), \qquad \tau(\{2,3\})-\tau(\{3\}), \qquad \tau(\{1,2\})-\tau(\{1\}), \qquad \tau(\{1,2,3\})-\tau(\{1,3\}).$$

All these terms measure the effect of the second input and hence it is natural to average them.

The same goes for interactions. The *interaction effect* between i and j is defined as

$$\mathrm{I}(\{i,j\}) = \frac{1}{2^{d-2}} \sum_{A\subset D\setminus\{i,j\}} (\tau(\{i,j\}\cup A) - \tau(\{j\}\cup A)) - (\tau(\{i\}\cup A) - \tau(A)). \tag{4}$$

Above input j is added to the set of fluctuating inputs to see if it affects the effect of input i. Note that the interaction effect is symmetric and hence the notation $I(\{i,j\})$ is unambiguous.

Interactions of higher-order can be defined in a similar fashion, recursively. Let $\mathbf{T}$ denote the set of all real maps on $\mathbf{2}^D$. If $B \in \mathbf{2}^D$ then define the operator $\Delta^B : \mathbf{T} \to \mathbf{T}$ by $(\Delta^B \tau)(A) = \tau(A \cup B) - \tau(A)$. In particular, $\Delta^B \tau(A) = \tau(B|A)$ if $A \cap B = \emptyset$. With the above notation, it holds that the main effect of j is $\sum_{A \subset D \setminus j} \Delta^j \tau(A)$ and the interaction between i and j is $\sum_{A \subset D \setminus \{i,j\}} \Delta^i \Delta^j \tau(A)$. Since $\Delta^B \tau \in \mathbf{T}$ for every $B \subset D$, we can compose the operators as many times as we please. For instance, if $B_1 \subset D$ and $B_2 \subset D$ then $\Delta^{B_2} \Delta^{B_1} \tau(A) = \Delta^{B_2}(\Delta^{B_1}\tau)(A) = \tau(A \cup B_2 \cup B_1) - \tau(A \cup B_2) - \tau(A \cup B_1) + \tau(A)$. Note the symmetry in B_1 and B_2. In general, we have the following formula.

Lemma 1. *If* $\{i_1, \dots, i_n\} =: B \subset D \setminus A$ *then*

$$\Delta^{i_n} \cdots \Delta^{i_1} \tau(A) = \sum_{A \subset C \subset A \cup B} (-1)^{|B| - |C \setminus A|} \tau(C) =: \Delta_B \tau(A). \tag{5}$$

The above formula is similar to [15]. Note that the operator $\Delta^{i_n} \cdots \Delta^{i_1}$ is symmetric and hence the notation Δ_B is unambiguous.

The factorial effects can now be defined as

$$I(B) := \frac{1}{2^{d-|B|}} \sum_{A \subset D \setminus B} \Delta_B \tau(A). \tag{6}$$

Setting $B = \{i\}$ and $B = \{i,j\}$ above yield (3) and (4), respectively. If we set $B = \{i,j,k\}$ then we get the difference between, on the one hand, the interaction between i and j in the presence of k, and, on the other hand, the interaction between i and j in the absence of k. That is, we get the average of the quantities

$$(\tau(\{i,k\}|\{j,k\} \cup A) - \tau(\{i,k\}|A \cup \{k\})) - (\tau(\{i\}|\{j\} \cup A) - \tau(\{i\}|A))$$

over all $A \subset D \setminus \{i,j,k\}$, where above $\tau(B|A) := \tau(A \cup B) - \tau(A)$. It is important to note that the factorial effects can be expressed with the alternative formula

$$I(B) = \sum_{A \subset D} (-1)^{|B \setminus A|} \tau(A) \frac{1}{2^{d-|B|}}.$$

This formula is implicit in, e.g. [36]. It is a particular case of a result given in the next section.

4 Weighted factorial effects

Here we extend factorial effects by taking weighted averages. General formulas are given in Section 4.1. Examples of weights are given in Section 4.2.

4.1 General formulas

For each $B \subset D$ let $p_B : \mathbf{2}^{D \setminus B} \to \mathbf{R}$ be a weight function such that $p_B(A) \geq 0$ for all $A \subset D \setminus B$ and

$$\sum_{A \subset D \setminus B} p_B(A) = 1. \tag{7}$$

Each weight function p_B can be seen as a function on $\mathbf{2}^{D\setminus B}$ or as a function on $\mathbf{2}^D$ by imposing $p_B(A) = 0$ if $A \not\subset D \setminus B$. We shall define the *weighted factorial effect* of B as

$$I(B) = \sum_{A\subset D\setminus B} p_B(A)\Delta_B\tau(A), \tag{8}$$

where $\Delta_B\tau(A)$ was given in (5). Comparing with (6), we see that weighted factorial effects are obtained by multiplying $\Delta_B\tau(A)$ with $p_B(A)$. For instance, if

$$p_B(A) = \begin{cases} 1/|\mathbf{2}^{|D\setminus B|}| = 1/2^{d-|B|} & \text{if } A \subset D \setminus B \\ 0 & \text{otherwise,} \end{cases} \tag{9}$$

then (8) coincides with standard factorial effects (6). Note that $I(\emptyset) = \sum_{A\subset D} p_\emptyset(A)\tau(A)$ is not zero in general.

Similarly to factorial effects, weighted factorial effects can be expressed as a linear combination of the values of the sensitivity map.

Proposition 2. *For every $B \subset D$, it holds*

$$I(B) = \sum_{A\subset D} (-1)^{|B\setminus A|} p_B(A \setminus B)\tau(A). \tag{10}$$

Standard factorial effects correspond to $p_B(A \setminus B) = 1/2^{d-|B|}$ for all $A \subset D$ and $B \subset D$.

4.2 Examples of weights

Three examples of families of weights are given below.

Möbius transform

Let

$$p_B(A \setminus B) = \begin{cases} 1 & \text{if } A \subset B \\ 0 & \text{otherwise,} \end{cases} \qquad p_B(A) = \begin{cases} 1 & \text{if } A = \emptyset \\ 0 & \text{otherwise.} \end{cases} \tag{11}$$

This family of weights satisfies (7). It yields

$$I(B) = \sum_{A\subset B} (-1)^{|B\setminus A|}\tau(A) \qquad \text{(for every } B \subset D). \tag{12}$$

The map I that with each $B \subset D$ associates $I(B)$ above is known as the *Möbius transform* of the map $\tau : \mathbf{2}^D \to \mathbf{R}$, see, e.g. [12]. An important property of the Möbius transform is that (12) is equivalent to

$$\tau(B) = \sum_{A\subset B} I(A) \qquad \text{(for every } B \subset D).$$

See, e.g. [1, 26, 34]. Two maps τ and I as above are sometimes called the Möbius inverses of one another [5].

Shapley value

Let

$$p_B(A) = \begin{cases} \frac{1}{(|D\setminus B|+1)\binom{|D\setminus B|}{|A|}} & \text{if } A \subset D \setminus B \\ 0 & \text{otherwise,} \end{cases} \tag{13}$$

$$p_B(A \setminus B) = \frac{1}{(|D \setminus B| + 1)\binom{|D\setminus B|}{|A\setminus B|}} \qquad \text{(for every } A \subset D \text{ and } B \subset D).$$

The weights (13) satisfy the condition (7) and yield

$$I(B) = \sum_{A\subset D\setminus B} \frac{1}{(|D \setminus B| + 1)\binom{|D\setminus B|}{|A|}} \Delta_B \tau(A).$$

In the particular case $B = \{j\}$, we have

$$I(\{j\}) = \frac{1}{d} \sum_{A\subset D\setminus\{j\}} \frac{1}{\binom{d-1}{|A|}} (\tau(A \cup \{j\}) - \tau(A)).$$

The map $I : D \to \mathbf{R}$ which with each $j \in D$ associates $I(\{j\})$ as above is known as the *Shapley value* corresponding to the map τ. The Shapley value appears in cooperative game theory for redistributing an overall payoff earned by a finite set of cooperative players [19, 30]. In cooperative game theory the set D is called the grand coalition, the map τ the characteristic function of the game; each $A \subset D$ is called a coalition. The value I($\{j\}$) is interpreted as the "fair" share attributed to player j and $\tau(A)$ the payoff of the coalition A. The map $\tau : \mathbf{2}^D \to \mathbf{R}$ is assumed to satisfy $0 = \tau(\emptyset)$. One property is that

$$\sum_{i=1}^{d} I(\{i\}) = \tau(D),$$

that is, the sum of the individual payoffs is equal to the overall payoff.

5 Decomposing the total output variability

The total output variability $\tau(D)$ can be decomposed using appropriate choices of weight families. Two decompositions are recovered: a Sobol-like decomposition (or Möbius-like, recall Section 4.2) decomposition and a Shapley-like decomposition.

5.1 Sobol-like decomposition

A feature of classical global sensitivity analysis, inherited from the Sobol-Hoeffding functional decomposition, is the ability to decompose the total output variance into a sum of main and interaction effects. We seek conditions on the weights to get a similar decomposition of the total output variability. That is, we seek weights such that

$$\sum_{B\subset A} I(B) = \tau(A) \qquad \text{(for every } A \subset D). \tag{14}$$

By the Möbius inversion formulas given in Section 4.2, we see that this problem is equivalent to finding the Möbius transform of τ. In other words, decomposing the total output variability amounts to finding its Möbius transform.

Proposition 3. *If $I(B)$ is the weighted factorial effect (8) then there is a unique set of weights such that* (14) *holds for all maps $\tau : \mathbf{2}^D \to \mathbf{R}$ with $\tau(\emptyset) = 0$. These weights are those given in* (11).

5.2 Shapley-like decomposition

We are now interested in characterising the weight families such that, for every sensitivity map τ,

$$\sum_{i=1}^{d} I(\{i\}) = \tau(D) \qquad \text{(for every sensitivity map } \tau). \tag{15}$$

A necessary and sufficient condition is given below.

Proposition 4. *If $I(B)$ is the weighted factorial effect (8) then a necessary and sufficient condition for (15) to hold is that*

$$\left\{ \begin{array}{rcl} \sum_{i=1}^{d} p_i(\emptyset) & = & 1 \\ \sum_{i=1}^{d} (-1)^{1-|A\cap\{i\}|} p_i(A \setminus \{i\}) & = & 0 \textit{ for every } A \in \mathbf{2}^D \setminus \{\emptyset \cup D\} \\ \sum_{i=1}^{d} p_i(D \setminus i) & = & 1. \end{array} \right. \tag{16}$$

An example of weight family that satisfies (16) is of course given by (13), since Shapley effects satisfy (15), see Section 4.2. But there are more than one family that satisfiy (16). See Example 2.

Example 2. *Let $d = 3$. Let the weights*

$$\begin{pmatrix} p_{\{1\}}(\emptyset \setminus \{1\}) & p_{\{2\}}(\emptyset \setminus \{2\}) & p_{\{3\}}(\emptyset \setminus \{3\}) \\ p_{\{1\}}(\{3\} \setminus \{1\}) & p_{\{2\}}(\{3\} \setminus \{2\}) & p_{\{3\}}(\{3\} \setminus \{3\}) \\ p_{\{1\}}(\{2\} \setminus \{1\}) & p_{\{2\}}(\{2\} \setminus \{2\}) & p_{\{3\}}(\{2\} \setminus \{3\}) \\ p_{\{1\}}(\{2,3\} \setminus \{1\}) & p_{\{2\}}(\{2,3\} \setminus \{2\}) & p_{\{3\}}(\{2,3\} \setminus \{3\}) \\ p_{\{1\}}(\{1\} \setminus \{1\}) & p_{\{2\}}(\{1\} \setminus \{2\}) & p_{\{3\}}(\{1\} \setminus \{3\}) \\ p_{\{1\}}(\{1,3\} \setminus \{1\}) & p_{\{2\}}(\{1,3\} \setminus \{2\}) & p_{\{3\}}(\{1,3\} \setminus \{3\}) \\ p_{\{1\}}(\{1,2\} \setminus \{1\}) & p_{\{2\}}(\{1,2\} \setminus \{2\}) & p_{\{3\}}(\{1,2\} \setminus \{3\}) \\ p_{\{1\}}(\{1,2,3\} \setminus \{1\}) & p_{\{2\}}(\{1,2,3\} \setminus \{2\}) & p_{\{3\}}(\{1,2,3\} \setminus \{3\}) \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

These weights satisfy (7) and (16) but differ from those given in (13).

6 The dual sensitivity map

Remember from Section 3 that the set of inputs is partitioned into a set of fluctuating variables A and a set of fixed variables $D \setminus A$. Suppose we add a set of inputs B to the set of fluctuating inputs A. The set of fluctuating inputs is now $A \cup B$, and we can measure the effect of adding more inputs by

$$\tau(B|A) := \tau(B \cup A) - \tau(A).$$

Above it is assumed that A and B are disjoint. We call this effect the *conditional effect of B given A*, or *the effect of B in the presence of A*.

Remark 3. *Conditional effects can be defined for arbitrary subsets A and B (not necessarily disjoint) through $\tau(A|B) = \tau((A \cap B^{\mathrm{c}}) \cup B) - \tau(B)$.*

Remark 4. *Since there is a one-to-one correspondence between conditional and unconditional effects, we could have well defined conditional effects* before *unconditional effects.*

Observe that $\tau(A)$, since it is equal to $\tau(A \cup \emptyset) - \tau(\emptyset)$, is in fact the conditional effect of A given no inputs, that is $\tau(A|\emptyset)$, *the effect of letting the inputs in A fluctuate while all where fixed*. Let

$$\tau^*(A) := \tau(D) - \tau(D \setminus A).$$

The map τ^* is called the *dual* of τ and $\tau(A)$ is interpreted as *the effect of fixing the inputs in A while all were fluctuating* (compare to preceding interpretation). The following properties hold:

(i) $\tau^*(A) \leq \tau^*(D)$ for all $A \subset D$, with equality if and only if f depends on its arguments indexed by A only—that is, if and only if $f(X) = \mathbf{E}(f(X)|X_A)$—, in which case $\tau^*(B) = \tau^*(D)$ for every B such that $A \subset B$;

(ii) $\tau^*(A) < 0$ if and only if $\tau(D \setminus A) > \tau(D)$;

(iii) $\tau^{**}(A) = \tau(A)$, that is, the dual of the dual of τ is τ itself.

Weighted factorial effects can be defined from τ^* as they were defined from τ. Denote by $I^*(B)$ the weighted factorial effect of B corresponding to τ^*, that is, by substituting τ^* for τ in (8). It is then natural to ask whether I^* and I are *self-dual*, that is, $I^*(B) = I(B)$.

Proposition 5. *If $|B|$ is odd, then a necessary and sufficient condition for $I(B)$ to be self-dual for every sensitivity map τ is that*

$$p_B(A \setminus B) = p_B(D \setminus (A \cup B))$$

for every $A \subset D$, $A \neq \emptyset$.

Corollary 1. *Weighted factorial effects $I(B)$ with $|B|$ odd and weights given by (9) or (13) are self-dual.*

7 Examples

Two well-known sensitivity indices of the literature are recovered.

7.1 Sobol indices

As seen in the Introduction, the Sobol indices are given by $\operatorname{Var} f_B(X_B) =: \operatorname{Sob}(B)$, $B \subset D$, where the random variables $f_B(X_B)$ are the components of the functional Sobol-Hoeffding decomposition. To express Sobol indices with sensitivity maps, the reasoning runs in three points. First, remember that it holds $\sum_{B\subset D} \operatorname{Sob}(B) = \operatorname{Var} f(X)$. Second, it is well-known that, if $B = \{j\}$ is a singleton then $f_j(X_j) = \mathbf{E}(f(X)|X_j)$. Finally, we know from Example 1 that if $\psi(x, y) = (x - y)^2/2$ then $\tau(A) = \mathbf{E}\operatorname{Var}(f(X)|X_{D\setminus A})$. Hence, remembering that $\tau^*(A) = \tau(D) - \tau(D \setminus A)$, we get

$$\sum_{B\subset D} \operatorname{Sob}(B) = \tau(D) = \tau^*(D), \qquad \operatorname{Sob}\{j\} = \tau^*\{j\}.$$

This suggests that Sob, the map that with each B associates the Sobol index of B, might be the Möbius transform of the dual of τ. This is indeed the case [17, 20]. In summary, the Sobol indices are obtained from (1) or from (2) by taking $\psi(x, y) = (x-y)^2/2$ and $p_B(A) = \mathbf{1}_{\{A=\emptyset\}}$. As a final comment, let us note that, in this case, the quantities $\tau^*(A)$ and $\tau(A)$ are known as the *closed Sobol index* and the *total Sobol index* of A, respectively [14, 25].

7.2 Shapley effects

It has been proposed that the problem of assessing the importance of inputs in both global sensitivity analysis and machine learning was akin to the problem of distributing an overall payoff to players in cooperative game theory [18, 24]. If this comparison is endorsed then it is natural to use the Shapley value (see Section 4.2) as a measure of input importance. To specify a Shapley value we need to specify the characteristic function from which it arises. In uncertainty quantification, it has been proposed

$$\tau(A) = \mathbf{E}\operatorname{Var}(f(X)|X_{D\setminus A}) \quad \text{and} \quad \tau^*(A) = \operatorname{Var}\mathbf{E}(f(X)|X_A),$$

leading to the so-called *Shapley effects* [24, 33]. By self-duality, both choices above lead to the same Shapley effect. (See [23, 33]; see also Proposition 5.) We have already seen that τ and τ^* above can be obtained with the divergence $\psi(x, y) = (x - y)^2/2$ and that Shapley values can be obtained with the weight family (13). Thus the Shapley effect is an example of weighted factorial effects.

8 Discussion

A new paradigm for global sensitivity analysis has been proposed. In this paradigm, we do not rely on the Sobol-Hoeffding decomposition to define main and interaction effects anymore, but instead use ideas and concepts of factorial experiments, in which the study of main and interaction effects has been a topic of interest for a long time [37].

In the paradigm proposed, global sensitivity analysis consists of the following key points:

1. we choose a divergence function ψ and build a sensitivity map τ;

2. we define the main effect of some given input, say $\{j\}$, by taking into account the presence/absence of the other inputs. That is, by averaging $\tau(j \cup A) - \tau(A)$ over all $A \subset D \setminus j$;

3. we multiply each $\tau(j \cup A) - \tau(A)$ by a weight $p_j(A)$;

4. we define interactions similarly.

The above approach has several direct benefits: (i) for inputs, arbitrary probability distributions can be considered; (ii) for outputs, arbitrary divergences; (iii) factorial effects are well-defined and interpretable; (iv) Sobol-like or Shapley-like decompositions can be recovered by choosing appropriate weights, if desired.

Beyond these direct benefits, the above paradigm brings a new perspective which can lead to new ideas and foster new research. For example, look at Table 3. The main effect $I(\{2\})$ is represented with three different weight families: the second column is the family of equal weights; the third and fourth columns are those corresponding to Sobol indices and Shapley effects, respectively. Observe that in the Sobol case, some conditional effects are simply ignored. This seems to be rather harsh. In the Shapley case, we may wonder why some effects have more weight than some others. What is reasonable in game theory may not necessarily be reasonable in uncertainty quantification. More natural seems to be the family of equal weights. From our new perspective it now seems paradoxical that the most natural weight family is in fact the one which did not lead to any sensitivity index known in the literature.

conditional effect	weight families		
$\tau\{2\}$	1/4	1	1/3
$\tau\{2,3\} - \tau\{3\}$	1/4	0	1/6
$\tau\{1,2\} - \tau\{1\}$	1/4	0	1/6
$\tau\{1,2,3\} - \tau\{1,3\}$	1/4	0	1/3

Table 3: Main effect of input 2 ($I(\{2\})$) in the three-dimensional factorial experiment with three possible weight families. The effect $I(\{2\})$ is obtained by multiplying, term by term, the first column by one of the last three columns—according to the chosen weight family—and adding up the numbers.

As a second example, note that one important advantage of connecting global sensitivity analysis with factorial experiments is that the methods and results of the latter becomes available to the former. This should help to address high-dimensional input spaces. Of course one can always perform some screening experiment to reduce the number of inputs, but now in addition we can consider *fractional factorial designs* to reduce the number of model runs while retaining the most effects possible. See for instance [2, 22, 36] for more about fractional factorial designs.

As a last example, note that in the present manuscript we focused on those indices that satisfy property (iii) of Definition 2, that is, an index associated with inputs A is null if and only if the function f does not depend on the inputs in A. They are (many) indices in the literature that do not satisfy this property, as for example indices based on divergences between probability distributions (rather than between scalar outputs) [3, 7, 8, 10, 11, 31]. Instead, these indices satisfy the property: "an index associated with inputs A is null if and only if X_A and $f(X)$ are independent". It is important to note that the paradigm proposed in the present manuscript applies to the latter case as well. In general it suffices to replace property (iii) of Definition 2 by any property of interest. What is important really is the correspondance between the indices and the implicit factorial experiment. Once we realize this, we also realize that factorial effects are already defined through the factorial experiment, and hence there may be no need to look for any functional Sobol-Hoeffding decomposition.

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A Proofs

Proof of Proposition 1

Suppose that $\tau(A) = 0$. Then it holds (almost surely, as implicitly understood throughout) $f(X) = f(X^{\setminus A})$. Taking expectations conditionally on X in both sides, we get

$$\begin{aligned} f(X) &= \mathbf{E}(f(X^{\setminus A})|X) \\ &= \mathbf{E}(\mathbf{E}(f(X^{\setminus A})|X, X_{D\setminus A})|X) \\ &= \mathbf{E}(\mathbf{E}(f(X^{\setminus A})|X_{D\setminus A})|X) \\ &= \mathbf{E}(f(X^{\setminus A})|X_{D\setminus A}) \end{aligned}$$

and the first part of the equivalence is proved. Suppose that $f(X) = \mathbf{E}(f(X)|X_{D\setminus A})$. Then

$$\begin{aligned} f(X) &= \mathbf{E}(f(X)|X_{D\setminus A}) \\ &= \mathbf{E}(f(X^{\setminus A})|X_{D\setminus A}) \\ &= \mathbf{E}(f(X^{\setminus A})|X^{\setminus A}_{D\setminus A}) \\ &= f(X^{\setminus A}). \end{aligned}$$

The second part is proved. The proof is complete.

Proof of Lemma 1

Choose $A \subset D$. The proof is by mathematical induction. Fix $n = 1$. It is clear that $\Delta^{i_1}\tau(A) = \Delta_{\{i_1\}}\tau(A)$ for every $i_1 \in D \setminus A$. Now let us assume that $\Delta^{i_n} \cdots \Delta^{i_1}\tau(A) = \Delta_{\{i_1,\dots,i_n\}}\tau(A)$ holds for some fixed n and for all $\{i_1, \dots, i_n\} \cap A = \emptyset$. Choose $\{i_1, \dots, i_{n+1}\} \in D \setminus A$ and put $B_n = \{i_1, \dots, i_n\}$ and $B_{n+1} = B_n \cup i_{n+1}$. We have

$$\begin{aligned}
&\Delta^{i_{n+1}} \cdots \Delta^{i_1}\tau(A) \\
&= \Delta^{i_{n+1}}\Delta_{B_n}\tau(A) \\
&= \Delta_{B_n}\tau(A \cup i_{n+1}) - \Delta_{B_n}\tau(A) \\
&= \sum_{(A\cup i_{n+1})\subset C\subset A\cup B_{n+1}} (-1)^{n-|C\setminus(A\cup i_{n+1})|}\tau(C) - \sum_{A\subset C\subset A\cup B_n} (-1)^{n-|C\setminus A|}\tau(C) \\
&= \sum_{A\subset C\subset A\cup B_{n+1}} \tau(C)\left((-1)^{n-|C\setminus(A\cup i_{n+1})|}\mathbf{1}_{\{i_{n+1}\in C\}} - (-1)^{n-|C\setminus A|}\mathbf{1}_{\{i_{n+1}\notin C\}}\right) \\
&= \sum_{A\subset C\subset A\cup B_{n+1}} \tau(C)(-1)^{n-|C|+|A|+1}\left(\mathbf{1}_{\{i_{n+1}\in C\}} + \mathbf{1}_{\{i_{n+1}\notin C\}}\right).
\end{aligned}$$

The proof is complete.

Proof of Proposition 2

The equality is correct for $B = \emptyset$. Suppose $B \neq \emptyset$. Plugging (5) into (8), we have

$$I(B) = \sum_{A\subset D\setminus B} \sum_{A\subset C\subset A\cup B} (-1)^{|B|-|C\setminus A|}\tau(C)p_B(A). \tag{17}$$

Clearly, for each $A' \subset D$, the term $\tau(A')$ appears exactly one time in the sum. Furthermore, if we denote $B = \{i_1, \dots, i_n\}$ then D can be partitioned into subsets $\{A : A \cap B = \emptyset\}$, $\{A : A \cap B = i_1\}$, ..., $\{A : A \cap B = B\}$. It then clear that (17) equals

$$\sum_{k=0}^{n} \sum_{A:|A\cap B|=k} (-1)^{n-k} p_B(A \setminus B)\tau(A).$$

The proof is complete.

Proof of Proposition 3

If we plug (11) into (8) then we get (12) and hence (14) by Möbius inversion. Now we shall show that (11) is the only choice that guarantees the correctness of (14) for every map τ. Since it is equivalent to (12), it is clear that (14) implies $I(\emptyset) = 0$. But then $\sum_{A\subset D} p_\emptyset(A)\tau(A) = 0$ by Proposition 2, which means that $p_\emptyset(A)$ is null unless $A = \emptyset$. Now, Combining (10) and (12),

$$\sum_{A\subset B} (-1)^{|B\setminus A|}\tau(A) = \sum_{A\subset D} (-1)^{|B\setminus A|} p_B(A \setminus B)\tau(A)(\text{ for all } B \neq \emptyset).$$

Since this equality must be true for every map $\tau : \mathbf{2}^D \to [0, \infty)$ with $\tau(\emptyset) = 0$, we have that

$$\mathbf{1}_{\{A\subset B\}} = p_B(A \setminus B)$$

for every $A \subset D$, $A \neq \emptyset$. This implies that $p_B(A) = \mathbf{1}_{\{A \cup B \subset B\}} = \mathbf{1}_{\{A=\emptyset\}}$ for all $A \subset D \setminus B$. The proof is complete.

Proof of Proposition 4

Put $l(A) = \sum_{i=1}^{d} (-1)^{|i \setminus A|} p_i(A \setminus i)$. Taking $B = \{i\}$ in (10), we have

$$\sum_{i=1}^{d} I(\{i\}) = \sum_{A \subset D} \tau(A) l(A).$$

Since it is required that the equality (15) be true for every τ, we have that $l(A)$ must be zero for every subset A which is not the empty set or D. If $A = D$ then $l(D)$ must be one. Hence, since $\sum_{A \subset D} l(A) = 0$, we have that $l(\emptyset)$ must be minus one. The proof is complete.

Proof of Proposition 5

Put $l(A, B) = (-1)^{|B \setminus A|} p_B(A \setminus B)$ so that $I^*(B) = \sum_{A \subset D} l(A, B)\tau^*(A)$. Since $\sum_{A \subset D} l(A, B) = 0$, it holds

$$\begin{aligned} I^*(B) &= -\sum_{A} l(A, B)\tau(D \setminus A) \\ &= -\sum_{A} l(D \setminus A, B)\tau(A) \\ &= \sum_{A} (-1)^{|A \cap B|+1} p_B(D \setminus (A \cup B))\tau(A). \end{aligned}$$

The equality $I(B) = I^*(B)$ is then equivalent to

$$\sum_{A} \tau(A) \Big((-1)^{|B \setminus A|} p_B(A \setminus B) - (-1)^{|A \cap B|+1} p_B(D \setminus (A \cup B)) \Big) = 0.$$

If $|B|$ is odd, it holds that $|B \setminus A|$ is even if and only if $|A \cap B| + 1$ is even, and hence $(-1)^{|B \setminus A|} p_B(A \setminus B)$ and $(-1)^{|A \cap B|+1} p_B(D \setminus (A \cup B))$ are always of the same sign. The claim follows because the equality must hold true for every map τ with $\tau(\emptyset) = 0$.