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Abstract

Performing (variance-based) global sensitivity analysis (GSA) with dependent inputs has recently benefited from cooperative game theory concepts, leading to meaningful sensitivity indices suitable with dependent inputs. The "Shapley effects", i.e., the Shapley values transposed to variance-based GSA problems, are an example of such indices. However, these indices exhibit a particular behavior that can be undesirable: an exogenous input (i.e., which is not explicitly included in the structural equations of the model) can be associated with a strictly positive index when it is correlated to endogenous inputs. This paper investigates using a different allocation, called the "proportional values" for GSA purposes. First, an extension of this allocation is proposed to make it suitable for variance-based GSA. A novel GSA index is then defined: the "proportional marginal effect" (PME). The notion of exogeneity is formally defined in the context of variance-based GSA. It is shown that the PMEs are more discriminant than the Shapley values and allow the distinction of exogenous variables, even when they are correlated to endogenous inputs. Moreover, their behavior is compared to the Shapley effects on analytical toy cases and more realistic use cases.

Keywords: Cooperative game theory, Dependence, Proportional values, Sobol' indices, Shapley effects.

1. Introduction

When using phenomenological numerical models in science and engineering, the uncertainty quantification (UQ) process allows one to consider and better quantify the various sources of uncertainties, most often using probabilistic modeling [18]. Global sensitivity analysis (GSA) is a crucial step of this process, aiming to understand the effects of each uncertain model input (or set of inputs) on the quantity of interest related to the output variable of interest obtained from the numerical model [41, 27]. From a practical viewpoint, GSA aims at investigating four primary settings [10]: (i.) model exploration, i.e., investigating the input-output relationship; (ii.) factor fixing, i.e., identifying non-influential inputs; (iii.) factor prioritization, i.e., quantifying the most important inputs using quantitative importance measures; (iv.) robustness analysis, i.e., quantifying the sensitivity of the quantity of interest with respect to probabilistic model uncertainty of the input distributions. The present paper focuses on the first three settings.

Among a large panel of GSA indices, the variance-based sensitivity measures, also called "Sobol' indices" [43], are derived from the functional analysis of variance (FANOVA) decomposition [11] between all the independent inputs. Thus, these indices provide interpretable answers to the previously mentioned GSA settings. Let $Y = G(X)$ denotes the input-output relationship under study, with $G(\cdot) : \mathbb{R}^d \longrightarrow \mathbb{R}$ a deterministic (often black-box) numerical model, Y a scalar output and $X = (X_1, \ldots, X_d)$ a vector of d scalar inputs. Moreover, let $\mathcal{P}(D)$ the set of all subsets of $D = \{1, \ldots, d\}$. For every

subset of input $X_A = (X_i)_{i \in A}$, $A \in \mathcal{P}(D)$, the Sobol' indices are defined as follows:

$$S_A = \frac{\sum_{B \subseteq A} (-1)^{|A|-|B|} \mathbb{V}\left(\mathbb{E}\left[G(X)|X_B\right]\right)}{\mathbb{V}\left(G(X)\right)} \tag{1}$$

where $|\cdot|$ denotes the number of elements in a subset. For mutually independent inputs, the FANOVA decomposition leads to a nonnegative allocation of shares of the output's variance (i.e., S_A) to every subset of inputs $A \in \mathcal{P}(D)$. Since they also sum to one, they can be interpreted as percentages of the output variance. Hence, Sobol' indices can determine which inputs of a numerical model contribute the most to the output's variability or, on the contrary, identify the ones that are not influential and possibly which inputs interact. Therefore, Sobol' indices are particularly relevant for factor fixing and prioritization (settings ii. and iii.).

However, in many applications, some inputs may have a statistical dependence structure, either initially imposed in their probabilistic modeling [31] or induced by physical constraints upon the input or the output space [30, 33]. In these cases, estimating and interpreting Sobol' indices is not trivial, as shown by many different analyses and interpretations proposed in the past (see [26] or [10] for an overview of this topic). In order to circumvent this issue, [36] proposed a new approach based on the "Shapley value" [42], an allocation developed in cooperative game theory and powerfully used in economic modeling. It distributes gains and costs to several players working in a coalition in an egalitarian way. Therefore, based on Shapley values and Sobol' indices, [36] proposed the so-called "Shapley effects" as new GSA indices in the context of dependent inputs. The underlying idea is to compute, similarly to a game involving coalitions of players, the value assigned to a coalition of inputs X_A as their explanatory power towards the output's variance. This value corresponds to the so-called "closed Sobol' indices" defined as:

$$S_A^{\text{clos}} = \frac{\mathbb{V}\left(\mathbb{E}\left[G(X)|X_A\right]\right)}{\mathbb{V}\left(G(X)\right)}. \tag{2}$$

In the GSA context, the two main properties and advantages of the Shapley effects are the following: firstly, they are nonnegative; secondly, their sum is equal to one, even for dependent inputs [37, 26]. These two properties correspond to the two main desirability criteria for importance measures of linear regression models as reviewed in [19].

In [26], it is claimed that the Shapley effects are relevant for the factor fixing setting since an effect close to zero means that the input has no significant contribution to the variance of the output. However, another phenomenon, observed by [26] and known as "Shapley's joke" [23], shows that the Shapley effects may not be suitable for factor fixing in certain situations: an exogenous variable (i.e., which is not explicitly included in the structural equations of the model) can receive a non-zero share of the output variance whenever it is sufficiently correlated with endogenous inputs. Note that other GSA techniques dedicated to screening [10, 3], such as one-at-a-time (OAT) design or derivative-based global sensitivity measures [29], can detect exogenous inputs. However, such methods either require specific designs of experiments that do not respect the underlying statistical dependence, or do not have theoretical guarantees for exogeneity detection.

In statistical learning, if G is a linear regression model, an analogy can be made between Sobol' indices and the squared value of the standardized regression coefficients (SRC^2). Moreover, the Shapley effect, corresponding to the so-called "LMG measure" (named after the authors' names, Lindeman-Merenda-Gold, see [32, 6]), is none other than the Shapley values of a cooperative game aimed at allocating the determination coefficient R^2. Hence, the Shapley effects developed in GSA generalize the LMG indices for non-linear deterministic models. In a different way, an analog of LMG called *proportional marginal variance decomposition* (PMVD) has been proposed by [15] in order to respect the exclusion property: an exogenous variable should receive no share of R^2. It is based on the proportional values, which are a different allocation. These importance measures have been extensively studied in [19, 20] and illustrated more recently in [25, 8].

This paper takes inspiration from the PMVD for linear regression and the Shapley effects for GSA. A generalization of the PMVD indices to non-linear deterministic models is proposed. It leads to the

proportional marginal effect (PME), based on the proportional values [34, 15]. These indices encompass the ability to detect exogenous variables. For clarity, Table 1 provides a preliminary analogy between linear regression and GSA to emphasize the problem addressed in the present paper.

R^2 decomposition (linear regression)	$\mathbb{V}(Y)$ decomposition (GSA)
SRC^2	Sobol' indices
LMG	Shapley effects
PMVD	**PME (proposed indices)**

Table 1: Analogy between linear regression importance measures (R^2 decomposition) and variance-based GSA.

The main drawback related to the Shapley effects' estimation is their computational cost, which has been studied in several papers. Estimates can be obtained via several techniques such as Monte Carlo-based algorithms (requiring the ability to simulate according to marginal and conditional laws) [44], k-nearest neighbors [5] or Möbius inverses [38], or by using surrogate models [26, 2, 1]. However, it requires the estimation of $2^d - 1$ closed Sobol' indices, which exponentially grow with the number of inputs. The proposed indices suffer from the same problems. However, if the practitioner is committed to estimating the Shapley effects, the PMEs can be computed with no additional cost (in terms of model evaluations).

The remainder of this paper is organized as follows. Section 2 focuses on the interaction between GSA and cooperative game theory and the existing literature. The Shapley effects are recalled, as well as their main shortcoming: the inability to detect exogenous inputs. To that end, the notion of L^2-*exogeneity* is formally defined. Then, Section 3 defines the proportional values and presents the main result of this paper, an extension allowing for well-defined novel GSA indices: the PMEs. Additionally, these novel indices allow the detection of exogenous inputs while remaining inherently interpretable. Section 4 illustrates the behavior of the novel PMEs by using analytical formulas obtained for particular forms of G with Gaussian inputs. Section 5 briefly recalls several strategies for estimating the PMEs and presents results obtained on a more challenging numerical use case. Section 6 discusses several possible improvements and some perspectives about the proposed work. A few appendices provide extra materials, such as information about the reproducibility of numerical results (Appendix Appendix A) and proofs (Appendix Appendix B). Finally, some supplementary materials contain details on random order model allocations and additional use-cases.

Throughout this paper, let $\mathbb{E}[\cdot]$ and $\mathbb{V}(\cdot)$ denote the expectation and variance, respectively. A *coalition of players* is a subset of the *grand coalition* denoted $D = \{1, \dots, d\}$. Moreover, $\forall A \subseteq D$, the restricted set of indices $A \setminus \{i\}$, for any $i \in A$, is denoted by A_{-i}. Additionally, for any $A \subseteq D$, $X_{D \setminus A}$ is denoted by $X_{\overline{A}}$. The distribution of the random inputs X is denoted by P_X and the marginal distribution of any subset of inputs X_A for any $A \subseteq D$ is denoted by P_{X_A}. The spaces $L^2(P_{X_A})$, for any $A \subseteq D$, denote the spaces of measurable functions with finite second-order moments. The nonnegative part of the real line $[0, \infty)$ is denoted $\mathbb{R}^+$, and the positive part $(0, \infty)$ is denoted $\mathbb{R}^+_*$. When a function is referred to as being nonnegative (resp. positive), it entails that it takes values in $\mathbb{R}^+$ (resp. $\mathbb{R}^+_*$). Whenever reference is made to a model G, it is always implicitly assumed that $G \in L^2(P_X)$. In this paper, almost sure statements are followed by the acronym "a.s.".

2. Cooperative game theory for variance-based global sensitivity analysis

This section presents the use of cooperative game theory to define variance-based GSA indices. A particular class of allocations is presented: the random order model allocations, which generalizes the Shapley values. Sobol' cooperative games are introduced to formalize the analogy between players and inputs of deterministic models. The Shapley effects are presented as the Shapley values of a Sobol' cooperative game. Duals of a cooperative game are also briefly discussed. Finally, a specific Shapley effects' drawback (for factor fixing setting) is illustrated as a motivation for the proposed work: their

inability to detect exogenous inputs. The interested reader is referred to the supplementary materials for a more in-depth discussion of these concepts.

2.1. Analogy between allocation and variance-based GSA indices

A cooperative game is a tuple (D, v) where $D = \{1, \dots, d\}$ is a set of d players and the set function $v : \mathcal{P}(D) \to \mathbb{R}$ is known as a *value function*. Usually, v is assumed to be *monotonically increasing*, meaning that, for any two sets T and A such that $T \subseteq A \in \mathcal{P}(D)$, one has $v(T) \leq v(A)$. In the following, cooperative games with monotonically increasing value functions are called "monotonic games". Moreover, if the value function v takes values in $\mathbb{R}_*^+$ (resp. in $\mathbb{R}^+$) for non-empty coalitions, the corresponding cooperative game is referred to as "positive (resp. nonnegative) games". By convention, it is always assumed that $v(\emptyset) = 0$.

The analogy between the players D of a cooperative game (D, v) and the inputs $(X_i)_{i \in D}$ involved in a numerical model has been first developed in [36]. The author proposed to use the closed Sobol' indices (see, Eq. (2)) as the value function. This choice of value function defines the Sobol' cooperative games.

Definition 1 (Sobol' cooperative game)**.** *Let $X = (X_1, \dots, X_d)^\top$ be random inputs, let $G \in L^2(P_X)$ be a model and denote $Y = G(X)$ the random output. The Sobol' cooperative game related to X and Y is the cooperative game with value function S^{clos} defined as follows:*

$$\begin{aligned} S^{\text{clos}} \colon \mathcal{P}(D) &\to \mathbb{R}^+ \\ A &\mapsto S_A^{\text{clos}} = \frac{\mathbb{V}\left(\mathbb{E}\left[Y \mid X_A\right]\right)}{\mathbb{V}\left(Y\right)}. \end{aligned}$$

Sobol' cooperative games are always nonnegative and monotonic. The choice of S^{clos} as a value function can be interpreted as measuring the value of every subset of players $A \subseteq D$ as the variance of the best approximation of Y in $L^2(P_{X_A})$, i.e., $\mathbb{V}\left(\mathbb{E}\left[Y \mid X_A\right]\right)$.

One of the main goals of cooperative game theory is to build *allocation* (or solution concepts) [35]. In general, allocations can be understood as a decomposition of the quantity $v(D)$ in d elements, each allocated to a specific player. Formally, an allocation can be understood as a mapping ϕ that associates, to a cooperative game (D, v), a real-valued vector $(\phi_1, \dots, \phi_d)^\top \in \mathbb{R}^d$.

Regarding Sobol' cooperative games, it entails assigning a share of the output's variance $\mathbb{V}\left(Y\right)$ to each input of the model. Allocations of Sobol' cooperative games require limited assumptions on the probabilistic structure between the inputs (i.e., mutual independence is not required) to provide a decomposition of the output variance, which made them particularly attractive for importance quantification with dependent inputs [37, 10]. Hence, variance-based GSA indices with dependent inputs can be defined by choosing an allocation related to a Sobol' cooperative game (D, S^{clos}).

For instance, *Shapley values* are a particular instance of allocations. For a cooperative game (D, v), they are defined $\forall i \in D$, as:

$$\text{Shap}_i\big((D, v)\big) = \frac{1}{d} \sum_{A \subseteq D_{-i}} \binom{d-1}{|A|}^{-1} \left[v(A \cup \{i\}) - v(A)\right], \tag{3}$$

This original formulation attributed to [42] can be interpreted as a weighted average, over every possible coalition A, of the "marginal contribution" of a player i to that coalition A, quantified by the quantity $v(A \cup \{i\}) - v(A)$. Two main properties make this allocation particularly attractive in practice:

- They are *efficient*: $\sum_{i=1}^{d} \text{Shap}_i\big((D, v)\big) = v(D)$.
- If the game is monotonic, they are *nonnegative*: $\forall i \in D, \text{Shap}_i\big((D, v)\big) \geq 0$.

Shapley values of Sobol' cooperative games lead to the definition of the *Shapley effects* [36]. They are defined for every $i \in D$, as:

$$\mathrm{Sh}_i := \mathrm{Shap}_i\big((D, S^{\mathrm{clos}})\big) \tag{4a}$$

$$= \frac{1}{d} \sum_{A \subseteq D_{-i}} \binom{d-1}{|A|}^{-1} \left(S^{\mathrm{clos}}_{A\cup\{i\}} - S^{\mathrm{clos}}_{A}\right) \tag{4b}$$

These indices have been extensively studied in [44, 37, 26] and are a valuable tool to quantify variable importance in the context of dependent inputs [9]. They allow for a decomposition of $\mathbb{V}(Y)$ into nonnegative shares attributed to each input, even when the inputs are not mutually independent.

The efficiency and nonnegativity properties are in fact guaranteed for an entire class of allocations, known as *random order models* (or Weber's set) [48, 16]. These allocations are based on players' different orderings (i.e., permutations). Formally, let $\mathcal{S}_D$ be the symmetric group on D (the set of all permutations of D). Let $\pi = (\pi_1, \ldots, \pi_d) \in \mathcal{S}_D$ be a particular permutation, and for any $i \in D$, denote $\pi(i) = \pi_i^{-1}$ its inverse (i.e., the position of i in π, such that $\pi_{\pi(i)} = i$). Let $C_i(\pi)$ be the set of the i-th first players in the ordering π, with the convention that, for any permutation, $C_0(\pi) = \emptyset$, i.e., :

$$C_i(\pi) = \{\pi_j : j \leq i\}. \tag{5}$$

As their names suggest, random order models endow $\mathcal{S}_D$ with a probabilistic structure. For any game (D, v), the set of random order models allocations contains every allocation $\phi\big((D, v)\big)$ that can be written, for any $i \in D$, as:

$$\begin{aligned}\phi_i &= \sum_{\pi \in \mathcal{S}_D} p(\pi) \left[v\left(C_{\pi(i)}(\pi)\right) - v\left(C_{\pi(i)-1}(\pi)\right)\right] \\ &= \mathbb{E}_{\pi\sim p}\left[v\left(C_{\pi(i)}(\pi)\right) - v\left(C_{\pi(i)-1}(\pi)\right)\right]\end{aligned}$$

where p is a probability mass function over the orderings of D. For a player i, its random order allocation can be interpreted as the expectation over the permutations π of D w.r.t. p, of the marginal contributions of i to the coalitions formed by $C_{\pi(i)-1}(\pi)$. The random order model allocations are always *efficient* and when dealing with monotonic games, *nonnegative* [48].

In particular, the Shapley values can be expressed as a random order model allocation. They are characterized by the choice of p as the discrete uniform distribution over $\mathcal{S}_D$:

$$\mathrm{Shap}_i\big((D, v)\big) = \frac{1}{d!} \sum_{\pi \in \mathcal{S}_D} \left[v\left(C_{\pi(i)}(\pi)\right) - v\left(C_{\pi(i)-1}(\pi)\right)\right]. \tag{6}$$

In this setting, Shapley values are a maximum entropy a priori (i.e., uniform over $\mathcal{S}_D$). In variance-based GSA, the equivalent formulation of the Shapley effects as a random order model allocation of a Sobol' cooperative game has been introduced by [44] for estimation purposes. For every $i \in D$, it writes:

$$\mathrm{Sh}_i = \frac{1}{d!} \sum_{\pi \in \mathcal{S}_D} \left[S^{\mathrm{clos}}_{C_{\pi(i)}(\pi)} - S^{\mathrm{clos}}_{C_{\pi(i)-1}(\pi)}\right]. \tag{7}$$

The notion of the *dual* of a cooperative game is also of interest in the present paper. In a nutshell, the dual of a cooperative game focuses on the "worth" of a coalition instead of its value, i.e., the shortfall due to a coalition [15, 16]. The dual of a cooperative game (D, v) is usually denoted by (D, w) where w is defined, for any $A \in \mathcal{P}(D)$ as:

$$w(A) = v(D) - v(D \setminus A). \tag{8}$$

In the following, one refers to $w(A)$ as the *marginal contribution of the coalition* A. The dual (D, w) of (D, v) is also a cooperative game, and thus one can seek to construct appropriate allocations for this game.

The Shapley values of a game and its dual are equal (see, [17] Lemma 2.7). However, it is essential to note that this is a particular property of the Shapley values and is not inherent to every random order model allocation.

The dual of a Sobol' cooperative game (D, S^{clos}) is the nonnegative, monotonic cooperative game (D, S^T), where S^T denotes the total Sobol' indices, given for any $A \in \mathcal{P}(D)$, by

$$S_A^T = \frac{\mathbb{E}\left[\mathbb{V}\left(Y \mid X_{\overline{A}}\right)\right]}{\mathbb{V}\left(Y\right)}. \tag{9}$$

In the variance-based GSA literature, the equivalence between the Shapley values of a Sobol' cooperative game and its dual has been highlighted and used for estimation purposes in [44].

2.2. Detecting exogenous inputs

As noted in [23], the main drawback (for factor fixing setting) of the Shapley effects is their behavior when dealing with exogenous (or spurious) inputs. Formally, exogenous inputs, in the context of variance-based GSA, can be defined as follows.

Definition 2 (L^2-exogeneity)**.** *Let $X = (X_1, \ldots, X_d)$ be random inputs of a model $G : \mathbb{R}^d \mapsto \mathbb{R}$ such that $Y = G(X)$, with Y the random output. Let $i \in D$. The random input X_i is said to be L^2-exogenous to G if, $\exists f \in L^2(P_{X_{D_{-i}}})$ such that $Y = f(X_{D_{-i}})$ a.s..*

Moreover, if for $E \in \mathcal{P}(D)$, $\exists f \in L^2(P_{X_{D_{\overline{E}}}})$ such that $Y = f(X_{\overline{E}})$ a.s. then X_E is said to form an L^2-exogenous vector.

For the sake of conciseness, in the following, L^2-exogenous inputs or vectors are referred to as being simply exogenous. It is important to note that, according to the proposed definition, a set of exogenous inputs does not necessarily form an exogenous vector. However, the following assumption allows avoiding such situations.

Assumption 1. *Let $E \in \mathcal{P}(D)$. If for every $i \in E$, X_i is exogenous, then X_E forms an exogenous vector.*

In situations where the random inputs are correlated, the Shapley effects can allocate shares of variance to exogenous inputs. This phenomenon, called *Shapley's joke*, has been illustrated in [26, 23] through the following example.

Example 1 (Shapley's joke)**.** *Let $X = (X_1, X_2)^\top \sim \mathcal{N}\left(\begin{pmatrix}0\\0\end{pmatrix}, \begin{pmatrix}1 & \rho\\ \rho & 1\end{pmatrix}\right)$, $-1 < \rho < 1$, and let the model be:*

$$Y = G(X) = X_1.$$

The Shapley effects of the random inputs are given by

$$Sh_1 = 1 - \frac{\rho^2}{2}, \quad Sh_2 = \frac{\rho^2}{2}.$$

Even if X_2 is exogenous, its Shapley effect is not zero as long as $\rho \neq 0$. While this behavior can be considered valuable for factor prioritization (effects due to correlation can be relevant), it can also be a drawback for spurious variable detection [10]. Another allocation called the proportional values provides us a direct solution to this drawback.

3. From proportional values to proportional marginal effects

The proportional values (PVs) are a random order model allocation initially designed for positive games. In this section, they are introduced and extended to nonnegative games to be suitable for GSA purposes. The extended allocation of the dual of Sobol' cooperative games is introduced as the *proportional marginal effects* (PMEs). It is shown that the PMEs enable the detection of exogenous inputs while offering an interpretable variance decomposition.

3.1. Proportional values as an alternative allocation strategy to Shapley values

The PVs are a random order model allocation associated to a particular probability mass function over $\mathcal{S}_D$ [15] (see also the section 1 of the supplementary materials). They can also be characterized recursively [13, 34].

Definition 3 (Proportional values)**.** *Let (D, v) be a positive game, where $v : \mathcal{P}(D) \to \mathbb{R}_*^+$. The proportional values of (D, v), are defined for every $i \in D$, as a random order model allocation:*

$$\mathrm{PV}_i\big((D,v)\big) = \sum_{\pi \in \mathcal{S}_D} p(\pi) \left[v\left(C_{\pi(i)}(\pi)\right) - v\left(C_{\pi(i)-1}(\pi)\right) \right] \tag{10}$$

where the probability mass function p is defined as:

$$p(\pi) = \frac{L(\pi)}{\sum_{\sigma \in \mathcal{S}_D} L(\sigma)}, \quad \text{where} \quad L(\pi) = \left(\prod_{j \in D} v\left(C_j(\pi)\right) \right)^{-1}. \tag{11}$$

Equivalently, PV can be characterized recursively, for every $i \in D$, as:

$$\mathrm{PV}_i\big((D,v)\big) = \frac{R(D,v)}{R(D_{-i},v)} \tag{12}$$

where, for all $A \in \mathcal{P}(D)$, $R(A,v) = v(A) \left(\sum_{j \in A} R(A_{-j},v)^{-1} \right)^{-1}$, and $R(\emptyset, v) = 1$. This recursive definition leads to the following identification [16]:

$$\mathrm{PV}_i\big((D,v)\big) = \frac{\sum_{\pi \in \mathcal{S}_{D_{-i}}} \prod_{j=1}^{d-1} v\left(C_j(\pi)\right)^{-1}}{\sum_{\sigma \in \mathcal{S}_D} \prod_{j=1}^{d} v\left(C_j(\sigma)\right)^{-1}}. \tag{13}$$

The PVs can also be characterized axiomatically (see [16]), as the unique allocation $\phi(D, v)$ respecting the following two axioms:

- **Efficiency**: $\sum_{i=1}^{d} \phi_i = v(D)$;
- **Equal proportional gains**: for all $A \in \mathcal{P}(D)$, and for all $i, j \in A$, $i \neq j$:

$$\frac{\phi_i\big((A,v)\big)}{\phi_j\big((A,v)\big)} = \frac{\phi_i\big((A_{-j},v)\big)}{\phi_j\big((A_{-i},v)\big)}.$$

These axioms characterize the choice of $L(\pi)$ in Eq. (11). We refer the interested reader to [15] for more details. If the game is monotonic, the PVs are efficient and nonnegative, allowing for a meaningful interpretation, as for the Shapley values. The equal proportional gains axiom sheds light on the redistribution dynamic of this particular allocation scheme. For any two different players i and j, the ratio of their allocations in any subgame (A, v) (for every $A \in \mathcal{P}(D)$ such that $i,\ j \in A$) must be invariant to removing each player's contribution to the other's allocation. In other words, the magnitude of the ratios must be preserved, independently of the possible interaction between i and j, within any coalition they can be a part of. It implies that the allocation favors the players proportionally to their (marginal) contributions to every possible coalition in the redistribution process.

As a frame of comparison, the Shapley values can also be characterized as the unique, efficient allocation respecting the following axiom (see [16]):

- **Balanced contributions:** for all $A \in \mathcal{P}(D)$, and for all $i, j \in A$, $i \neq j$:

$$\phi_i(A,v) - \phi_i(A_{-j},v) = \phi_j(A,v) - \phi_j(A_{-i},v).$$

This axiom entails that for any two different players i and j, the difference in each allocation by removing the other player to any sub-game (A, v) such that $i,\ j \in A$ must remain equal, for any $A \in \mathcal{P}(D)$. In other words, the difference in allocation of the two players induced by the removal of the other player must be equal, implicitly entailing a balanced redistribution process where individual and coalitional contributions are favored equally.

Remark 1. *In a nutshell, one can remark that the redistribution processes in both allocations (Shapley values* vs. *PVs) are fundamentally different: the PVs redistribution process is* proportional *while the Shapley values are* egalitarian*.*

The different behaviors between PVs and Shapley values can be illustrated in a two-player game, i.e., $(D = \{1, 2\})$. The allocations are given, for any $i \in D$, by

$$\mathrm{PV}_i\Big((D, v)\Big) = v(\{i\}) + \frac{v(\{i\})}{v(\{1\}) + v(\{2\})}\Big(v(D) - v(\{1\}) - v(\{2\})\Big) \tag{14a}$$

$$\mathrm{Shap}_i\Big((D, v)\Big) = v\big(\{i\}\big) + \frac{1}{2}\Big(v(D) - v(\{1\}) - v(\{2\})\Big). \tag{14b}$$

For both PVs and Shapley values, each player receives its individual value plus a weighted share of the value surplus generated due to their cooperation. In the literature, this surplus is referred to as the *Harsanyi dividend* of the coalition $\{1, 2\}$ [21]. The Shapley values redistribute precisely half of this dividend to each player (i.e., egalitarian way). In contrast, the PVs redistribute them proportionally (i.e., proportional way) to each player's individual contribution.

Remark 2. *Eq. (14a) is equivalent to another allocation, namely the* proportional Shapley values *[7]. However, they differ from the PVs as soon as more than two players are involved in a game. Intuitively, the proportional Shapley values are a "proportional redistribution with respect to the individual values of the players", whereas the proportional values are "proportional with respect to the value added by the players to every possible coalition".*

It is important to notice that this allocation is only well-defined for positively defined value functions v. However, as stated in Definition 1, Sobol' cooperative games' value function is nonnegative. The following section presents a continuous extension of the PVs to nonnegative games, enabling their use for variance-based GSA purposes.

3.2. Extension of proportional values to nonnegative games

This section proposes an extension of the PVs to nonnegative and monotonic games. Initially, the PVs are only defined for positive games. However, Sobol' cooperative games are inherently nonnegative. By leveraging the method of [14], it is possible to define a continuous extension of the PVs for games with coalitions of zero value. The following result builds upon this extension.

Theorem 1 (PV extension to monotonic nonnegative games)**.** *Let (D, v) be a nonnegative and monotonic game with value function $v : \mathcal{P}(D) \to \mathbb{R}^+$. Denote $\mathcal{K}$ the set of largest (w.r.t. their cardinality) zero coalitions,* i.e., *, $\mathcal{K} = \underset{A \in \mathcal{P}(D)\ s.t.\ v(A)=0}{\operatorname{argmax}} |A|$. Additionally, the sets of largest zero coalitions that do not contain $i \in D$ is denoted by $\mathcal{K}_{-i}$,* i.e., *, $\mathcal{K}_{-i} = \Big\{A \in \mathcal{K} : i \notin A\Big\}$. Define, for any $A \in \mathcal{K}$, the positive set function:*

$$\begin{aligned} v_A : \mathcal{P}\left(D \setminus A\right) &\to \mathbb{R}_*^+ \\ B &\mapsto v(B \cup A). \end{aligned}$$

Let $\mathrm{PV}^0\left((D, v)\right) = \left(\mathrm{PV}_1^0, \ldots, \mathrm{PV}_d^0\right)$ be the allocation defined as:

$$\mathrm{PV}_i^0 = \frac{\sum_{A \in \mathcal{K}_{-i}} R\left(D_{-i} \setminus A, v_A\right)^{-1}}{\sum_{A \in \mathcal{K}} R\left(D \setminus A, v_A\right)^{-1}} \quad \text{if } i \notin \bigcap_{A \in \mathcal{K}} A \text{ and } \quad \mathrm{PV}_i^0 = 0 \text{ otherwise.} \tag{15}$$

Then, PV^0 *is a continuous extension of* PV *to the set of nonnegative monotonic games,* i.e., *for a positive monotonic game* (D, v)*,*

$$\mathrm{PV}^0\left((D,v)\right) = \mathrm{PV}\left((D,v)\right).$$

A proof of this result is available in Appendix Appendix B. Interestingly, the definition of this extension precisely identifies the players whose allocation is zero. For a player $i \in D$, $\mathrm{PV}_i^0 = 0$ if and only if it is part of every largest zero coalition.

Remark 3. *From this point forward, for conciseness, any mention of the PVs refers to their extension to nonnegative games (*i.e., PV^0*).*

3.3. Proportional marginal effects and exogeneity detection

Thanks to Eq. (15), one can see that the PVs of a cooperative game and its dual are different, contrarily to the case of the Shapley values. The duals of Sobol' cooperative games are more relevant for exogenous variable detection. This fact becomes clear thanks to the following result, in a similar manner to [22].

Lemma 1. *Let* $X = (X_1, \ldots, X_d)^\top$ *be random inputs and* $G \in L^2(P_X)$ *denote a model such that* $\mathbb{V}\left(G(X)\right) > 0$*. One has,* $\forall A \subseteq D$*,*

$$S_A^T = \frac{\mathbb{E}\left[\mathbb{V}\left(G(X) \mid X_{\overline{A}}\right)\right]}{\mathbb{V}\left(G(X)\right)} = 0 \quad \Longleftrightarrow \quad G(X) = \mathbb{E}\left[G(X) \mid X_{\overline{A}}\right] \ \ a.s.$$

A proof of this result can be found in Appendix Appendix B. For $A \subseteq D$, S_A^T being equal to zero indicates that $G(X)$ is almost surely equal to some $f(X_{\overline{A}})$ where $f \in L^2\left(P_{X_{\overline{A}}}\right)$. However, S_A^{clos} being equal to zero is only equivalent to the fact that $\mathbb{E}\left[G(X) \mid X_A\right]$ is constant almost surely. It leads to the proposed cooperative game theory-inspired GSA indices called *proportional marginal effects* (PMEs), which are none other than the (extended) PVs of the dual of Sobol' cooperative games. They are defined as follows:

Definition 4 (Proportional marginal effects)**.** *Let* $X = (X_1, \ldots, X_d)^\top$ *be random inputs, and let* $Y = G(X)$ *be the random output of a model. The proportional marginal effects are the proportional values of the dual of the monotonic Sobol' cooperative game related to the model* G*. They are defined as:*

$$\mathrm{PME} = \mathrm{PV}\big((D, S^T)\big) \in \mathbb{R}^d.$$

Naturally, these indices are efficient, and since Sobol' cooperative games are monotonic, they result in nonnegative allocations. Thus they offer interpretable shares of the output variance in the context of dependent inputs. As Section 3.1 presents, they differ from the Shapley effects on the underlying redistribution principle. More importantly, thanks to the following result, they allow exogenous input detection.

Proposition 1. *Let* $X = (X_1, \ldots, X_d)^\top$ *be random inputs and* $G \in L^2(P_X)$ *be a model such that Assumption 1 holds. For any input* $i \in D$*, the following equivalence holds:*

$$X_i \text{ is } L^2\text{-exogenous to } G \Longleftrightarrow PME_i = 0$$

A proof of this result can be found in Appendix Appendix B. In addition to offering an interpretable tool for factor prioritization, the PMEs allow the detection of exogenous inputs by granting them a zero share. Hence, these novel indices circumvent Shapley's joke, presented in Section 2.2.

4. Illustration on analytical cases

Two toy cases are studied, where it is possible to compute analytical values for the PMEs. The first one aims at illustrating the exogeneity detection property of the PMEs ensured by Proposition 1. The second toy case introduces a trade-off between individual and interaction effects between two inputs and highlights the difference in repartition between the Shapley effects and the proposed PMEs. An additional toy case is presented in the supplementary materials.

4.1. A linear model with an exogenous input

This first toy case illustrates the exogeneity detection property of the PMEs (i.e., Proposition 1). This first model reads:

$$Y = G(X) = X_1 + X_2, \quad X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & \rho \\ 0 & 1 & 0 \\ \rho & 0 & 1 \end{pmatrix} \right) \tag{16}$$

where $-1 < \rho < 1$. One can notice that X_3 is exogenous but linearly correlated to X_1. Since the inputs are not mutually independent, traditional GSA tools such as first- and second-order Sobol' indices fail to be interpreted as shares of variance [10]. Hence, one can resort to cooperative game theory-inspired tools, such as the Shapley effects and PMEs. Analytical values can be computed (since the inputs are multivariate Gaussian) and are given in Table 4.1.

$\mathrm{Sh}_1 = 1/2 - \rho^2/4$	$\mathrm{PME}_1 = 1/2$
$\mathrm{Sh}_2 = 1/2$	$\mathrm{PME}_2 = 1/2$
$\mathrm{Sh}_3 = \rho^2/4$	$\mathrm{PME}_3 = 0$

Table 2: Reference analytical values for Shapley effects and PMEs (toy-case 4.1).

One can first notice that X_3 can receive a non-zero Shapley effect, dependent on the value of ρ. In highly correlated settings, X_3 is interpreted as being almost as important as X_1. This interpretation can be meaningful because the correlation between X_3 and X_1 may be relevant to the underlying studied phenomenon. However, in GSA, the practitioner usually supposes that the model G is black-box and only has access to the input's distribution. Hence, relying only on the Shapley effects, the practitioner would not be able to determine the exogenous nature of X_3. If the aim of the sensitivity study is focused on better understanding the relationship between the model and its inputs, independently from their probabilistic structure, the Shapley effects are hence not suitable alone.

Contrarily, the PMEs do indeed detect X_3 as being an exogenous input by granting it a zero allocation. Moreover, the PMEs are not influenced by the linear correlation ρ between X_1 and X_3. In combination with the Shapley effects, additional insights on G can be extracted from the initial study: while X_3 can affect G through its correlation with other inputs (supposedly known by the practitioner), it is exogenous to G. Additionally, by allocating half the output's variance to both X_1 and X_2, the PMEs also indicate an equal influence.

Hence, by combining the interpretation of both indices, one can interpret these results as follows: X_3 is an exogenous variable (PMEs), but it bears an effect on G through its correlation with X_1 (Shapley effects) and X_1 and X_2 seem to bear an equal influence on the output's variance, whenever X_3 is detected as exogenous (PMEs). In this setting, both indices complement each other and provide a more precise interpretation of the studied model and its interaction with the inputs and their probabilistic structure.

4.2. Unbalanced linear model with interactions

This toy case aims at studying and comparing the behavior in a trade-off between individual and interaction effects. This particular unbalanced linear model is given as follows:

$$Y = G(X) = X_1 + (1-\alpha)X_2 + \alpha X_1 X_2, \quad X = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \right), \tag{17a}$$

$$\mathbb{V}(Y) = 2 + (1-\alpha)^2 + 2(1-\alpha)\rho + \rho^2. \tag{17b}$$

The parameter α aims at controlling the "trade-off" between the individual effect of X_2 and its interaction term with X_1. When $\alpha = 0$, there is no interaction term between X_1 and X_2, and when $\alpha = 1$, X_2 does not have any individual effect. Analytical formulas for the Shapley effects and the PMEs are given in Table 4.2. In addition, both inputs are correlated through their covariance $\rho \in (-1, 1)$.

$2\mathbb{V}(Y) \times \mathrm{Sh}_1 = 3 + \rho^2(1-\alpha)^2 + 2\rho(1-\alpha)$	$\mathrm{PME}_1 = \frac{2}{3+(1-\alpha)^2}$
$2\mathbb{V}(Y) \times \mathrm{Sh}_2 = 1 + 2\rho^2 + (2-\rho^2)(1-\alpha)^2 + 2\rho(1-\alpha)$	$\mathrm{PME}_2 = \frac{(1-\alpha)^2+1}{3+(1-\alpha)^2}$

Table 3: Reference analytical values for Shapley effects and PMEs (toy-case 4.2).

To illustrate the redistribution differences between the Shapley effects and the PMEs w.r.t. both correlation and interaction, (α, ρ)-plane plots are provided in Figure 1. First, one can notice that, when $\alpha = 0$, the Shapley effects and the PMEs are equal, granting each input half of the output's variance. However, when α deviates from zero, both indices display different behaviors. Secondly, and interestingly, the analytical formulas of the PMEs do not depend on the correlation coefficient ρ.

Focusing on the behavior of both effects w.r.t. the interaction, one can first focus on the α-axis of the plots in Figure 1. Whenever α is close to 0, one can notice that both indices tend to allocate an equal share of the output variance to both inputs. As α increases, the PME grants an increasing share of the output variance to X_1, independently of ρ. However, on the other hand, the Shapley effects display a sharing mechanism dependent on ρ. When ρ is between -0.5 and 0.5, and α is close to 1, Sh_1 increases, with a maximum allocation of 0.75 taken at $(\rho = 0, \alpha = 1)$, while Sh_2 decreases, with a minimum allocation of 0.25 at the same point on the plane. Additionally, one can notice that when both inputs are highly correlated, the Shapley effects redistribute the output's variance equally, whatever the value of α is.

This toy case illustrates the difference in behavior between the Shapley effects and the PMEs. The PMEs are not impacted by the correlation and may be preferred if the study's goal is to gather insights on the intricacies of the model G. On the other hand, the Shapley effects even the importance of the correlated inputs whenever their correlation levels are relatively high.

4.3. First conclusions

From these two toy cases, the following conclusions can be drawn:

- whenever the inputs are correlated, the Shapley effects do not detect exogenous inputs, while the PMEs do;
- in the highly correlated cases, the Shapley effects can lead to an equalized importance ranking, while the PMEs allow for a more pronounced discriminatory power;
- overall, the PMEs seem less sensitive to high levels of correlation, while the Shapley effects can vary greatly.

However, these conclusions are subject to the presented toy cases and are not universal.

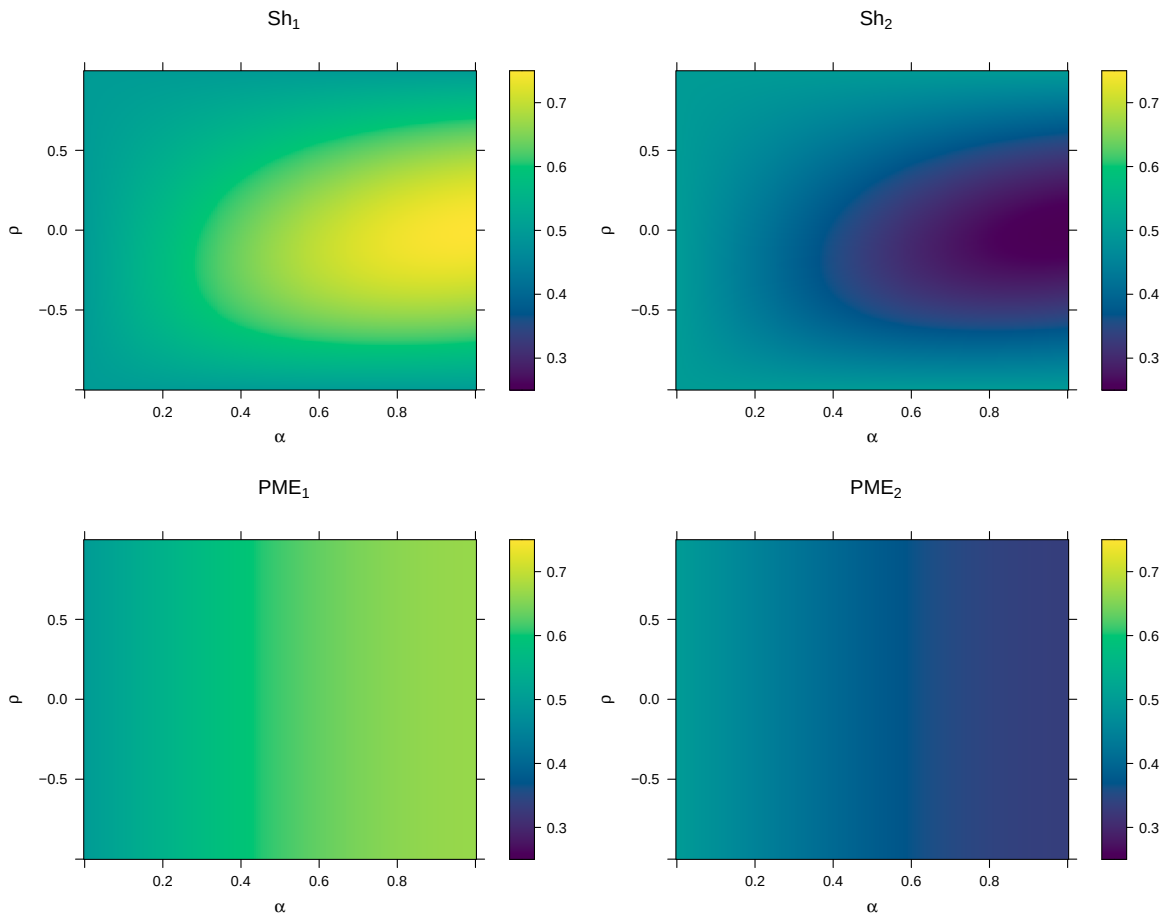

Figure 1: PMEs and Shapley effects in the (α, ρ)-plane for test-case 4.2.

5. Estimation and numerical results

This section presents estimation schemes of the PME: they rely on the same ingredients as the Shapley effects. Then, a practical use case is studied: a model of optical system interference.

5.1. Estimation strategies

The plug-in estimation of the PME relies on the same elements as the estimation of the Shapley effects. For the sake of completeness, the classical estimation framework is briefly stated. Following the two-steps methodology presented in [4], initially developed for Shapley effects' estimation, one can estimate the PMEs in two distinct steps:

- Step 1: Estimate the *conditional elements*, i.e., S_A^T, $\forall A \in \mathcal{P}(\mathcal{D})$;
- Step 2: Perform an *aggregation procedure* via a direct plug-in of the estimated conditional elements in Eq. (15).

Only the aggregation procedure differs between the estimation of the PMEs and the Shapley effects. It entails that the estimation cost in terms of model evaluations is the same for the PMEs as for the Shapley effects. Furthermore, both indices can be evaluated "at once" using the same conditional elements estimates. Two situations the practitioner may encounter are defined.

First, if the practitioner can randomly sample from (i) every possible conditional distribution of the conditional random variables $X_A|X_{\overline{A}}$ and (ii) every marginal distribution, i.e., to simulate

i.i.d. observations of X_A, for all $A \in \mathcal{P}(\mathcal{D})$, then the conditional elements can be estimated via a Monte Carlo scheme. This estimation scheme has been studied and proven to yield consistent estimates in [44, 5, 10, 24]. This estimation method is applied in Section 2.2 of the supplementary materials on a toy case, illustrating the correct capabilities of exogeneity detection by PMEs. However, it is essential to note that the ability (i) to sample from the conditional distributions can be difficult in practice (especially if the inputs are dependent).

Second, if the practitioner can only access an i.i.d. input-output sample (coming from the joint distribution of the inputs), they can perform a given-data estimation scheme. Such a scheme has been proposed in the literature and relies on approximating the conditional samples using a nearest-neighbor [5]. One can refer to [5, 10, 24] for additional theoretical and computational details on this estimation method. This estimation method is applied in Section 2.3 of the supplementary materials on a simple application case containing an exogenous input, illustrating the problem of the bias induced by this estimation method. Indeed, the PME of the exogenous input is low but not zero.

In both situations, the practitioner must estimate $2^d - 1$ conditional elements, which is exponential w.r.t. the number of inputs. As stated in [44, 4, 24], some Monte Carlo-inspired methods can require a number of evaluations proportional to $d!(d-1)$, which may be prohibitive for costly numerical models. The given-data procedure avoids the need to simulate and evaluate data, but the sheer number of elements to estimate can render the estimation very long. It is important to note that the Shapley effects suffer from the same computational burden. However, both indices can be estimated with the same set of conditional elements, with the only differentiating factor being the aggregation procedures, which are less computationally expensive in comparison.

Given estimates of every conditional element, i.e., $\widehat{S_A^T}$ for every $A \subseteq D$, the aggregation procedure for the PME can be computed using its recursive definition (see, Eq. (15)). It relies on the computation of the ratio potential, i.e., the function R in Eq. (12).

Ratio potential computation. First, recall that for any value function v, $R(\emptyset, v) = 1$ and for any $i \in D$, $R(i, v) = v(\{i\})$. The computation of $R(A, v)$ can be broken down as follows:

1. Let $A \in \mathcal{P}(D)$, $A \neq \emptyset$, $|A| \geq 2$.
2. Compute $v(B)$, for every $B \in \mathcal{P}(A)$.
3. For $m = 1, \ldots, |A| - 1$:
   - ↪ For $B \subseteq A$ such that $|B| = m$:
     - ↪ Compute $R(B, v) = v(B) \left(\sum_{j \in B} R(B_{-j}, v)^{-1} \right)^{-1}$.
4. Compute $R(A, v) = v(A) \left(\sum_{j \in A} R(A_{-j}, v)^{-1} \right)^{-1}$.

Following this algorithm and given conditional element estimates, one can then compute $R\left(A, \widehat{S^T}\right)$ for any $A \in \mathcal{P}(D)$.

Aggregation procedure for PME computation. With the ability to compute the ratio potential $R(A, \widehat{S^T})$ for any $A \in \mathcal{P}(D)$ and any set function v, one can proceed to compute the PME. First, define the function, $\forall A \in \mathcal{P}(D)$:

$$\begin{aligned} \widehat{\zeta_A} : \mathcal{P}(D \setminus A) &\to \mathbb{R}^+ \\ B &\mapsto \widehat{\zeta_A}(B) := \widehat{S^T_{A \cup B}} \end{aligned}$$

The aggregation procedure of the PME can then be broken down as follows:

1. Compute $\widehat{S_A^T}$, for every $A \in \mathcal{P}(D)$.

2. Compute $\mathcal{K} = \underset{A \in \mathcal{P}(D) \text{ s.t. } \widehat{S_A^T}=0}{\operatorname{argmax}} |A|$.

3. For every $A \in \mathcal{K}$, compute $R\left(D \setminus A, \widehat{\zeta_A}\right)$.

4. Let $R_{\mathcal{K}} = \sum_{A \in \mathcal{K}} R\left(D \setminus A, \widehat{\zeta_A}\right)^{-1}$.

5. For $i = 1, \ldots, d$:

   (a) If $i \in \underset{A \in \mathcal{K}}{\cap} A$, set $\mathrm{PME}_i = 0$.

   (b) If $i \notin \underset{A \in \mathcal{K}}{\cap} A$:

      i. Compute $\mathcal{K}_{-i} = \left\{A \in \mathcal{K} : i \notin A\right\}$.

      ii. For every $A \in \mathcal{K}_{-i}$, compute $R\left(D_{-i} \setminus A, \widehat{\zeta_A}\right)$.

      iii. Let $\mathrm{PME}_i = \sum_{A \in \mathcal{K}_{-i}} R\left(D_{-i} \setminus A, \widehat{\zeta_A}\right)^{-1} / R_{\mathcal{K}}$.

This algorithmic procedure is used in order to estimate PMEs in the following use case.

5.2. Transmittance performance of optical filters

In this use case, inspired by [46], the transmittance of an optical filter is studied. The studied system comprises 13 layers stacked on each other, each having the same thickness but varying refractive indices.

This filter aims at splitting a light wave into two or more parts, each taking different paths through the system before coming together. Due to the refraction of the wave on each successive layer of the system, the paths' length and amplitude can vary, resulting in varying system transmittance values. The ability to determine which layer is influential is crucial for optical filters and remains a complicated problem due to high levels of interaction between the layers. In the literature, previous GSA studies (see, e.g., [46, 45]) allowed providing some answers but with independence hypothesis between refractive indices.

In this study, each of the 13 inputs $I_1, \ldots, I_{13}$ represents the refractive index error of a layer in the optical filter, which is assumed to vary uniformly between $[-0.05, 0.05]$. These errors are correlated, which may be due to the same deviation in the manufacturing process of the layers. The dependence structure is modeled using a Gaussian copula, where each pair of inputs exhibit a 0.9 correlation coefficient.

As depicted in [46], several light waves of varying frequencies are passed through the filter. The transmittance is then computed for each frequency, and their squared error w.r.t. the "perfect filter" (i.e., with no error) is computed. The model's output is the square root over the sum of these squared errors.

A unique i.i.d. sample of size 1000 of these 13 inputs has been simulated, on which the model's output has been computed. A given-data estimation method is used since this model is fairly expensive to evaluate (then applying the Monte Carlo scheme is not feasible). Hence, the Shapley effects and PMEs are computed using the nearest-neighbor procedure (see Section 5.1), with an arbitrarily chosen number of neighbors equal to 6.

5.2.1. Importance quantification

Figure 2 displays the Shapley effects and PMEs estimates. The intervals are the 5% and 95% empirical quantiles computed on 100 estimation repetitions. For each repetition, both indices have been estimated on a random selection of 80% of the initial dataset.

The Shapley effects of the different inputs vary between 5% and 11%, while the PMEs vary between 2% and 24%. Even if the Shapley effects of I_5 and I_9 are slightly larger than the others, no particular

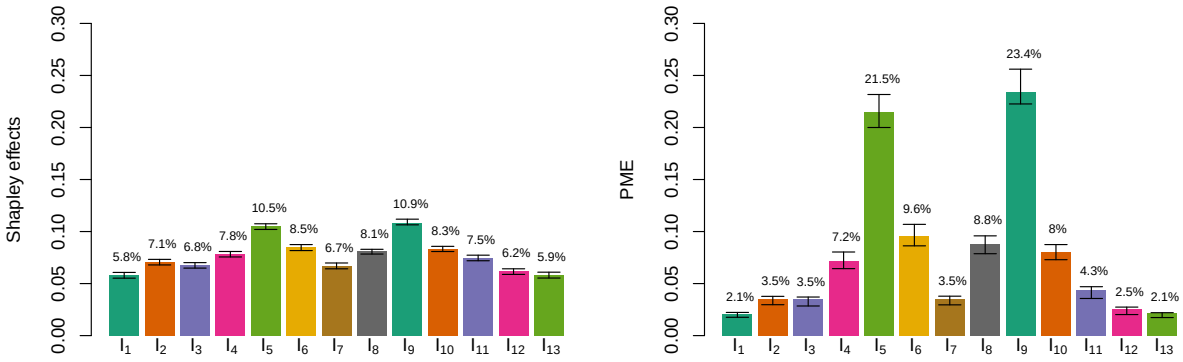

Figure 2: Shapley effects and PMEs estimates using the nearest-neighbor procedure for the interference filter model. The vertical error bars represent the 90% intervals of the estimates.

input emerges as predominantly influential, and none emerges as fairly non-influential. However, the PME is more discriminant in the influence repartition. I_5 and I_9 stand out as very influential, I_4, I_6, I_8 and I_{10} seem to bear some importance, while I_1, I_2, I_3, I_7, I_{11}, I_{12} and I_{13} can be considered as non-influential.

This more pronounced discriminating power can be explained by the difference in the redistribution process of the PMEs and the Shapley effects, especially in this case where the inputs are highly correlated. It highlights the more discriminatory ability of the PMEs for influence ranking in situations of highly correlated inputs, where the Shapley effects tend to equalize the influence between the inputs in this situation.

5.2.2. Input selection and surrogate model performance

The PME values of non influential inputs are not worth zero but are relatively close to zero (the PMEs of I_1 and I_{13} are smaller than 2%, and the PMEs of I_2, I_3, I_7, I_{11}, and I_{12} are smaller than 3%). However, as the nearest-neighbor procedure used to estimate the PME is known to have a bias, we cannot infer the non-exogeneity of these inputs. To verify if these inputs can be considered spurious, the impacts of including them in reduced models have to be measured.

The predictive capabilities of three different Gaussian process (GP) surrogate models [40] are compared. For each model, dimension reduction is performed by selecting subsets of inputs according to the previously discussed importance rankings:

- **$\mathbf{GP_1}$** - The inputs are selected with a 5% importance threshold applied on the Shapley effects: the 13 inputs are kept in the GP. Then, this GP corresponds to the one without dimension reduction;
- **$\mathbf{GP_2}$** - The inputs are selected with a 5%-threshold applied on the PMEs: only 6 inputs (I_4, I_5, I_6, I_8, I_9 and I_{10}) are kept to train the GP;
- **$\mathbf{GP_3}$** - The inputs are selected with a 2.2%-threshold applied on the PMEs: 2 inputs (I_1 and I_{13}) are removed from the initial 11 to train the GP.

The three surrogate models are trained on the initial 1000 observations and are parameterized by a constant trend and a 5/2-Matérn covariance kernel. The parameters have been estimated using a maximum likelihood scheme, by means of the `DiceKriging` R package [39].

To measure the predictive power of the models, their "predictivity coefficients" (i.e., the Q^2-metric, see, e.g., [12]) are computed and displayed in Table 4. Removing the two inputs with the lowest PMEs has a negligible impact on the model predictivity (shortfall in Q^2 of less than 0.4%), and removing the seven inputs with the lowest PMEs has a minor impact on the model predictivity (shortfall in Q^2 of less than 1%).

Model	Number of inputs	Selection Threshold	Q^2
$\mathbf{GP_1}$	13	Shapley Effects - 5%	99.48%
$\mathbf{GP_2}$	6	PMEs - 5 %	98.79%
$\mathbf{GP_3}$	11	PMEs - 2.2%	99.14%

Table 4: Predictivity coefficient of the three GP surrogate models.

This use case clearly illustrates the PMEs' usefulness in variable selection with highly correlated inputs for dimension reduction and surrogate modeling purposes. Overall, the PMEs favor the already influential inputs at the expense of the inputs they are correlated with, while the Shapley effects equalize importance amongst them. Combined with the ability to detect exogenous inputs, it makes the PME particularly suitable for screening purposes.

6. Discussion and perspectives

The main contribution of this paper is the adaptation to GSA of the proportional values. An extension of the original allocation is proposed for Sobol' cooperative games, leading to novel GSA indices: the proportional marginal effects. They fundamentally differ from the Shapley effects in two ways. First, it is proved that they detect exogenous inputs by granting them zero allocation, even when the inputs are dependent. Second, they are more discriminant than the Shapley values for highly correlated inputs. They remain intrinsically interpretable as shares of variance of the model's output. It is illustrated through analytical toy cases and use cases that the proposed PMEs, used in conjunction with the Shapley effects, can draw a more precise picture of the intricacies of black-box models.

These indices can be estimated in two ways: based either on a Monte Carlo sampling scheme or given data using nearest-neighbor procedures. Moreover, their computation relies on the same conditional elements' estimations as the Shapley effects: both indices can be computed simultaneously without additional model evaluations. However, the computational burden associated with their estimation remains a drawback. They require calculating an exponential number $(2^d - 1)$ of Sobol indices. The same problem has been highlighted for the Shapley effects estimation. An avenue to alleviate some of the computations would be to use surrogate models to estimate the conditional elements. For instance, random forests [1] or Gaussian process-based meta-models [26, 2] can be leveraged for that task, potentially reducing the need for costly numerical model evaluations. Additionally, the bias induced by using the nearest neighbor estimation method (which is the only one usable in costly application cases) does not guarantee the detection of exogenous inputs by PMEs. New given-data algorithms are required.

As seen in this paper, the Shapley effects and the PMEs are designed to extract different insights, the interest of which depends on the UQ task one is dealing with. While the PMEs are a reasonable option for factor fixing and factor prioritization, the Shapley effects provide a tool for model exploration that allows for a good overview of all the inputs that might impact the output, even though it is only due to correlation with other inputs. Other allocations, such as weighted Shapley values [28] or proportional Shapley values [7], may be defined with different specific UQ tasks in mind, allowing for domain-specific tools for more accurate and relevant indices. In the machine learning interpretability literature, recent works, such as the one of [47] which calls correlation distorsion the Shapley's joke, have also proposed modified versions of Shapley values but only in an heuristic way.

Finally, while cooperative game theory is a relevant source for producing novel GSA indices, its intricacies remain poorly understood by both the UQ and ML interpretability communities. Cooperative games, in general, and the construction of allocations in particular, are inherently player-centric, while UQ and interpretability studies have historically been model-centric. Even if cooperative game theory is beneficial to define relevant and interpretable tools for GSA with dependent inputs, further work must be put into theoretically justifying their use in critical industrial studies.

Appendix A. Software and reproducibility of results

All the numerical tests have been performed using the `R` programming language. Every results and figures presented in this paper can be reproduced by means the openly accessible codes in a GitLab repository[1], as well as details on the packages used.

Appendix B. Proofs

Proof of Theorem 1. Let (D, v) be a nonnegative, monotonic cooperative game, let $A \subseteq D$ be a coalition, and denote $|A|$ the cardinality of A. Denote $\mathcal{S}_A$ the set of permutations of players in A. Let $\pi \in \mathcal{S}_A$, and for the sake of clarity, denote $|\pi| = |A|$, i.e., the number of elements in the permutation. Moreover, by convention,$v\left(C_0(\pi)\right) = v(\emptyset) = 0$ for any $\pi \in \mathcal{S}_D$. By monotonicity, $\forall j \in \{0, \ldots, |\pi| - 1\}$, one has,

$$0 \leq v\left(C_j(\pi)\right) \leq v\left(C_{j+1}(\pi)\right).$$

For any permutation $\pi \in \mathcal{S}_A$, let:

$$k_\pi(v) = \max\left\{j \in \{0, \ldots, |\pi|\} : v(C_j(\pi)) = 0\right\}.$$

For the sake of conciseness and readability, the argument v is omitted and the notation $k_\pi := k_\pi(v)$ is adopted. Let $(\epsilon_p)_{p\in\mathbb{N}}$ be a sequence such that:

$$\forall p \in \mathbb{N}, \epsilon_p > 0, \quad \text{and} \quad \lim_{p\to\infty} \epsilon_p = 0.$$

Let $\left((D, v_p)\right)_{p\in\mathbb{N}}$ be a sequence of positive, monotonic cooperative games defined, for any $p \in \mathbb{N}$ and for any $A \subseteq D$, as:

$$v_p(A) = \begin{cases} \epsilon_p & \text{if } v(A) = 0, \\ v(A) & \text{otherwise.} \end{cases}$$

Alternatively, one can notice that, for any $A \subseteq D$, $\forall \pi \in \mathcal{S}_A$, $\forall j \in \{0, \ldots, |\pi|\}$,

$$v_p\big(C_j(\pi)\big) = \begin{cases} \epsilon_p & \text{if } j \leq k_\pi, \\ v(C_j(\pi)) & \text{otherwise.} \end{cases} \tag{B.1}$$

Let $p \in \mathbb{N}$, and from the recursive definition of the PV (see, Definition 3) of the positive games (D, v_p), one has, for any $i \in D$:

$$\mathrm{PV}_i = \frac{\sum_{\pi\in\mathcal{S}_{D_{-i}}} \prod_{m=1}^{d-1} v_p\left(C_m(\pi)\right)^{-1}}{\sum_{\sigma\in\mathcal{S}_D} \prod_{m=1}^{d} v_p\left(C_m(\sigma)\right)^{-1}}.$$

For the sake of conciseness and clarity, for any $\pi \in \mathcal{S}_A$, $A \subseteq D$, let us introduce the following notation:

$$\Upsilon_k^l(\pi, v) = \begin{cases} \prod_{j=k}^{l} v\left(C_j(\pi)\right)^{-1} & \text{if } k \leq l, \\ 1 & \text{otherwise.} \end{cases}$$

One then has that, for any $i \in D$:

$$\begin{aligned} \mathrm{PV}_i &= \frac{\sum_{\pi\in\mathcal{S}_{D_{-i}}} \Upsilon_1^{d-1}(\pi, v_p)}{\sum_{\sigma\in\mathcal{S}_D} \Upsilon_1^{d}(\sigma, v_p)} = \frac{\sum_{\pi\in\mathcal{S}_{D_{-i}}} \Upsilon_1^{k_\pi}(\pi, v_p)\Upsilon_{k_\pi+1}^{d-1}(\pi, v_p)}{\sum_{\sigma\in\mathcal{S}_D} \Upsilon_1^{k_\sigma}(\sigma, v_p)\Upsilon_{k_\sigma+1}^{d}(\sigma, v_p)} \\ &= \frac{\sum_{\pi\in\mathcal{S}_{D_{-i}}} \epsilon_p^{-k_\pi}\Upsilon_{k_\pi+1}^{d-1}(\pi, v_p)}{\sum_{\sigma\in\mathcal{S}_D} \epsilon_p^{-k_\sigma}\Upsilon_{k_\sigma+1}^{d}(\sigma, v_p)}, \end{aligned}$$

[1] https://gitlab.com/milidris/PME

since, from Eq. (B.1), for any $\pi \in \mathcal{S}_A$, $A \subseteq D$:

$$\Upsilon_1^{k_\pi}(\pi, v_p) = \prod_{j=1}^{k_\pi} v_p\big(C_j(\pi)\big)^{-1} = \epsilon_p^{-k_\pi}.$$

Denote, for any $i \in D$, $k_{\max}^{-i}$ the size of the largest null coalition in D_{-i}, i.e.,

$$k_{\max}^{-i} = \max_{A \in \mathcal{P}(D_{-i}) \text{ s.t. } v(A)=0} |A|,$$

and let $k_{\max}$ be the size of the largest null coalition in D, and notice that necessarily,

$$\forall i \in D, \forall \pi \in \mathcal{S}_{D_{-i}}, \quad k_{\max}^{-i} \leq k_{\max}. \tag{B.2}$$

Moreover, denote, $\mathcal{R}_{\max}$ and $\mathcal{R}$, the two following sets of permutations:

$$\mathcal{R}_{\max} = \{\pi \in \mathcal{S}_D : k_\pi = k_{\max}\}, \quad \text{and} \quad \mathcal{R} = \{\pi \in \mathcal{S}_D : k_\pi < k_{\max}\}$$

Since $\mathcal{R}_{\max} \cup \mathcal{R} = \mathcal{S}_D$, one has that:

$$\begin{aligned}\sum_{\pi \in \mathcal{S}_D} \epsilon_p^{-k_\pi} \Upsilon_{k_\pi+1}^d(\pi, v) &= \sum_{\pi \in \mathcal{R}_{\max}} \epsilon_p^{-k_{\max}} \Upsilon_{k_\pi+1}^d(\pi, v) + \sum_{\pi \in \mathcal{R}} \epsilon_p^{-k_\pi} \Upsilon_{k_\pi+1}^d(\pi, v) \\ &= \epsilon_p^{-k_{\max}} \left(\sum_{\pi \in \mathcal{R}_{\max}} \Upsilon_{k_\pi+1}^d(\pi, v) + \sum_{\pi \in \mathcal{R}} \epsilon_p^{k_{\max}-k_\pi} \Upsilon_{k_\pi+1}^d(\pi, v) \right).\end{aligned}$$

Similarly, for any $i \in D$, denote $\mathcal{R}_{\max}^{-i} = \{\pi \in \mathcal{S}_{D_{-i}} : k_\pi = k_{\max}^{-i}\}$, and $\mathcal{R}^{-i} = \{\pi \in \mathcal{S}_{D_{-i}} : k_\pi < k_{\max}^{-i}\}$. Since $\mathcal{R}_{\max}^{-i} \cup \mathcal{R}^{-i} = \mathcal{S}_{D_{-i}}$, one has that:

$$\begin{aligned}\sum_{\pi \in \mathcal{S}_{D^{-i}}} \epsilon_p^{-k_\pi} \Upsilon_{k_\pi+1}^{d-1}(\pi, v) &= \sum_{\pi \in \mathcal{R}_{\max}^{-i}} \epsilon_p^{-k_\pi} \Upsilon_{k_\pi+1}^{d-1}(\pi, v) + \sum_{\pi \in \mathcal{R}^{-i}} \epsilon_p^{-k_\pi} \Upsilon_{k_\pi+1}^{d-1}(\pi, v) \\ &= \sum_{\pi \in \mathcal{R}_{\max}^{-i}} \epsilon_p^{-k_{\max}^{-i}} \Upsilon_{k_\pi+1}^{d-1}(\pi, v) + \sum_{\pi \in \mathcal{R}^{-i}} \epsilon_p^{-k_\pi} \Upsilon_{k_\pi+1}^{d-1}(\pi, v)\end{aligned}$$

It entails that:

$$\mathrm{PV}_i = \frac{\sum_{\pi \in \mathcal{R}_{\max}^{-i}} \epsilon_p^{k_{\max}-k_{\max}^{-i}} \Upsilon_{k_\pi+1}^{d-1}(\pi, v) + \sum_{\pi \in \mathcal{R}^{-i}} \epsilon_p^{k_{\max}-k_\pi} \Upsilon_{k_\pi+1}^{d-1}(\pi, v)}{\sum_{\sigma \in \mathcal{R}_{\max}} \Upsilon_{k_\sigma+1}^d(\sigma, v) + \sum_{\sigma \in \mathcal{R}} \epsilon_p^{k_{\max}-k_\sigma} \Upsilon_{k_\sigma+1}^d(\sigma, v)}.$$

Denote $\tilde{D} = D \cup \{0\}$ and use the convention that $\mathcal{R}^{-0} = \mathcal{R}$. Then, notice that for any $i \in \tilde{D}$:

$$\forall \pi \in \mathcal{R}^{-i}, \quad k_\pi < k_{\max}. \tag{B.3}$$

From Eq. (B.3), one can notice, for any $i \in \tilde{D}$:

$$\lim_{p \to \infty} \sum_{\pi \in \mathcal{R}^{-i}} \epsilon_p^{k_{\max}-k_\pi} \Upsilon_{k_\pi+1}^{d-i}(\pi, v) = 0$$

and additionally, from Eq. (B.2), notice that for any $i \in D$:

$$\lim_{p \to \infty} \sum_{\pi \in \mathcal{R}_{\max}^{-i}} \epsilon_p^{k_{\max}-k_{\max}^{-i}} \Upsilon_{k_\pi+1}^{d-1}(\pi, v) = \begin{cases} \sum_{\pi \in \mathcal{R}_{\max}^{-i}} \Upsilon_{k_\pi+1}^{d-1}(\pi, v) & \text{if } k_{\max} = k_{\max}^{-i} \\ 0 & \text{otherwise.} \end{cases}$$

Denote:

$$\mathrm{PV}^0\big((D, v)\big) = \lim_{p \to \infty} \mathrm{PV}\big(D, v_p\big),$$

and notice that, for any $i \in D$:

$$\mathrm{PV}_i^0 = \begin{cases} \dfrac{\sum_{\pi \in \mathcal{R}_{\max}^{-i}} \Upsilon_{k_\pi+1}^{d-1}(\pi, v)}{\sum_{\sigma \in \mathcal{R}_{\max}} \Upsilon_{k_\sigma+1}^{d-1}(\sigma, v)} & \text{if } k_{\max} = k_{\max}^{-i}, \\ 0 & \text{otherwise.} \end{cases}$$

For any $i \in D$, the condition $k_{\max} = k_{\max}^{-i}$ is equivalent to having a coalition $A \subseteq D_{-i}$ such that $|A| = k_{\max}$ and $v(A) = 0$. On the other hand, the complement of this condition is that i must be in every coalition $A \subseteq D$ such that $|A| = k_{\max}$ and $v(A) = 0$. In the following, the set containing all such coalitions is denoted $\mathcal{K} = \underset{A \in \mathcal{P}(D) \text{ s.t. } v(A)=0}{\operatorname{argmax}} |A|$.

For any $i \in D$, and assuming that $k_{\max}^{-i} = k_{\max}$, one can notice that $\mathcal{R}_{\max}^{-i}$ only contains the permutations $\pi \in \mathcal{S}_{D_{-i}}$ such that $v\left(C_{k_{\max}}(\pi)\right) = 0$, and by monotonicity, this implies that for any $\pi \in \mathcal{R}_{\max}^{-i}$:

$$v\left(C_1(\pi)\right) = v\left(C_2(\pi)\right) = \cdots = v\left(C_{k_{\max}-1}(\pi)\right) = v\left(C_{k_{max}}(\pi)\right) = 0,$$

and that for $k_{\max} < k \leq |\pi|$,

$$v\left(C_k(\pi)\right) > 0.$$

For any $i \in D$, denote $\mathcal{K}_{-i} = \left\{A \in \mathcal{K} : i \notin A\right\}$, and notice that $\mathcal{R}_{\max}^{-i}$ is necessarily composed of permutations having permutations of elements in $\mathcal{K}_{-i}$ as their first $k_{\max}$ elements. In other words, for every $\pi \in \mathcal{R}_{\max}^{-i}$,

$$C_{k_{\max}}(\pi) \in \mathcal{K}_{-i}.$$

Thus, for any $i \in D$, one has that:

$$\begin{aligned} \sum_{\pi \in \mathcal{R}_{\max}^{-i}} \Upsilon_{k_\pi+1}^{d-1}(\pi, v) &= \sum_{A \in \mathcal{K}_{-i}} k_{\max}! \sum_{\pi \in \mathcal{S}_{D_{-i} \setminus A}} \Upsilon_1^{|\pi|}(\pi, v_A) \\ &= k_{\max}! \sum_{A \in \mathcal{K}_{-i}} \sum_{\pi \in \mathcal{S}_{D_{-i} \setminus A}} \prod_{k=1}^{|\pi|} v(A \cup C_k(\pi))^{-1} \\ &= k_{\max}! \sum_{A \in \mathcal{K}_{-i}} R(D_{-i} \setminus A, v_A)^{-1} \end{aligned}$$

where for any $B \subseteq D \setminus A$, $v_A(B) = v(A \cup B)$, and using results from [16] on the ratio potential. This leads to the following rewriting of PV^0, for any $i \in D$:

$$\mathrm{PV}_i^0 = \begin{cases} 0 & \text{if } i \in \bigcap\limits_{A \in \mathcal{K}} A \\ \dfrac{\sum_{A \in \mathcal{K}_{-i}} R(D_{-i} \setminus A, v_A)^{-1}}{\sum_{A \in \mathcal{K}} R(D \setminus A, v_A)^{-1}} & \text{otherwise.} \end{cases}$$

Finally, notice that for any positive game (D, v), i.e., , where v is positively valued, then necessarily, for any permutation and sub-permutations π of players $k_\pi = k_{\max} = 0$ and thus $\mathcal{K} = \{\emptyset\}$. Then for any $i \in D$, $\mathcal{K}_{-i} = \{\emptyset\}$ and,

$$\mathrm{PV}_i^0 = \frac{R(D, v)}{R(D_{-i}, v)} = \mathrm{PV}_i,$$

and hence the allocation $\mathrm{PV}^0\big((D, v)\big)$ is a continuous extension of $\mathrm{PV}\big((D, v)\big)$ to cooperative games with nonnegative value function. □

Proof of Lemma 1. Let $A \subseteq D$. First, assume that $S_A^T = 0$, then necessarily,

$$\mathbb{V}\left(G(X) \mid X_{\overline{A}}\right) := \mathbb{E}\left[\left(G(X) - \mathbb{E}\left[G(X) \mid X_{\overline{A}}\right]\right)^2 \mid X_{\overline{A}}\right] = 0 \text{ a.s.}$$

which can only be attained, by non-negativity of the squared distance, if

$$G(X) = \mathbb{E}\left[G(X) \mid X_{\overline{A}}\right] \text{ a.s.}$$

Now assume that $G(X) = \mathbb{E}\left[G(X) \mid X_{\overline{A}}\right]$ a.s.. Then necessarily,

$$\mathbb{V}\left(G(X) \mid X_{\overline{A}}\right) = 0 \text{ a.s.}$$

implying that $S_A^T = 0$, which proves Lemma 1. □

Proof of Proposition 1. Let $E \subseteq D$ be a subset of variables. Assume that X_E is an L^2-exogenous vector. This entails that $\exists f \in L^2(P_{X_{\overline{E}}})$ such that:

$$G(X) = f(X_{\overline{E}}) \text{ a.s.}$$

Recall that the conditional expectation of $G(X)$ w.r.t. $X_{\overline{E}}$ is the unique projection defined as:

$$\mathbb{E}\left[G(X) \mid X_{\overline{E}}\right] = \underset{h \in L^2\left(P_{X_{\overline{E}}}\right)}{\operatorname{argmin}} \mathbb{E}\left[\left(G(X) - h\left(X_{\overline{E}}\right)\right)^2\right],$$

One can notice that, since $f \in L^2(P_{X_{\overline{E}}})$ and $Y = f(X_{\overline{E}})$ a.s., then it necessarily minimizes the projection of $G(X)$ onto $L^2(P_{\overline{E}})$, leading to

$$G(X) = f(X_{\overline{E}}) = \mathbb{E}\left[G(X) \mid X_{\overline{E}}\right] \text{ a.s.}$$

and by Lemma 1, it entails that $S_E^T = 0$. Reciprocally, if $S_E^T = 0$, by Lemma 1, $G(X) = f(X_{\overline{E}})$ *a.s.* with $f(X_{\overline{E}}) = \mathbb{E}\left[G(X) \mid X_{\overline{E}}\right]$ and E is an exogenous vector. Then E is an exogenous vector is equivalent to $S_E^T = 0$.

Now let E be the coalition containing all the exogenous variables. Under Assumption 1, E is an exogenous vector and then, from the previous equivalence, $S_E^T = 0$. Suppose that there exists another subset $A \subseteq D$ such that $A \neq E$ and $|A| \geq |E|$ veryfing $S_A^T = 0$. Then, $A \setminus (A \cap E) \neq \emptyset$ and for any variable $i \in A \setminus (A \cap E)$, one has $0 \leq S_i^T \leq S_A^T = 0$ since S^T is monotonic w.r.t. set inclusion. Then $S_i^T = 0$ and from the previous equivalence, i is an exogenous variable, which is impossible since $i \notin E$ and E contains all the exogenous variables. Then one can not find any coalition A such that $|A| \geq |E|$, $A \neq E$ and $S_A^T = 0$.

Then, for the value function $v = S^T$, one has that $\mathcal{K} = \underset{A \in \mathcal{P}(D) \text{ s.t. } v(A)=0}{\operatorname{argmax}} |A| = \{E\}$. Also, from Theorem 1 one has that $PV_i = 0 \iff i \in \underset{A \in \mathcal{K}}{\cap} A$. Then , $PME_i = 0 \iff i \in E$. □

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Proportional marginal effects for global sensitivity analysis: Supplementary materials

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Contents

1 Random order model allocations

1.1 Cooperative game theory and allocations

A cooperative game is a tuple (D, v) where $D = \{1, \dots, d\}$ is a set of d players and $v : \mathcal{P}(D) \to \mathbb{R}$ is the *value function*, i.e., an application that maps a value to every possible coalition of players. Usually, v is assumed to be *monotonically increasing*, meaning that, for any two sets T and A such that $T \subseteq A \in \mathcal{P}(D)$, one has $v(T) \leq v(A)$. In other words, the value of a coalition A cannot be lower than the value of a sub-coalition $T \subseteq A$. In the following, cooperative games with monotonically increasing value functions are referred to as "monotonic cooperative games". Moreover, if the value function v takes values in $\mathbb{R}_*^+$ (resp. in $\mathbb{R}^+$), the corresponding cooperative game is referred to as "positive (resp. nonnegative) cooperative game".

One of the key aspects of cooperative games is the notion of *allocation*. In general, allocations can be understood as a decomposition of the quantity $v(D)$ in d elements, each one being allocated to a specific player. When it comes to Sobol' cooperative games, it translates to assigning a share of the output's variance $\mathbb{V}(Y)$ to each input in the model, with limited assumptions on the probabilistic structure between the inputs (in particular, no independence is assumed between the inputs). Formally, an allocation can be understood as a mapping ϕ that associates, to a cooperative game (D, v), a real-valued vector $(\phi_1, \dots, \phi_d)^\top \in \mathbb{R}^d$.

The *Shapley values*, are a particular example of allocations. For any cooperative game (D, v), it is uniquely characterized as the allocation $\phi\big((D, v)\big)$ verifying a set of four distinct axioms:

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1. **Efficiency**: $\sum_{i=1}^{d} \phi_i = v(D)$;
2. **Symmetry**: $\forall i, j \in D$ with $i \neq j$, if $v(A \cup \{i\}) = v(A \cup \{j\})$ for all $A \in \mathcal{P}(D)$, then $\phi_i = \phi_j$;
3. **Null player**: $\forall i \in D$, if $v(A \cup \{i\}) = v(A)$ for all $A \in \mathcal{P}(D)$, then $\phi_i = 0$;
4. **Additivity**: If two cooperative games (D, v) and (D, v') have Shapley values ϕ and ϕ' respectively, then the cooperative game $(D, v + v')$ has Shapley values $\phi_j + \phi'_j$ for $j \in D$.

For any cooperative game (D, v), its Shapley values can be expressed analytically, for any $i \in D$, as:

$$\text{Shap}_i\big((D, v)\big) = \frac{1}{d} \sum_{A \subseteq D_{-i}} \binom{d-1}{|A|}^{-1} \left[v(A \cup \{i\}) - v(A)\right]. \tag{1}$$

This original formulation attributed to [6] can be interpreted as a weighted average, over every possible coalition A, of the contribution of a player i to that coalition A. This contribution is quantified by the quantity $v(A \cup \{i\}) - v(A)$, often called the "*marginal contribution*" of the player i to the coalition A in the literature. The weighting scheme can be understood as the proportion of permutations (or orderings) of D such that i appears after the players in A. While this interpretation can be hard to understand, defining the Shapley values in terms of players permutations allows for a better understanding of its underlying sharing mechanism, as it is done in the following.

1.2 Random order models

A particular class of allocations, known as *random order models* [8, 3], allows to define allocations based on orderings of players, instead of reasoning in terms of coalitions as in Eq. (1). Let $\mathcal{S}_D$ be symmetric group on D (the set of all permutations of D). Let $\pi = (\pi_1, \ldots, \pi_d) \in \mathcal{S}_D$ be a particular permutation, and for any $i \in D$, denote $\pi(i) = \pi_i^{-1}$ its inverse (i.e., the position of i in π, such that $\pi_{\pi(i)} = i$). Then, one can define the following set of players, for any $i \in \{0, \ldots, d\}$:

$$C_i(\pi) = \{\pi_j : j \leq i\}. \tag{2}$$

$C_i(\pi)$ is the set of the i-th first players in the ordering π, with the convention that, for any permutation, $C_0(\pi) = \emptyset$. As an illustration, let $D = \{1, 2, 3\}$, and let $\pi = (2, 1, 3) \in \mathcal{S}_D$. Then,

$$\pi(1) = 2, \quad \pi(2) = 1, \text{ and } \quad \pi(3) = 3.$$

Moreover,

$$C_{\pi(1)}(\pi) = C_2(\pi) = \{1, 2\}, \quad C_{\pi(2)}(\pi) = C_1(\pi) = \{2\}, \quad C_{\pi(3)}(\pi) = C_3(\pi) = \{1, 2, 3\}$$

As their names suggest, random order models endow $\mathcal{S}_D$ with a probabilistic structure. For any game (D, v), the set of random order model allocations (or probabilistic allocations) contains every allocation $\phi\big((D, v)\big)$ that can be written, for any $i \in D$, as:

$$\begin{aligned}\phi_i &= \sum_{\pi \in \mathcal{S}_D} p(\pi) \left[v\left(C_{\pi(i)}(\pi)\right) - v\left(C_{\pi(i)-1}(\pi)\right)\right] \\ &= \mathbb{E}_{\pi \sim p}\left[v\left(C_{\pi(i)}(\pi)\right) - v\left(C_{\pi(i)-1}(\pi)\right)\right]\end{aligned}$$

where p is a probability mass function over the orderings of D. For a player i, its random order allocation can be interpreted as the expectation over the permutations π of D with respect to p, of the marginal contributions of i to the coalitions formed by $C_{\pi(i)-1}(\pi)$. The random order model allocations are always *efficient* and, when dealing with monotonic games, *nonnegative* (i.e., $\phi_i \geq 0$ for any $i \in D$)

[8]. The Shapley values, in particular, can be expressed as a random order model allocation, under the particular choice of p as a discrete uniform distribution over $\mathcal{S}_D$, which echoes Eq. (1):

$$\mathrm{Shap}_i\big((D,v)\big) = \frac{1}{d!}\sum_{\pi\in\mathcal{S}_D}\left[v\left(C_{\pi(i)}(\pi)\right) - v\left(C_{\pi(i)-1}(\pi)\right)\right]. \tag{3}$$

Random order models allow to apprehend allocations *dynamically* (see Section 1.3), meaning that coalitions are formed regarding orderings, as opposed to the pure coalition point of view displayed in Eq. (1). In this setting, Shapley values can then be understood as a maximum entropy a priori (i.e., uniform over $\mathcal{S}_D$) about this dynamic. In the light of this equivalent expression, L. S. Shapley himself interpreted the Shapley values as "*[...] an a priori assessment of the situation, based on either ignorance or disregard of the social organization of the players*" [7].

1.3 Random order model allocations and dual games

The notion of the *dual* of a cooperative game is also of interest in the present paper. On the one hand, under the game theory paradigm presented previously, the aim of the value function v is to quantify the "value produced" by a coalition of players (e.g., the monetary value). On the other hand, the dual of a cooperative game focuses on the "worth", or "bargaining power" of a coalition, i.e., the shortfall in value due to a coalition [2, 3]. The dual of a cooperative game (D,v) is usually denoted by (D,w) where w is defined, for any $A\in\mathcal{P}(D)$ as:

$$w(A) = v(D) - v(D\setminus A). \tag{4}$$

The quantities $w(A)$ are often referred to as the *marginal contribution of a coalition A to the grand coalition D* in the literature, and is often interpreted as a measure of how crucial a coalition is in producing $v(D)$. For the sake of conciseness, in the following, one refers to $w(A)$ as the *marginal contribution of the coalition A*. The dual (D,w) of (D,v) is also a cooperative game, and thus one can seek to construct relevant allocations for this game.

Following up this idea of dual game, one can draw a parallel between random order model allocations and the well-known "forward" and "backward" variable selection procedures. Figure 1 illustrates this similarity. Formally, one can notice that, for a player i and any permutation $\pi\in\mathcal{S}_d$, one has:

$$w\left(C_{\pi(i)}(\pi)\right) - w\left(C_{\pi(i)-1}(\pi)\right) = v\left(D\setminus C_{\pi(i)-1}(\pi)\right) - v\left(D\setminus C_{\pi(i)}(\pi)\right). \tag{5}$$

A random order model allocation of the dual of a cooperative game can be understood as the expected (with respect to a probability mass function p over $\mathcal{S}_D$) marginal contribution of a player i to the players that *follows* in the orderings' dynamic, whereas for the initial cooperative game, it is the expected marginal contribution of i to the players that *precedes* in the orderings' dynamic.

It is important to note that the Shapley values of a cooperative game are equal to the ones of its dual (see, [4] Lemma 2.7), however, this behavior do is not intrinsic to every random order model allocation.

2 Additional use-cases

2.1 Analytical toy-case : Unbalanced linear model

Beyond the detection of exogenous inputs, the Shapley effects and the PMEs fundamentally differ on their redistribution process. While the Shapley effects allocate importance in an egalitarian fashion, the PME follows a proportional principle. This toy-case aims at highlighting this difference, by introducing a coefficient in a linear model with three correlated Gaussian inputs. This use-case is referred to as

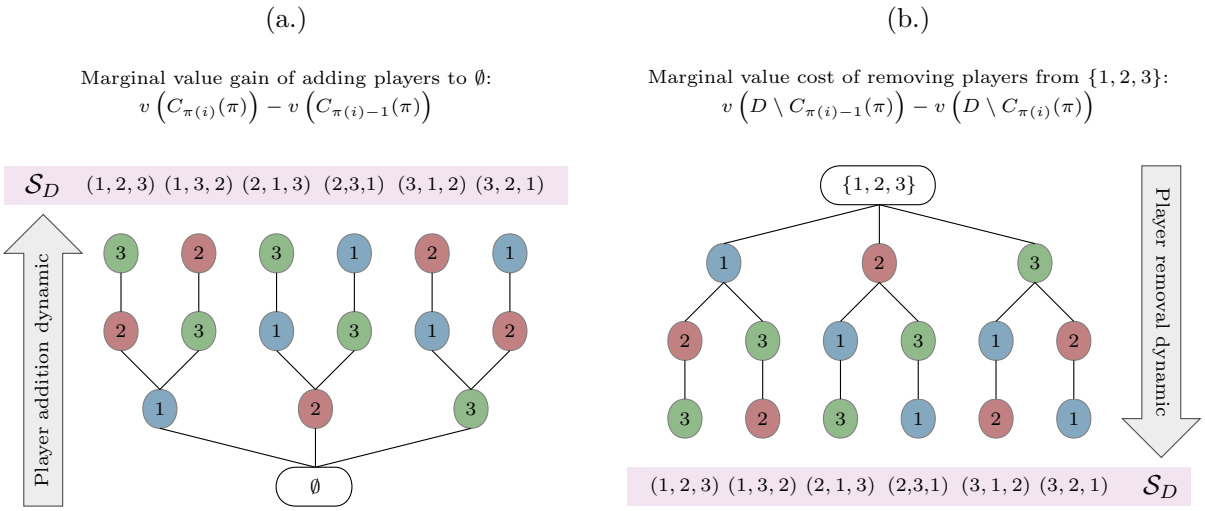

Figure 1: Analogy between random order model allocations and the forward-backward procedures for $D = \{1, 2, 3\}$: (a.) represents the allocation of a cooperative game as a forward procedure; (b.) illustrates the allocation of its dual as a backward procedure. The allocation of player 1 (resp. player 2 and 3) is the expected marginal gain (for a cooperative game (D, v)) or cost (for its dual (D, w)) computed for the blue (resp. red and green) ordering positions, weighted according to a probabilistic distribution over $\mathcal{S}_D$.

unbalanced since the three linear coefficient are different. This toy-case writes:

$$Y = G(X) = X_1 + \beta X_2 + X_3, \quad X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \rho \\ 0 & \rho & 1 \end{pmatrix} \right), \tag{6a}$$

$$\mathbb{V}(Y) = 2 + \beta^2 + 2\rho\beta. \tag{6b}$$

The analytical shares of output variance, according to the Shapley effects and the PMEs, are given in Table 2.1.

$\mathbb{V}(Y) \times \mathrm{Sh}_1 = 1$	$\mathbb{V}(Y) \times \mathrm{PME}_1 = 1$
$\mathbb{V}(Y) \times \mathrm{Sh}_2 = \beta^2 + \beta\rho + \frac{1}{2}\rho^2(1-\beta^2)$	$\mathbb{V}(Y) \times \mathrm{PME}_2 = \frac{\beta^2(1+\beta^2+2\rho\beta)}{(1+\beta^2)}$
$\mathbb{V}(Y) \times \mathrm{Sh}_3 = 1 + \beta\rho - \frac{1}{2}\rho^2(1-\beta^2)$	$\mathbb{V}(Y) \times \mathrm{PME}_3 = \frac{(1+\beta^2+2\rho\beta)}{(1+\beta^2)}$

Table 1: Reference analytical values for Shapley effects and PMEs (toy-case 2.1).

One can notice that, by considering the *balanced* case (i.e., $\beta = 1$), the Shapley effects and PMEs are equal. However, as soon as the model is unbalanced, one can notice that both allocations behave in a completely different fashion as soon as ρ approaches 1. Using an asymptotic-analysis-based reasoning,

one can obtain the following set of resulting approximation:

$$\mathrm{Sh}_1 = \mathrm{PME}_1 \xrightarrow[\rho\to 1]{} \frac{1}{2+\beta^2+2\beta} \xrightarrow[\beta\to\infty]{} 0, \tag{7a}$$

$$\mathrm{Sh}_2, \mathrm{Sh}_3 \xrightarrow[\rho\to 1]{} \frac{\frac{1}{2}\beta^2+\beta+\frac{1}{2}}{2+\beta^2+2\beta} \xrightarrow[\beta\to\infty]{} \frac{1}{2}, \tag{7b}$$

$$\mathrm{PME}_2 \xrightarrow[\rho\to 1]{} \frac{\beta^2(1+\beta^2+2\beta)}{(2+\beta^2+2\beta)(1+\beta^2)} \xrightarrow[\beta\to\infty]{} 1, \tag{7c}$$

$$\mathrm{PME}_3 \xrightarrow[\rho\to 1]{} \frac{(1+\beta^2+2\beta)}{(2+\beta^2+2\beta)(1+\beta^2)} \xrightarrow[\beta\to\infty]{} 0. \tag{7d}$$

In other words, in extreme cases of positive linear correlation between X_2 and X_3, the Shapley effects allocates half the importance to each input despite a fairly high β value in favor of X_2. The PMEs, on the other hand, tend to favor X_2 by granting it the whole variance, despite the high correlation with X_3. This behavior highlights the "egalitarian vs. proportional" behavior of both types of effects: the Shapley effects tend to consider X_2 and X_3 as equally important due to their high correlation, while the PMEs favor X_3 in regards of its high linear coefficient.

While these results inform on the asymptotic behavior of both indices, their difference can also be highlighted for punctual values of ρ and β. Figure 2 illustrates the behavior of both indices w.r.t. ρ, for two different values of β (namely, 2 and 10). Whenever $\beta = 2$, one can notice that PME_2 increases w.r.t. ρ, while Sh_2 decreases after $\rho \simeq -0.24$, and both indices are concave w.r.t. ρ. On the other hand, Sh_3 is convex w.r.t. ρ and becomes increasing at $\rho \simeq -0.54$, while PME_3 remains concave increasing. At extreme values of ρ (i.e., close to -1 or to 1), one can notice that Sh_2 and Sh_3 are considered equally important. Furthermore, one can notice that $\mathrm{PME}_2 > \mathrm{PME}_3$, whatever the magnitude of their correlation. Increasing β to 10 exacerbates this behavior of the Shapley effects. However, the PMEs behave differently: X_1 and X_3 are given a negligible part of variance, while X_2 is granted a seemingly constant share, w.r.t. ρ, hovering around 98%.

In conclusion, in this unbalanced case, the proportional redistribution property of the PME allows for a clearer importance hierarchy, even in situation of extreme correlation. On the other hand, the Shapley effect tends to the even importance out between the correlated inputs, leading to a potentially indecisive importance hierarchy.

2.2 Modified Ishigami model with a correlated exogenous input

In order to further study the behavior of the PME, the Ishigami model, well-known in GSA (see, e.g., [1]), is first considered. The Ishigami model is given by

$$G(X) = \sin(X_1) + 7\sin^2(X_2) + 0.1X_3^4\sin(X_1).$$

In our study, the following probabilistic structure of the inputs is considered:

$$X = \begin{pmatrix} X_1 \\ \vdots \\ X_4 \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}, \begin{pmatrix} (\pi/3)^2 & 0 & 0 & \rho \\ 0 & (\pi/3)^2 & 0 & 0 \\ 0 & 0 & (\pi/3)^2 & 0 \\ \rho & 0 & 0 & (\pi/3)^2 \end{pmatrix} \right).$$

One can notice that X_4 is, by design, an exogenous input, but it is linearly correlated to X_1 by means of the parameter $\rho \in (-1, 1)$. The Shapley effects and the PMEs are estimated using a Monte Carlo procedure, with chosen sample sizes $N_v = 10^5$, $N_o = 2 \times 10^3$ and $N_i = 300$, for various values of ρ (from -0.99 to 0.99 with a step of 0.01). Each Monte Carlo estimation has been independently repeated 200 times in order to obtain confidence intervals. The results are provided in Fig. 3.

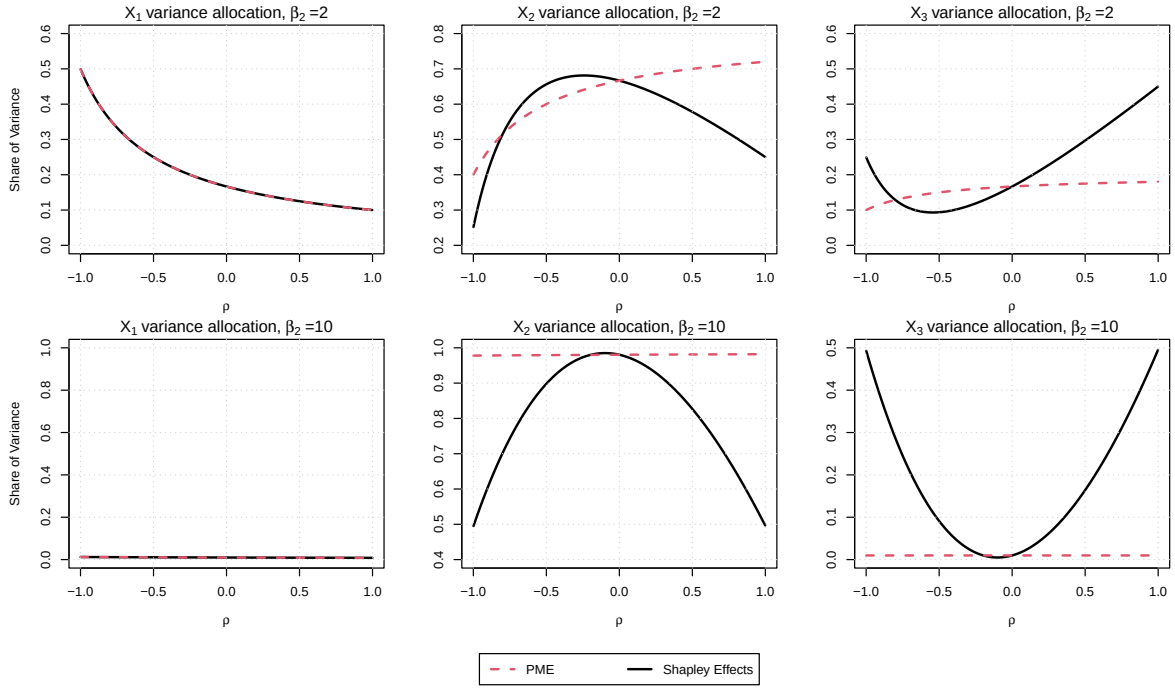

Figure 2: PMEs and Shapley effects w.r.t. ρ (toy-case 2.1). Top row depicts the allocations for $\beta = 2$ while the bottom row is for $\beta = 10$.

First, one can notice a strong influence of X_2, whose PMEs and Shapley effects are equal and constant along ρ. This result is expected, since X_2 has no interaction or correlation with other inputs in the Ishigami model, and hence its importance should not be subject to variation w.r.t. the correlation intensity. Second, focusing on X_1 and X_4, one can notice the same behavior of the Shapley effects as depicted previously. Despite the fact that X_4 is exogenous, in situation of extreme correlation, Sh_4 can be as high as Sh_1, which echoes the results in [5], but effectively grants a zero allocation to X_4 whenever both inputs are independent (i.e., $\rho = 0$). However, their PMEs differ, in the sense that PME_1 is constant w.r.t. ρ, while PME_4 is equal to zero whatever the correlation value. Hence X_4 is effectively detected as being exogenous. Third, one can notice that Sh_3 does vary w.r.t. ρ, which can be understood by the fact that X_3 interacts with X_1 in the model, which is itself correlated to X_4. However, since the PMEs detects X_4 as being exogenous, PME_3 remains constant w.r.t the correlation structure. Finally, focusing on X_3 and X_1 whenever $\rho = 0$ (i.e., the inputs are independent), one can notice that $\mathrm{Sh}_1 > \mathrm{PME}_1$, and $\mathrm{Sh}_3 < \mathrm{PME}_3$. This can be understood as the expression of the proportional versus the egalitarian redistribution schemes. While the Shapley effects effectively grants half the interaction surplus to both inputs, the PMEs tend to favor X_3. This can be understood by the fact that X_1 does not have an overwhelmingly higher overall effect on G than X_3.

Overall, the PMEs are less sensitive to the correlation of exogenous inputs than the Shapley effects. In conclusion, this toy-case highlights further the fact that both effects are complementary when it comes to a more precise interpretation of the model when its inputs are correlated. It reinforces the previously found behavioral tendencies in a less straightforward model.

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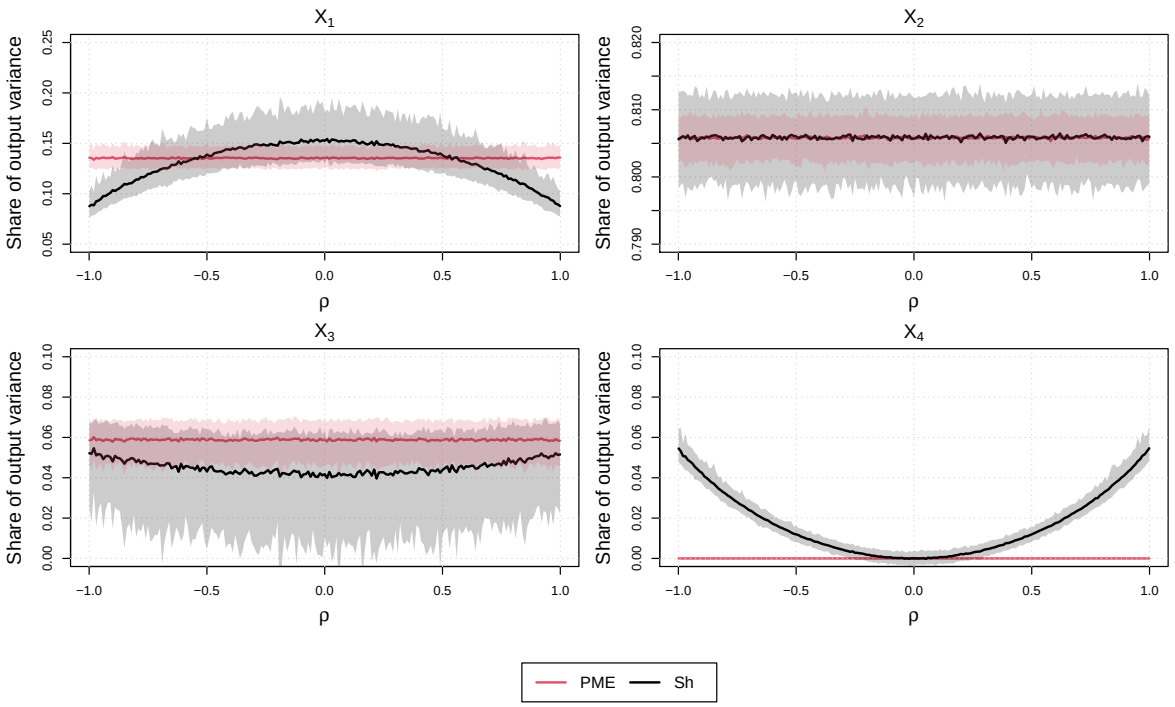

Figure 3: PMEs and Shapley effects for the Ishigami model with a spurious variable, with respect to the correlation coefficient ρ between X_1 and X_4. The grey and red areas around the solid plots give the 95%-confidence intervals of the estimates.

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