Moment Independent Importance Measures: New Results and Analytical Test Cases

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Abstract

Moment independent methods for the sensitivity analysis of model output are attracting growing attention among both academicians and practitioners. However, the lack of benchmarks against which to compare numerical strategies forces one to rely on ad-hoc experiments in estimating the sensitivity measures. This paper introduces a methodology that allows one to obtain moment independent sensitivity measures analytically. We illustrate the procedure by implementing four test cases with different model structures and model input distributions. Numerical experiments are performed at increasing sample size to check convergence of the sensitivity estimates to the analytical values.

Keywords: Global Sensitivity Analysis; Importance Measures; Moment Independent Sensitivity Analysis; Uncertainty Analysis; Density Function Distance.

1 Introduction

In complex risk assessment problems, quantitative models become central towards risk-informing the decision-process [Dillon et al (2003)]. However, both the model building and result interpretation phases need to cope with different sources of uncertainty [Kaplan and Garrick (1981), Apostolakis (1990), Paté-Cornell (1996), de Rocquigny et al (2008), Helton et al (2010), Aven (2010), Garrick (2010)]: *i*) aleatory uncertainty, namely the uncertainty provoked by the intrinsic randomness of the phenomena under investigation; *ii*) model uncertainty, namely uncertainty related to the structure of the prediction model itself; and *iii*) epistemic uncertainty, namely uncertainty deriving from our lack of knowledge about the numerical values of the model inputs. The above-mentioned works have established the awareness that proper uncertainty quantification is essential to inform decisions. Examples of this attitude can be found in several fields. The Florida Commission on Hurricane Loss Projection Methodology (FCHLPM) "*has established a professional team to perform onsite (confidential) audits of computer models developed by several different companies in the United States that seek to have their models approved for use in insurance rate filings in Florida. . . . an important part of the auditing process requires uncertainty and sensitivity analyses to be performed with the applicant's proprietary model* [Iman et al (2005a); p. 1277]." The US Environmental Protection Agency recommends both model developers and model users to perform proper sensitivity and uncertainty analysis to determine "*when a model, despite its uncertainties, can be appropriately used to inform a decision* [US EPA, 2009; p. vii]." Saltelli et al (2010) (p. 1) reports a statement from the White House's Office of Management and Budget underlying the role of SA as a "*a minimum, necessary component of a quality risk assessment report.*"

Sensitivity analysis (SA) methods have evolved towards the creation of techniques capable of taking uncertainty into account so as to reflect a decision-maker's state of information [Saltelli (1999), Saltelli (2002b), Borgonovo (2006)]. Local SA techniques prove ineffective when "*there is uncertainty about the true values of the inputs that should be used for a particular application* [Oakley and O'Hagan (2004)]." Global methods, instead, account for the entire model input and output distributions. Among global methods, non-parametric methods [McKay et al (1979), Saltelli and Marivoet (1990), Helton and Davis (2003), Helton et al (2006), Storlie et al (2009)] and variance-based methods [Saltelli and Tarantola (2002), Saltelli et al (2000), Saltelli (2002a), Owen (2003), Oakley and O'Hagan (2004), Saisana et al (2005), Saltelli et al (2010)] are widely studied and employed. However, variance is sometimes considered as fully representative of uncertainty, assuming "*that this moment is sufficient to describe output variability* [Saltelli (2002b)]." It is not uncommon that variance-based sensitivity indices are interpreted as "*the expected percentage reduction in the uncertainty ... that is attributable to each of the input variables* [Iman et al (2005b); p. 1299]." Nonetheless, several recent works have pointed out that identifying variance with uncertainty leads to misleading conclusions. Huang and Litzenberger (1988) underline that variance is sufficient to characterize uncertainty under normality assumptions. In applications, however, distributions can be skewed or, even, multi-modal. Cox (2008) and next Huber (2010) illustrate the pitfalls encountered by decision-makers, if they rely on variance as a measure of risk. Borgonovo (2006) shows an example in which a model output variance increases while fixing a model input at a certain value.

These limitations have contributed to renewing interest towards the utilization of moment independent approaches[1] for two main reasons. First, by removing the dependence on a single moment, the associated sensitivity measures thoroughly accounting for a decision-maker's uncertainty about the decision criterion. Second, the properties of moment independent importance measures are not affected by the presence of correlations.

Moment independent sensitivity measures have been applied in different sectors: Park and Ahn (1994), Chun et al (2000), Borgonovo (2007), and Liu and Homma (2009) in probabilistic safety assessment; Borgonovo and Tarantola (2008) in chemical system risk analysis; Borgonovo and Peccati (2010) in investment project risk analysis. However, in all these works, the sensitivity measures are estimated based on ad-hoc numerical experiments, because test cases against which to compare the efficacy of numerical estimation strategies are missing. In turn, this gap is linked to the absence of a methodology for obtaining moment independent sensitivity measures analytically.

To set forth such a methodology, we proceed as follows. Our first step is to establish a formal

[1] A method is said to be moment independent, if it does not rely on any moment of the model output distribution to define the sensitivity measures [Borgonovo and Tarantola (2008)].

connection between moment independent SA and probability density separation measurement. By studying the properties of the distance between density functions from a global SA perspective, we obtain two new properties for moment independent sensitivity measures. The first is invariance for model output monotonic transformation, the second is computation via cumulative distribution functions. The former property is relevant in numerical applications. Let y denote the model output (decision criterion or risk metric). In practical applications, due to uncertainty, y may range over several orders of magnitude. Analysts then resort to re-scaling (typically using $log_a(y)$) for improving numerical processing. Invariance insures that moment independent sensitivity measures are unaffected by any re-scaling. Thus, one can compute the sensitivity measures either, say, on y or $log_a(y)$ without altering the SA results[2]. The latter property allows us to formalize a 4-step procedure for obtaining moment independent sensitivity measures analytically.

By applying the methodology, we obtain four case studies: additive models with dependent or independent multivariate normally distributed model inputs, power-multiplicative models with lognormally distributed model inputs, additive models with uniformly distributed inputs, and non-additive-non-multiplicative model with gamma random variables. These case studies cover different model structures (from additive to completely interactive) and different model input support (from finite to infinite). This yields an assessment of the behavior of moment independent sensitivity measures in a broad variety of input-output combinations. Furthermore, by providing for each case study the corresponding variance-based sensitivity indices, our results shed further light about the differences between moment independent and variance-based sensitivity measures.

Finally, we perform numerical experiments based on a Latin hypercube sampling strategy for all case studies.

The remainder of the paper is organized as follows. Section 2 offers a literature review on variance-based and moment independent SA methods. Section 3 presents a methodology for obtaining moment independent importance measures analytically. Sections 4, 5 and 6, and 7 illustrate the four case studies. Section 8 discusses numerical experiments. Section 9 provides conclusions and outlines further research perspectives.

2 Variance-Based and Moment Independent Approaches in Probabilistic Sensitivity Analysis

One considers a risk metric (or, more in general, a decision-support criterion) Y, which is estimated via a model $[t(\mathbf{X})]$ dependent on n uncertain inputs (the random vector $\mathbf{X}$)[3]. In global SA, "*We assume to have information about the factors' probability distribution, either joint or marginal,*

[2] We note that the type of monotonic transformation we are referring to is connected with the re-scaling or the changes in units of measure of y. These changes are most often adopted for bettering numerical processing of model output ranging over several orders of magnitudes. This type of rescaling is not related to rank transformations. We recall the central role of rank transformation as introduced in Iman and Conover (1979) and Conover and Iman (1981) in regression and non-parametric sensitivity analysis. However, while rank transformation "*works quite well on monotonic data* [Iman and Conover (1979), p. 499]," it is a non-monotonic transformation.

[3] $y = t(\mathbf{x})$, $t : \Omega_X \subseteq \mathbb{R}^n \to \Omega_Y \subseteq \mathbb{R}$, is the relationship that links the model inputs to the model output. $t(\cdot)$ can be a simple expression or a complex computer code. Ω_Y, the image of t, coincides with the model output (y) support. Uncertainty in $\mathbf{x}$ makes y a random variable, which we denote by Y.

with or without correlation, and that this knowledge comes from measurements, estimates, expert opinion, physical bounds, output from simulations, analogy with factors for similar species, and so forth. [Saltelli and Tarantola (2002), p. 704]." In the light of the recent works by Aven (2010) and Garrick (2010), the above statement is equivalent to saying that the risk-analyst has assessed probability distributions on the random inputs consistent with her state of information about the problem at hand. In the remainder, μ_X denotes the probability distribution of $\mathbf{X}$.

Among the most widely studied methods to assess the influence of $\mathbf{X}$ on Y are variance-based techniques. Their theoretical aspects are developed in a vast literature, among which we recall Cukier et al (1978), Efron and Stein (1981), Sobol' (1993), Bedford (1998), Saltelli (1999), Rabitz and Alis (1999), Saltelli and Tarantola (2002), Saltelli et al (2000), Saltelli (2002a), Owen (2003), Oakley and O'Hagan (2004), and Saltelli et al (2010). Applications of global SA can be found in many areas of science (the following is a non-exhaustive list): operational research [Wagner (1995)], macroeconomics [Saisana et al (2005)], food safety [Patil and Frey (2004)], hurricane loss projections [Iman et al (2005a), Iman et al (2005b)], finance [Wang (2006)], physical chemistry [Hayes et al (2006)], probabilistic safety assessment [Aven and Nokland (2010)].

In variance-based SA, "*we are asked to bet on the factor that, if determined (i.e., fixed to its true value), would lead to the greatest reduction in the variance of* Y [Saltelli and Tarantola (2002), p. 705]." The corresponding importance measures are defined as [Iman and Hora (1990), Homma and Saltelli (1996) and Saltelli and Tarantola (2002)][4]

$$S_i = \frac{V_Y - \mathbb{E}_{X_i}[V_{Y|x_i}]}{V_Y} = \frac{V_{X_i}(\mathbb{E}[Y|X_i])}{V_Y} \tag{1}$$

where V_Y is the model output variance. $S_i > S_j$ implies that, on average, fixing X_i leads to a greater reduction in V_Y than fixing X_j.

Homma and Saltelli (1996) show that, if the parameters are independent, S_i coincides with Sobol' global sensitivity indices of order 1 [Sobol' (1993)]. A global sensitivity index of order r is defined as

$$S_{i_1,i_2,\ldots,i_r} = \frac{V_{i_1,i_2,\ldots,i_r}}{V_Y} \tag{2}$$

where

$$V_{i_1,i_2,\ldots,i_r} = \int t^2_{i_1,i_2,\ldots,i_r} \mathrm{d}\mu_{i_1} \mathrm{d}\mu_{i_2} \ldots \mathrm{d}\mu_{i_r} \tag{3}$$

is a partial variance in the functional ANOVA expansion of t:

$$t = t_0 + \sum_{r=1}^{n} \sum_{i_1<i_2<\ldots<i_r} t_{i_1,i_2,\ldots,i_r}(x_{i_1}, x_{i_2}, \ldots, x_{i_r}) \tag{4}$$

In eq. (4), $t_0 = \mathbb{E}[t]$ and the functions $t_{i_1,i_2,\ldots,i_r}(x_{i_1}, x_{i_2}, \ldots, x_{i_r})$ are obtained by conditional expectations and nested subtractions following a Grahm-Schmidt orthogonalization procedure [Hoeffding

[4]In the remainder, $f_{Y|x_i}(y)$ is used to denote the conditional density of Y given that X_i is fixed at x_i. Also, instead of $Y|X_i = x_i$, we shall adopt the shorter $Y|x_i$.

(1948), Sobol' (1969), Efron and Stein (1981), Takemura (1983), Owen (2003).] By subtracting t_0 from t in eq. (4) and squaring, one obtains

$$V_Y = \sum_{r=1}^{n} \sum_{i_1 < i_2 < \ldots < i_r} V_{i_1, i_2, \ldots, i_r} \tag{5}$$

By eqs. (3) and (4), $S_{i_1,i_2,\ldots,i_r}$ [eq. (2)], is the fraction of V_Y associated with the interaction among factors $X_{i_1}, X_{i_2}, \ldots, X_{i_r}$. As Oakley and O'Hagan (2004) (p. 754) note, eqs. (3) and (4) grant "*a tidy decomposition of the total variance into component variances that are directly related to* model structure." This correspondence is synthesized in the concept of function dimension distribution by Owen (2003).

The numerical estimation of global sensitivity indices has been extensively studied and constantly improved since the work of Sobol' (1993). Relevant results from the computational side are achieved in: *a*) Sobol' (1993), Homma and Saltelli (1996) and Saltelli (2002a) developing the sample and re-sample matrix strategy; *b*) Saltelli et al (1999) formalizing the use of the Fourier amplitude sensitivity test; *c*) Oakley and O'Hagan (2004) proposing a Bayesian approach to variance-based importance measures.

However, in the presence of correlated model inputs, much of the computational advantages connected with the previous methods are lost; for instance, the sample and re-sample strategy becomes no more applicable. Methods for computing variance-based sensitivity indices in the presence of correlations are proposed in Bedford (1998), Saltelli and Tarantola (2002), Lewandowski et al (2007) and Rabitz (2010). The method of Lewandowski et al (2007) is applied by Duintjer Tebbens et al (2008) in a medical decision-making context.

Bedford (1998) shows that, with correlated model inputs, eqs. (4) and (5) lose uniqueness, and variance-based importance measures become dependent on the lexicographical ordering of the parameters. Oakley and O'Hagan (2004) observe that eq. (4) is no more reflective of model structure for dependent inputs. By considering $Y = t(x_1, x_2) = x_1$, Oakley and O'Hagan (2004) show that a term containing x_2 is generated in eq. (4) by the correlation of x_1 and x_2. In the presence of correlations, Saltelli and Tarantola (2002) show that variance-based measures still retain their meaning based on the variance-reduction setting reported above. However, variance is not necessarily a good summary of a decision-maker's uncertainty. Consider the model [Borgonovo (2006)]

$$y = t(x_1, x_2) = e^{x_1} \left| \sin x_2 \right|, \tag{6}$$

with $\mu_{\mathbf{X}} = \mu_{X_1} \cdot \mu_{X_2}$, $\mu_{X_1} = N(1,1)$ and $\mu_{X_2} = N(2,1)$. The unconditional model output variance is $V_Y = 11.18$. The decision-maker is next informed that $X_2 = 1$. She now possesses full information about X_2, and is uncertain only about X_1. However, if she represents uncertainty by variance, she concludes that the new information has increased her uncertainty, since $V[Y|X_2 = 1] = 12.58 > V_Y$. Indeed, for the model output distribution is skewed in this case, violating the assumption that variance is sufficient to characterize uncertainty [Savage (1972), Huang and Litzenberger (1988).]

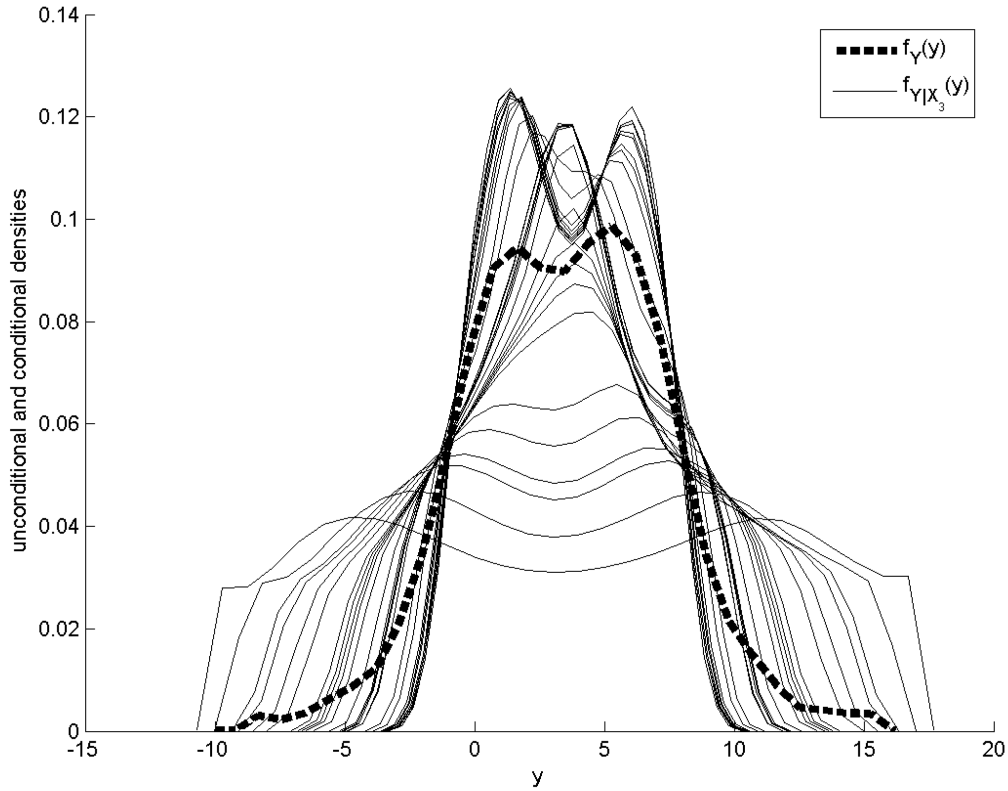

Figure 1: $f_{Y|x_3}$ for different values of x_3, for the density of the Ishigami function [eq (7)].

Several works have also pointed out the limitations of variance as a measure of risk. In particular, Theorem 1 in Cox (2008) shows that "*mean-variance decision-making violates the principle that a rational decision-maker should prefer higher to lower probabilities of receiving a fixed gain, all else being equal* [Cox (2008), p. 925]." This result is also generalized in Huber (2010).

The question then splits into: *a*) what is the effect of getting to know that $X_i = x_i$? and *b*) how can we measure this effect?

Concerning *a*), after conditioning on $X_i = x_i$, the decision-maker's uncertainty about the model output is given by the conditional model output density [$f_{Y|x_i}(y)$]. Figure 1 shows the different conditional densities $f_{Y|x_3}(y)$, obtained by conditioning on X_3 for the model

$$y = \sin(x_1) + 7\sin^2(x_2) + 0.1x_3^4 \sin(x_1) \tag{7}$$

with X_i ($i = 1, 2, 3$) uniformly iid on $[-\pi, \pi]$. Eq. (7) is the Ishigami function, a widely utilized test case in global SA [Homma and Saltelli (1996), Crestaux et al (2009), Iooss and Ribatet (2009)].

Suppose we measure the effect of X_3 using variance. For the Ishigami function, $\mathbb{E}_{Y|x_3}$ is independent of X_3. In fact, when one conditions on x_3 and averages, the third summand in eq. (7)

disappears, since $\mathbb{E}[\sin x_1] = 0$. Hence, $\mathbb{E}_{Y|x_3}$ is constant in X_3 and, correspondingly, its variance is null ($V_{X_3}\left[\mathbb{E}_{Y|x_3}\right] = 0$.) By eq. (1), $S_3 = \dfrac{V_{X_3}\left[\mathbb{E}_{Y|x_3}\right]}{V_Y} = 0$. Therefore, one would conclude that evidence on X_3 does not provide any information, if she considers the expected reduction in V_Y provoked by X_3. Nonetheless, Figure 1 shows that fixing X_3 changes the distribution of Y. The effect of knowing X_3 would become non-null, if one measured the expected shift between the conditional and unconditional densities of y.

In global SA, Park and Ahn (1994) introduce the idea of measuring the shift between model output densities first. Park and Ahn (1994) base their sensitivity measure on the Kullback-Leibler divergence (Kullback and Leibler (1951)), defining

$$I_i^{KL} = \int_{\Omega_Y} f_Y(y) \ln \frac{f_Y}{f_{Y|x_i}} \mathrm{d}y \tag{8}$$

However, the following problem connected with I_i^{KL} emerges. Consider eq. (7). By the functional form of eq. (7), $\Omega_Y = [-10.741, 17.741]$. Hence, in eq. (8) one writes $I_i^{KL} = \int_{-10.741}^{17.741} f_Y \ln \frac{f_Y}{f_{Y|x_i}} \mathrm{d}y$. By conditioning on any $x_1 \in [0, \pi]$, the support of the model output changes to $[0, 17.741]$. Thus, $f_{Y|x_i} = 0$ for $y \in [-10.741, 0)$. Consequently, the integral in eq. (8) I_i^{KL} is not defined. This problem is encountered every time the support of y changes. This makes I_i^{KL} not suitable in global SA, because the support of the model output varies, in principle, at each conditioning.

To overcome this issue, Chun et al (2000) utilize a distance rather than a divergence for separation measurement. This choice has also the advantage of making the sensitivity measures independent of the order according to which $f_Y(y)$ and $f_{Y|x_i}(y)$ are considered[5]. Both Park and Ahn (1994) and Chun et al (2000), however, define their sensitivity measures for a specific sensitivity case $X_i = x_i$. Because X_i is not known with certainty, fixing it at just one of its possible values is only partially informative. This limitation is overcome by Borgonovo (2007), where the sensitivity measure is defined as

$$\delta_i := \frac{1}{2} \mathbb{E}_{X_i}[s_i(X_i)] \tag{9}$$

with

$$s_i(X_i) := \int \left| f_Y(y) - f_{Y|x_i}(y) \right| \mathrm{d}y \tag{10}$$

The expectation $\mathbb{E}_{X_i}[s_i(X_i)]$ accounts for the decision-maker's degree of belief about X_i. $s_i(X_i)$ [eq. (10)] quantifies the separation between the unconditional and conditional output densities (see Glick (1975); please refer to the next section for further technical details). δ_i [eq. (9)] measures the expected shift in decision-maker's degree of belief on Y provoked by coming to know X_i.

The corresponding setting is, then: "*We are asked to bet on the model input that, if determined, would lead to the greatest expected shift in the distribution of* Y [Borgonovo and Tarantola (2008).]"

Let us examine the definitions of S_i [eq. (1)] and δ_i [eq. (9)] further. In both eqs. (9) and (1),

[5] In fact, $I_i^{KL}(f_Y, f_{Y|X_i}) \neq I_i^{KL}(f_{Y|X_i}, f_Y)$ since $\int f_Y(y) \ln \frac{f_Y}{f_{Y|X_i}} \mathrm{d}y \neq \int f_{Y|X_i} \ln \frac{f_{Y|X_i}}{f_Y} dy$.

internal statistics — $V_{Y|x_i}$ and $s_i(X_i)$, respectively — are estimated. An external expectation is next carried out to account for uncertainty in X_i. Hence, as shown in Borgonovo and Tarantola (2008), S_i and δ_i can be estimated from the same Monte Carlo sample. However, $V_{Y|x_i}$ synthesizes the conditional distribution of Y in its variance, in agreement with the variance-based setting; $s_i(X_i)$ measures the separation between the conditional and unconditional model output densities, in agreement with the moment independent SA setting.

The above literature review reveals that global SA methods have been extensively studied from both the theoretical and numerical perspectives, whilst several aspects of moment independent approaches are still open to further research. In particular, a methodology for obtaining moment independent sensitivity measures analytically has not been established yet. This is the subject of the next sections.

3 New Properties and a Procedure for Obtaining Moment Independent Importance Measures Analytically

This section introduces two new properties of moment independent importance measures and presents a procedure for determining them analytically.

We start with some notation. Denoting an open interval in $\mathbb{R}$ by Ω, and any two probability density functions by $f, g : \Omega \to \mathbb{R}^+$, we let

$$\|f - g\| = \int |f - g| \, \mathrm{d}\omega \tag{11}$$

define their distance. As proven in Glick (1975), the operation $\int |f - g| \mathrm{d}\omega$ [eq. (11))] is a "*separation measurement with respect to the L_1 norm, for the set of all probability densities*." In other words, eq. (11) measures the shift between any two density functions.

Let us now study eq. (11) more closely. As shown in Borgonovo and Peccati (2009), the operation $|f - g|$ sets forth the piecewise defined function

$$u(\omega) = \begin{cases} f - g & \omega \in \Omega_+ \\ 0 & \omega \in \Sigma \\ g - f & \omega \in \Omega_- \end{cases} \tag{12}$$

$\Sigma = \{\omega : f(\omega) = g(\omega)\}$ is the set of points where $f = g$, Ω_+ is the set of points where $f > g$ and Ω_- the set of points where $f < g$. Let us now denote by F and G the cumulative distribution functions associated with f and g, respectively: $F(\omega) = \int_{-\infty}^{\omega} f(\xi) d\xi$ and $G(\omega) = \int_{-\infty}^{\omega} g(\xi) d\xi$. In Appendix A, we show that the following holds:

Proposition 1

$$\|f - g\| = 2F(\Omega_+) - 2G(\Omega_+) = 2G(\Omega_-) - 2F(\Omega_-) \tag{13}$$

Eq. (13) states that $\|f - g\|$ is equal to twice the difference between *a*) the probability that $\omega \in \Omega_+$ under F and *b*) the same probability under G. By symmetry, eq. (13) states that

$\|f-g\|$equals twice the difference between the probabilities of $\omega \in \Omega_-$ under G and F, respectively.

Proposition 1 plays a central role in the explicit derivation of moment independent sensitivity measures, as we are to discuss later in this section.

Let us now consider the case in which g is the Dirac-δ density (δ^{Dirac}). The Dirac-δ expresses the case in which the support of a random variable (the space Ω) collapses into a unique point, say, ω_0. In this case, the decision-maker is certain that ω_0 is the value assumed by the random variable.

Corollary 1 *Let f be a generic density. Then,*

$$\left\|f-\delta^{Dirac}\right\| = 2 \tag{14}$$

Eq. (14) can be interpreted as follows. The density f reflects the current decision-maker's uncertainty about ω. When the decision-maker becomes informed that $\omega = \omega_0$, the decision-maker's uncertainty is described by a δ^{Dirac} density. Eq. (14) states that it is equal to 2 the shift from: *i*) the situation in which the decision-maker is uncertain about ω, to *ii*) the situation in which she knows that $\omega = \omega_0$.

The next property of $\|f-g\|$concerns monotonically increasing transformations.

Proposition 2 *Let $z = z(\omega)$, $z : \Omega \to \mathbb{R}$, be a monotonically increasing function of ω. Denoting by $f_\Omega(\omega)$ and $g_\Omega(\omega)$ any two density functions on ω and by $f_Z(z)$ and $g_Z(z)$ the corresponding densities on Z, one obtains:*

$$\|f_Z - g_Z\| = \|f_\Omega - g_\Omega\| \tag{15}$$

Proposition 2 expresses the fact that the distance between any two densities as defined in eq. (11) is invariant for monotonic transformations of the random variable. For instance, if $\Omega = \mathbb{R}^+ - \{0\}$, and $z = \ln(\omega)$, then $\left\|f_{\ln(\omega)} - g_{\ln(\omega)}\right\| = \|f_\Omega - g_\Omega\|$.

The above findings can be generalized in moment independent global SA as follows. Moment independent importance measures quantify the effect of coming to know X_i by measuring the separation between f_Y and $f_{Y|x_i}(y)$. Therefore, in moment independent SA, Ω becomes the range of $t(\mathbf{x})$, Ω_Y. The densities f and g are substituted by f_Y and $f_{Y|x_i}$, respectively. We denote by F_Y and $F_{Y|X}$ the corresponding cumulative distribution functions. The partition $\Omega = \{\Omega_+, \Omega_-\}$ is replaced by $\Omega_Y = \{Y_+, Y_-\}$, with $Y_+ = \left\{y : f_Y > f_{Y|x_i}\right\}$ and $Y_- = Y \backslash Y_+$. In moment independent SA, Y_+ varies with X_i. To evidence this dependence, we use the notation $Y_+^{x_i}, Y_-^{x_i}$. We then have the following properties.

Proposition 3 *1. Let $z(y)$ be a monotonic transformation of the model output. Let δ_i^y, $\delta_i^{z(y)}$ denote the importance of X_i with respect to (w.r.t.) y and $z(y)$ respectively. Then,*

$$\delta_i^y = \delta_i^{z(y)} \tag{16}$$

2.

$$\delta_{1,2,\ldots,n} = 1 \tag{17}$$

Table 1: Steps for the analytical derivation of the delta importance measure.

Step nr	Head
1	Identification of the unconditional and conditional model cumulative distribution functions
2	Identification of $Y_+^{x_i}$ and $Y_-^{x_i}$
3	Evaluation of $s_i(X_i)$ by eq. (19).
4	Evaluation of δ_i by eq. (20).

where

$$\delta_{1,2,...,n} = \frac{1}{2}\mathbb{E}[|\int f_Y - f_{Y|x_1,x_2,...,x_n}(y)dy|] \tag{18}$$

3.

$$s_i(X_i) = 2F_Y(Y_+^{x_i}) - 2F_{Y|x_i}(Y_+^{x_i}) \tag{19}$$

and

$$\delta_i = \mathbb{E}_{X_i}[F_Y(Y_+^{x_i}) - F_{Y|x_i}(Y_+^{x_i})] \tag{20}$$

Point 1 in Proposition 3 states that δ_i does not change if the model output undergoes a monotonic transformation. Correspondingly, the model input ranking is invariant. When the model output spans several order of magnitudes, analysts re-scale the output (typically resorting to a logarithmic scale) to manage and elaborate results. Item 1 insures that computing δ before or after the re-scaling does not alter the SA results. This property is not shared by variance-based sensitivity measures, since, in general, $V_{Y|x_i} \neq V_{Z(Y)|x_i}$, which implies $S_i^y \neq S_i^{z(y)}$.

Point 2 has the following interpretation. $f_{Y|x_1,x_2,...,x_n}(y)$ is the model output density obtained when all parameters are fixed, say at $\mathbf{x}^0$. In that case, $y = t(\mathbf{x}^0)$ with certainty, and $f_{Y|x_1,x_2,...,x_n}(y) = \delta^{Dirac}(t(\mathbf{x}^0))$. The shift $|\int f_Y - f_{Y|x_1,x_2,...,x_n}(y)\mathrm{d}y|$, then, measures the separation from the current degree of belief to the state in which one comes to know that $\mathbf{x}^0$ is "*the true value of the inputs* [Oakley and O'Hagan (2004)]." Point 2 states that this expected shift is normalized to unity. We note that the way in which we have derived this result, namely via Corollary 1, generalizes previous literature findings (see, in particular, Borgonovo (2007), p. 782.). Finally, we observe that Proposition 3 adds two new properties to previous literature results [Borgonovo (2007)].

Point 3 can be turned into a methodology for deriving δ analytically by exploiting the knowledge of the conditional cumulative distribution functions. We summarize the steps in Table 1.

The first step consists of deriving the explicit expressions of the conditional and unconditional cumulative distribution functions Y. The second step consists of determining $Y_+^{x_i}$ and $Y_-^{x_i}$ by studying the inequality $f_Y \geq f_{Y|x_i}$. The third step consists of computing $s_i(X_i)$ by eq. (19). In this respect, Proposition 3 allows one to obtain $s_i(X_i)$ by evaluating $F_Y(Y_+^{x_i})$ and $F_{Y|x_i}(Y_+^{x_i})$ at a limited number of points, resulting in notable computational simplification. The final step consists of taking the expected value of $s_i(X_i)$.

In the next sections, we apply the methodology and obtain four analytical test cases, with different model structures and different assumptions on the random model inputs.

4 Normal Random Variables and Additive Model Output

In this section, we apply the procedure in Table 1 and obtain the explicit expression of moment independent importance measures for the case of additive model and normally distributed inputs.

Proposition 4 *Let*

$$y = \sum_{i=1}^{n} a_i x_i \tag{21}$$

with $\mathbf{X} \sim N(\mathbf{x}, \mathbf{m}, \Sigma)$ *with parameters* $\mathbf{m} = (m_1, m_2, ...m_n)$, *(*$m_i = \mathbb{E}[X_i]$*) and non degenerate covariance matrix* Σ *(*$\det \Sigma \neq 0$*). Then*

1. $$F_Y = N(y; m_Y, V_Y) \text{ and } F_{Y|x_i}(y) = N(y; m_{Y|x_i}, V_{Y|x_i}) \tag{22}$$

   where

   $$\begin{gathered} V_Y = \mathbf{a}\Sigma\mathbf{a}^T \\ V_{Y|x_i} = \mathbf{a}\Sigma_{Y|x_i}\mathbf{a}^T \\ m_Y = \sum\nolimits_{s=1}^{n} a_s m_s \\ m_{Y|x_i} = \sum_{s=1, s\neq i}^{n} a_s \left[m_s + (x_i - m_i)\frac{\sigma_{s,i}}{\sigma_i} \right], \quad i = 1, 2, ..., n \end{gathered} \tag{23}$$

   and

   $$\Sigma_{Y|x_i} = \left[\sigma_{j,s} - \frac{\sigma_{j,i} \cdot \sigma_{i,s}}{\sigma_{i,i}}, \quad j, s, i = 1, 2, ..., n \right] \tag{24}$$

2. $Y_+^{x_i} = (-\infty, y_1] \cup [y_2, +\infty)$ *and* $Y_-^{x_i} = (y_1, y_2)$ *with*

   $$y_{1,2} = \frac{1}{V_Y - V_{Y|x_i}} \left(V_Y m_{Y|x_i} - V_{Y|x_i} m_Y \pm \sqrt{V_Y V_{Y|x_i} \left[(a_i x_i)^2 + (V_Y - V_{Y|x_i}) \ln(\frac{V_Y}{V_{Y|x_i}}) \right]} \right) \tag{25}$$

3. $$s_i(X_i) = 2[N(y_1; m_Y, V_Y) + N(y_2; m_{Y|x_i}, V_{Y|x_i}) - N(y_2; m_Y, V_Y) - N(y_1; m_{Y|x_i}, V_{Y|x_i})] \tag{26}$$

4. *and*

   $$\delta_i = \mathbb{E}_{X_i}[N(y_1; m_Y, V_Y) + N(y_2; m_Y|\omega_i, V_{Y|x_i}) - N(y_2; m_Y, \Sigma_Y) - N(y_1; m_{Y|x_i}, V_{Y|x_i})] \tag{27}$$

Proposition 4 has the following interpretation. Item 1 states that both the conditional and unconditional model output densities are normal, and with parameters displayed in eq. (23). Item 2 identifies the two points at which f_Y and $f_{Y|x_i}$ intersect. Item 3 determines $s_i(X_i)$ by Proposition 1. Item 4 obtains δ_i by conditional expectation over the normal density of X_i.

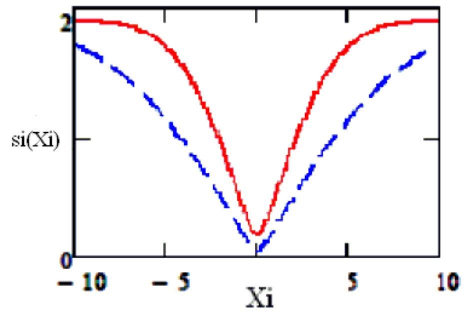

Figure 2: $s_i(X_i), i = 1, 2, ..., n$,for $n = 3$ (continuous) and $n = 10$ (dotted).

Proposition 4 is readily implemented in a software as Matematica or Mathcad (used by the authors), delivering $s_i(X_i)$ and δ_i [eqs. (26), (27)] for all $\mathbf{a}$, $\mathbf{m}$, Σ and n.

Let us then study the separation between the conditional and unconditional densities, $s_i(X_i)$, as a function of X_i. We recall that $s_i(x_i)$ measures how far the conditional density of y shifts from the unconditional density, given that the decision-makers gets to know that $X_i = x_i$.

Figure 2 displays $s_i(X_i)$ in eq. (26), for $\mathbf{a} = \mathbf{1}$ ($\mathbf{1} = 1\,1\ldots 1$), $\mathbf{m} = \mathbf{0}$ and $\Sigma = I$ (identity matrix), for two model sizes ($n = 3$, continuous and $n = 10$, dotted.)

$s_i(X_i)$ (Figure 2) is symmetric around the expected value of X_i. This symmetry stems from the symmetric structure of the model and from the identity of the conditional and unconditional normal densities. One notes (Figure 2) that the left limit of $s_i(X_i)$ is 2, then $s_i(X_i)$ decreases to a minimum value, which is reached at $\mathbb{E}[X_i]$ and next increases to its maximum value, 2. The fact that the separation reaches its minimum at $\mathbb{E}[X_i]$ signals that getting to know that X_i is fixed at its expected value provokes the smallest change in the decision-maker's uncertainty about y; the more the value of X_i differs from $\mathbb{E}[X_i]$, the bigger the shift between the conditional and unconditional model output densities. We observe that the limiting values do not depend on the choice of the parameters of the distributions (see Appendix A for the proof.)

Corollary 2 *Given the model input distribution and the model output in Proposition 4, it holds*

$$\lim_{X_i \to \pm\infty} s_i(X_i) = 2 \qquad \forall \mathbf{a}, \mathbf{m}, \Sigma \tag{28}$$

Let us then examine the behavior of $s_i(X_i)$ as the model size changes, namely, as n increases. The continuous and dotted lines in Figure 2, report $s_i(X_i)$ in the cases $n = 3$ and $n = 10$, respectively. One notes that $s_i(X_i)$ grows to its asymptotic value less rapidly for $n = 10$ than for $n = 3$ — the same behavior is obtained for other values of n, although not displayed. — In other words, $s_i(X_i)$ grows faster to its limit as n decreases. This behavior is relevant to the results for importance measures.

By our choice of the parameters, it is $s_i(x^*) = s_j(x^*)$, $\forall x^* \in \mathbb{R}$, and $\forall i, j = 1, 2, ..., n$, that is, getting to know that one out of n standard normally iid random variables is fixed at x^* provokes the same shift in the distribution of their sum, independently of whether this variable is labeled X_i or X_j. By the fact that the X_i are iid, $\delta_i = \delta_j$ $\forall i, j = 1, 2, ..., n$. Furthermore, by $\mathbf{a} = \mathbf{1}$, $\mathbf{m} = \mathbf{0}$ and $\Sigma = I$, δ_i is obtained by averaging $s_i(X_i)$ via a standard normal density [eq. (9)] as follows:

$$\delta_i = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{\frac{-v^2}{2}} \cdot s_i(v) \mathrm{d}v \tag{29}$$

In eq. (29), $\frac{1}{\sqrt{2\pi}} e^{\frac{-v^2}{2}}$ does not vary with n. Because $s_i(X_i)$ grows at a lower pace as n increases, the measure of the region intercepted by the product $\left(\frac{1}{\sqrt{2\pi}} e^{\frac{-v^2}{2}}\right) \cdot s_i(v)$ decreases with n. Consequently, δ_i decreases with n. This result is also in accordance with intuition: getting to know one out of 100 (to be summed) iid variables has a lower impact on a decision-maker's degree of belief than getting to know 1 out of 3 (to be summed) variables.

Lines $2-4$ in Table 2 report the importance measures for several values of n ($\mathbf{a} = 1$, $\mathbf{m} = \mathbf{0}$ and $\Sigma = I$). The decreasing values of δ in the second line of Table 2 show that the impact of getting to know X_i decreases with n, as expected. The same happens to variance-based measures, S (third row in Table 2.) For the model in eq. (21), one writes

$$S_i = \frac{\mathbf{a}\Sigma_{Y|x_i}\mathbf{a}^T}{\mathbf{a}\Sigma\mathbf{a}^T} \tag{30}$$

By $\mathbf{a} = 1$ and the fact that the random inputs are iid, $S_i = 1/n$ [see also Owen (2003)].

This section has involved an additive model — its superimposition dimension equals unity [Owen (2003)] — with infinite support of the random inputs. In the next section, we discuss a case study with a different superimposition dimension, namely a completely interactive model, with semi-infinite support of the random inputs.

Table 2: Moment Independent (delta) and Variance-Based (S) Importance Measures with growing model size (n). Lines 2-4: additive model with normally distributed inputs. Lines 5-6: power-multiplicative model with lognormally distributed inputs. Lines 8-11: additive model with uniformly distributed inputs

n	2	3	4	5	6	7	8	9	10	100
Normal	**Additive**	$\mathbf{a} = 1$	$\mathbf{m} = \mathbf{0}$	$\Sigma = I$						
δ	0.306	0.224	0.185	0.160	0.144	0.131	0.121	0.114	0.107	0.032
S	0.5	0.333	0.25	0.2	0.167	0.142	0.125	0.111	0.10	0.01
Lognormal	**Multiplicative**	$\mathbf{a} = \boldsymbol{\eta} = \mathbf{1}$	$\boldsymbol{\xi} = \mathbf{1}$	$\Sigma = I$						
δ	0.306	0.224	0.185	0.160	0.144	0.131	0.121	0.114	0.107	0.032
S	0.268	0.090	0.032	0.012	$4.27E-3$	$4.7E-3$	$1.73E-3$	$6.36E-4$	$2.34E-4$	$2.52E-29$
Uniform	**Additive**	$\mathbf{a} = \mathbf{1}$								
δ analytical	0.333	0.228	0.186	0.166	0.149	0.137	0.128	0.120	0.113	0.032
δ normal approx.	0.306	0.224	0.185	0.160	0.144	0.131	0.121	0.114	0.107	0.032
S	0.5	0.333	0.25	0.2	0.167	0.142	0.125	0.11	0.1	0.01
Non-Additive	**Non-Multiplicative**									
α	1	2	3	10	20	30	50			
δ	0.33	0.319	0.315	0.309	0.3073	0.3069	0.3065			
S	0.478	0.492	0.496	0.499	0.5	0.5	0.5			

5 Lognormal Random Variables and Multiplicative Model Output

In this section, we consider a model with completely different structure in respect of the model of Section 4, i.e.,

$$Y = \prod_{i=1}^{n} X_i^{a_i} \tag{31}$$

The model in eq. (31) is characterized by the presence of interactions among the model inputs, generated by their multiplication — it is constituted by a unique interaction term. — We let X_i be independently distributed with lognormal distributions $LN(x_i; \eta_i, \xi_i)$, where η_i and ξ_i are the mean value and standard deviation of $ln(X_i)$, respectively. For clarity, we report the density function of $\mathbf{X}$:

$$\mu_{\mathbf{X}}(\mathbf{x}; \boldsymbol{\eta}, \boldsymbol{\xi}) = \prod_{i=1}^{n} \mu_i(x_i; \eta_i, \xi_i) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\xi_i x_i} e^{-\frac{1}{2}\left[\frac{\ln(x_i)-\eta_i}{\xi_i}\right]^2} \tag{32}$$

The next result reports the expression of the sensitivity measures. The proof makes use of the invariance properties of Propositions 2 and 3 and is discussed in Appendix A.

Proposition 5 *Let Y be defined by eq. (31) and $\mathbf{X}$ a random vector with the density given in eq. (32). Then*

1.

$$f_Y(y) = \frac{1}{y\sqrt{2\pi\xi_Y^2}} e^{-\frac{[\ln(y)-\sum_{i=1}^{k}\eta_i]^2}{2\xi_Y^2}} \text{ and } f_{Y|x_i}(y) = \frac{1}{y\sqrt{2\pi\xi_{Y|x_i}^2}} e^{-\frac{[\ln(y)-\eta_{Y|x_i}]^2}{2\xi_{Y|x_i}^2}} \tag{33}$$

where

$$\begin{gathered} \xi_Y^2 = \textstyle\sum_{i=1}^{n} a_i^2 \xi_i^2 \\ \xi_{Y|x_i}^2 = \textstyle\sum_{\substack{s=1 \\ s\neq i}}^{n} a_s^2 \xi_s^2 \\ \eta_Y = \mathbf{a}\boldsymbol{\eta}^T \\ \eta_{Y|x_i} = \eta_Y - a_i\eta_i + a_i \ln x_i \end{gathered} \tag{34}$$

2. $Y_+^{x_i} = (0, e^{y_1}] \cup [e^{y_2}, +\infty)$ *and* $Y_-^{x_i} = (e^{y_1}, e^{y_2})$ *with* y_1 *and* y_2 *obtained by eq. (25) where* V_Y, $V_{Y|x_i}$, m_Y *and* $m_{Y|x_i}$ *are replaced by* ξ_Y^2, *by* $\xi_{Y|x_i}^2$, η_Y, *and* $\eta_{Y|x_i}$, *respectively.*

3.

$$\begin{gathered} s_i(X_i) = \\ 2[LN(e^{y_1}; \eta_Y, \xi_Y^2) - LN(e^{y_2}; \eta_Y, \xi_Y^2) + LN(e^{y_2}; \eta_{Y|x_i}, \xi_{Y|x_i}^2) - LN(e^{y_1}; \eta_{Y|x_i}, \xi_{Y|x_i}^2)] \\ = 2[N(y_1; \eta_Y, \xi_Y^2) - N(y_2; \eta_Y, \xi_Y^2) + N(y_2; \eta_{Y|x_i}, \xi_{Y|x_i}^2) - N(y_1; \eta_{Y|x_i}, \xi_{Y|x_i}^2)] \end{gathered} \tag{35}$$

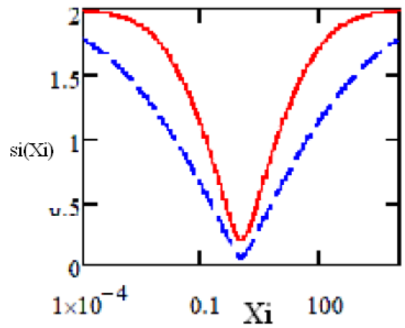

Figure 3: $s_i(X_i)$ for $Y = \prod_{i=1}^{n} X_i$, X_i lognormally iid; $n = 3$ (continuous) and $n = 10$ (dotted). The horizontal axis is in logarithmic scale.

4.

$$\begin{aligned}\delta_i &= \\ &= \mathbb{E}_{X_i}[LN(e^{y_1};\eta_Y,\xi_Y^2) - LN(e^{y_2};\eta_Y,\xi_Y^2) + LN(e^{y_2};\eta_{Y|x_i},\xi_{Y|x_i}^2) - LN(e^{y_1};\eta_{Y|x_i},\xi_{Y|x_i}^2)] \\ &= \mathbb{E}_{X_i}[N(y_1;\eta_Y,\xi_Y^2) - N(y_2;\eta_Y,\xi_Y^2) + N(y_2;\eta_{Y|x_i},\xi_{Y|x_i}^2) - N(y_1;\eta_{Y|x_i},\xi_{Y|x_i}^2)]\end{aligned} \tag{36}$$

Concerning the asymptotic properties of $s_i(X_i)$, one obtains

$$\lim_{X_i \to 0^+} s_i(X_i) = 2 \quad \text{and} \quad \lim_{X_i \to +\infty} s_i(X_i) = 2 \tag{37}$$

Eq. (37) follows by the second of the equalities in eq. (35)[6]. Figure 3 displays $s_i(X_i)$ [eq. (35)] for the cases $n = 3$ and $n = 10$ (continuous and dotted graphs respectively), with $\mathbf{a} = \boldsymbol{\eta} = \mathbf{1}, \boldsymbol{\xi} = \mathbf{1}$.

Figure 3 displays $s_i(X_i)$. The continuous and dotted lines refer to $n = 3$ and $n = 10$, respectively. A logarithmic scale is used in the horizontal axis. Figure 3 shows that, unlike in the normal-additive case, the density separation is no more a symmetric function of X_i. It is, instead, symmetric in $\ln X_i$. Similarly to the normal-additive case, $s_i(X_i)$ reaches its minimum at the expected value of X_i, and it increases towards its asymptotic value at a lower pace when the number of parameters is higher (compare the dotted to the continuous lines in Figure 3.) We therefore expect a decreasing value of δ_i as n increases. Lines $5-7$ in Table 2 illustrate the numerical values of the importance measures for different model sizes. The values of the sensitivity measures show that the importance of model inputs decreases with n also in the multiplicative-lognormal case. In particular, δ (sixth line) assumes the same values as in the normal-additive case. This result follows by the monotonic invariance property of δ (Proposition 2). However, a notable difference is registered among the values of the variance-based sensitivity measures between the additive-normal case study and the multiplicative-lognormal one. This discrepancy is a consequence of the different model structure.

[6] The proof is close to the one of Corollary 2, and is omitted for the sake of brevity.

Variance-based importance measures, can be found analytically also for this type of model (see Appendix A for the derivation):

$$S_i = 1 - \frac{(e^{\xi_Y^2} - e^{\xi_i^2})}{(e^{\xi_Y^2} - 1)} \tag{38}$$

Line 6 in Table 2 shows that S_i decreases very rapidly with model size. As an example, take the case $n = 5$. Determining X_i reduces variance by around 1%. Hence, by looking at variance reduction, the decision-maker would conclude that being able to know X_i with certainty has an almost negligible effect on her uncertainty (if this is made coincide with variance). Instead, fixing one-out-of the 5 model inputs provokes a non-negligible shift in the model output distribution, as testified by $\delta_i = 0.160$. Its interpretation in terms of density separation measurement is as follows: the expected impact of getting to know a random variable in the sum of n standard normally iid random variables is the same as that of getting to know a random variable in the product of n standard lognormally iid random variables. However, variance based importance measures would not deliver this information.

In the next section, we deal with a classical case: additive model and uniformly distributed random variables in $[0, 1]^n$.

6 Uniform Random Variables and Additive Model Output

In this section, we consider the case in which $\mathbf{X} \in [0, 1]^n$ is a random vector of iid uniformly distributed random variables X_i, and the model is additive:

$$y = \sum_{i=1}^{n} x_i \tag{39}$$

By the works of Mitra (1971) and Sadooghi-Alvandi et al (2007), the unconditional density of Y is the piecewise-defined function:

$$u_Y^n(y) = \begin{cases} \frac{1}{(n-1)!}(y)^{n-1} & if \quad 0 \leq y < 1 \\ \frac{y^{n-1}}{(n-1)!} - \frac{n}{(n-1)!}(y-1)^{n-1} & if \quad 1 \leq y < 2 \\ \dots & \dots \quad \dots \\ \sum_{l=0}^{n-1} (-1)^l \binom{n}{l} \frac{1}{(n-1)!}(y-l)^{n-1} & if \; n-1 \leq y < n \\ 0 & otherwise \end{cases} \tag{40}$$

In order to utilize Proposition 1, the cumulative distribution function of the sum of uniformly distributed random variables is needed. We write it as follows (the proof is in Appendix A).

Lemma 1 *Let $y \in [k^* - 1, k^*]$, $k^* = 1, 2, ..., n$. Then, the cumulative distribution function of the* *sum of n uniform iid random variables is given by*

$$U_Y^n(y) = \sum_{m=0}^{k^*-2} (\sum_{l=0}^{m} (\frac{(-1)^l}{l!(n-l)!}((m+1-l)^n - (m-l)^n) + \sum_{l=0}^{k^*-1} \frac{(-1)^l}{l!(n-l)!}((y-l)^n - (k^*-1-l)^n) \quad (41)$$

We then have the following results.

Proposition 6 *Given the model output in eq. (39),* $\mathbf{X} \in [0,1]^n$*, with* X_i *uniformly iid random variables, then:*

1.
$$F_Y = U_Y^n(y) \ \ and\, F_{Y|x_i} = U_Y^{n-1}(y - x_i) \quad (42)$$
where $U_Y^n(y)$ *is given in eq. (41).*

2. $Y_+^{x_i} = [0, a_i^n(x_i)] \cup [b_i^n(x_i), n]$ *and* $Y_-^{x_i} = [0, n] \backslash Y_+^{x_i}$*, where* $a_i^n(x_i)$ *and* $b_i^n(x_i)$ *are the solutions of the equation*
$$u_Y^{n-1}(y - x_i) = u_Y^n(y) \quad (43)$$

3.
$$s_i(x_i) = 2[U_Y^n(a_i^n(x_i)) - U_{Y|x_i}^{n-1}(a_i^n(x_i)) + U_{Y|x_i}^{n-1}(b_i^n(x_i)) - U_Y^{n-1}(b_i^n(x_i))] \quad (44)$$

4.
$$\delta_i = \int_0^1 \left[U_Y^n(a_i^n(s)) - U_{Y|x_i}^{n-1}(a_i^n(s)) + U_{Y|x_i}^{n-1}(b_i^n(s)) - U_Y^{n-1}(b_i^n(s))\right] ds \quad (45)$$

We note that item 1 extends previous results proven in Mitra (1971) and Sadooghi-Alvandi et al (2007). In particular, it introduces the conditional distributions of the sum of independently distributed uniform random variables. Item 3, furthermore, provides a general explicit expression of the separation between the conditional and unconditional densities of the sum of uniformly iid random variables.

Let us now illustrate Proposition 6. Given $n = 2$, by Item 1 in Proposition 6, the conditional and unconditional model output distributions are

$$u_Y^2(y) = \begin{cases} y \quad if \quad x_i \leq y < x_i + 1 \\ 2 - y\, if\, x_i + 1 \leq y < 2 + x_i \\ 0 \qquad\qquad otherwise \end{cases} \quad (46)$$

and

$$u_{Y|x_i}^1(y) = \begin{cases} 1\, if\, x_i \leq y < x_i + 1 \\ 0 \qquad otherwise \end{cases} \text{, respectively.} \quad (47)$$

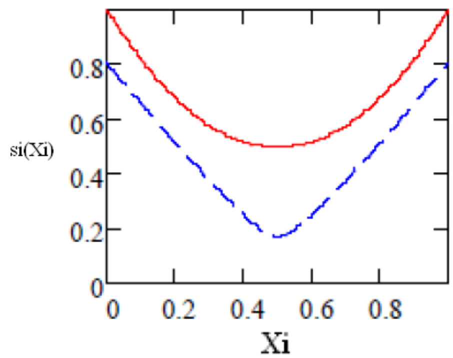

Figure 4: $s_i(X_i)$ in eq. (48) ($n = 2$, continuous line) and eq. (50) ($n = 3$, dotted line).

By solving eq. (43) (Item 2 in Proposition 6), one obtains $Y_+^{x_i} = [0, x_i] \cup [1 + x_i, 2]$, and $Y_+^{x_i} = (x_i, 1 + x_i)$. By eq. (44), one obtains the following closed form expression for the separation:

$$s_i(x_i) = 2x_i^2 - 2x_i + 1 \tag{48}$$

The left graph in Figure 4 displays $s_i(X_i)$ in eq. (48).

Finally, by Item 4 in Proposition 6, one obtains

$$\delta_i = \frac{1}{2} \int_0^1 s_i(v) dv = \frac{1}{3}. \tag{49}$$

For the case $n = 3$, by Proposition 6, we have (the derivation is Appendix A):

$$s_i(x_i) = \begin{cases} 2x_i - 2x_i^2 - \frac{1}{3} + (-x_i + \frac{1}{\sqrt{2}} + 1 - \sqrt{2}x_i)\sqrt{1 - 2x_i} - (\frac{\sqrt{2}}{6} + \frac{1}{3})\,(1 - 2x_i)^{\frac{3}{2}} \; if\; 0 \leq x_i < \frac{1}{2} \\ 2x_i - 2x_i^2 - \frac{1}{3} + (2x_i - \frac{1}{\sqrt{2}} - 1 + \sqrt{2}x_i)\sqrt{2x_i - 1} - (\frac{1}{3\sqrt{2}} + \frac{1}{3})\,(2x_i - 1)^{\frac{3}{2}} \; if\; \frac{1}{2} < x_i \leq 1 \end{cases} \tag{50}$$

One notes that, for $n = 3$, $s_i(x_i)$ is continuous, albeit piecewise-defined. δ_i is then found by integrating eq. (50) in $[0, 1]$. One obtains $\delta_i = 0.228$.

Figure 4 displays $s_i(X_i)$ for $n = 2$ and 3 (continuous and dotted lines, respectively). One notes the symmetric shape of $s_i(X_i)$ around $\mathbb{E}[X_i]$ (namely, $\frac{1}{2}$). As in the previous case studies, the minimum of the separation is reached when X_i is fixed at $\mathbb{E}[X_i]$.

The above analysis has concerned $n = 2$ and 3. For large n, by a result proven in Mitra (1971), Y is approximately normally distributed, with density

$$f_Y(y) \simeq \sqrt{\frac{3}{2\pi n}} e^{-\frac{3(y - \frac{n}{2})^2}{2n}} \tag{51}$$

Therefore, provided that the approximation in eq. (51) is accurate, one is brought back to a normal-additive problem and can apply the results of Section 4, namely Proposition 4. However, neither Mitra (1971), nor later on Sadooghi-Alvandi et al (2007), provide a numerical indication about the value of n for which such approximation becomes accurate. Our calculations allow us to verify the accuracy of the approximation. The results are reported in Table 2, lines $9-11$.

Table 2 shows that the normal approximation is accurate after $n=3$. A slight bias is, however, always present. The bias is caused by the missed truncation of the normal distribution tails. Lines $9-11$ in Table 2 also show that the relative importance of an uncertain input decreases with model size (both when considered with variance-based and moment independent importance measures), in accordance with intuition and with the results of the previous sections.

In the next section, we introduce a further analytical test case, in which the model output is a non-additive-non-multiplicative function of the model inputs.

7 Non Additive and Non-Multiplicative Model

In this section, we show the application of the procedure in Table 1 for obtaining moment independent importance measures analytically in the case of a non-additive and non-multiplicative model. The model equation is

$$Y=\frac{X_1}{X_1+X_2} \tag{52}$$

The random inputs are $X_1 \sim Gamma(\alpha,\theta)$ and $X_2 \sim Gamma(\beta,\theta)$, independently distributed. We write the Gamma densities as follows:

$$f_{X_1}(x_1;\alpha,\theta)=x_1^{\alpha-1}\frac{e^{-\frac{x_1}{\theta}}}{\theta^{\alpha}\Gamma(\alpha)}\,and\,f_{X_2}(x_2;\beta,\theta)=x_1^{\beta-1}\frac{e^{-\frac{x_1}{\theta}}}{\theta^{\beta}\Gamma(\beta)} \tag{53}$$

Before coming to the values of the sensitivity measures, let us study the behavior of the uncertainty in y deriving from the selected distributions. The resulting distribution of the model output [see also Appendix A] is Beta with parameters α and β. Thus, the model output assumes values between 0 and 1. Figure 5 displays the unconditional density of y for increasing values of $\alpha=\beta$.

Figure 5 shows that the distribution of y is symmetric when $\alpha=\beta$. In this case, the random inputs x_1 and x_2 are identically distributed. However, the mathematical expression of y is not symmetric in x_1 and x_2, although the resulting distribution of y is. This observation impacts the sensitivity measures, as we are to see later in this section. Furthermore, Figure 5 shows that the density of y tends to collapse on its expected value ($\mathbb{E}[y]$) as $\alpha=\beta$ increase. This implies that, for the model in eq. (52), while the variance of the model inputs increases (the variance of a gamma random variable increases linearly with α), the variance of the model output decreases.

Let us then come the global sensitivity analysis of this case study. As far as moment independent sensitivity measures are concerned, by applying the Procedure in Table 1, one finds the following results.

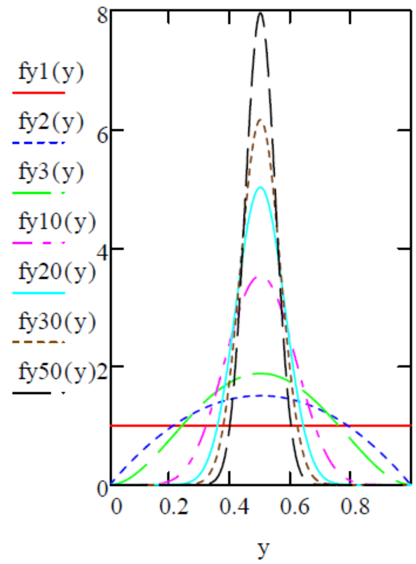

Figure 5: Density of y as $\alpha = \beta$ increase from 1 to 50. One notes that the density tends to a Dirac-δ density concentrated on the expected value of y, namely $\mathbb{E}[y] = 0.5$.

Proposition 7 *Given the model in eq. (52), X_1 and X_2 distributed according with the densities in eqs. (53), one obtains:*

1. *The unconditional and conditional distributions given x_1 and x_2 are, respectively:*

$$F_Y(y) = \frac{\int_0^y u^{\alpha-1}(1-u)^{\beta-1}dy}{\int_0^1 s^{\alpha-1}(1-s)^{\beta-1}ds}$$
$$F_{Y|x_1}(y) = \int_0^y \frac{(1-s)^{\beta-1}}{s^{\beta+1}} x_1^\beta \frac{e^{-\frac{x_1}{\theta}(\frac{1-s}{s})}}{\theta^\beta \Gamma(\beta)} dy \tag{54}$$
$$F_{Y|x_2}(y) = \int_0^y \frac{(s)^{\alpha-1}}{(s-1)^{\beta+1}} x_1^\beta \frac{e^{-\frac{x_1}{\theta}(\frac{1-s}{s})}}{\theta^\beta \Gamma(\beta)} dy$$

2. *Let $i = 1, 2$. $Y_+^{x_i} = [0, a_1(x_i)] \cup [a_2(x_i), 1]$ and $Y_-^{x_i} = [0,1] \backslash Y_+^{x_i}$, where $a_1(x_i)$ and $a_2(x_i)$ are the two points at which the conditional and unconditional densities intersect [they are given in Appendix A]*

3. $$s_i(x_i) = 2[F_Y(a_1(x_i)) - F_{Y|x_i}(a_2(x_i)) + F_{Y|x_i}(a_2(x_i)) - F_Y(a_2(x_i))] \tag{55}$$

4. $$\delta_i = \int_0^1 [F_Y(a_1(x_i)) - F_{Y|x_i}(a_2(x_i)) + F_{Y|x_i}(a_2(x_i)) - F_Y(a_2(x_i))] ds \tag{56}$$

It is possible to see (Appendix A) that, when $\alpha = \beta$, then $s_1(x_1)$ becomes identical to $s_2(x_2)$ — in the remainder we shall simply write $s(x)$ when $\alpha = \beta$. — By $s_1(x_1) = s_2(x_2)$, $\delta_1 = \delta_2$ when $\alpha = \beta$. This finding is in agreement with the symmetry effect discussed earlier.

Figure 6 displays $s(x)$ for increasing values of $\alpha = \beta$.

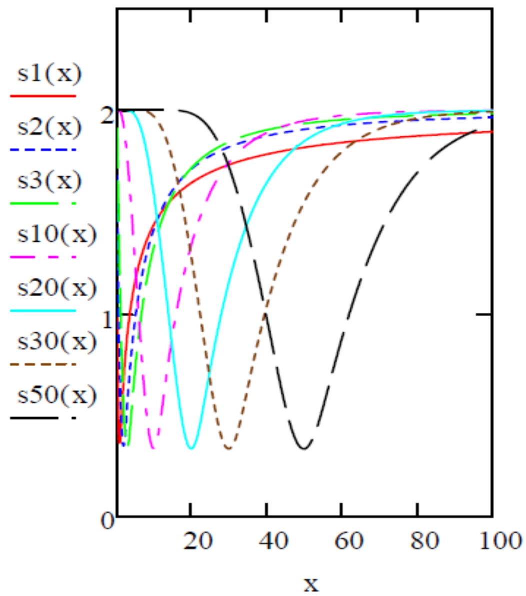

Figure 6: $s(x)$ for different choices of $\alpha = \beta$. The figure besides s on the vertical axes denotes the value. Hence, $s1(x)$ means the $s(x)$ for $\alpha = \beta = 1$; $s2(x)$ means $s(x)$ for $\alpha = \beta = 2$, and, similarly, $s2(x)$ means $s(x)$ for $\alpha = \beta = 50$.

Figure 6 shows that the separation reaches its minimum at $x = \alpha \cdot \theta$ ($\theta = 1$ in our case), which is the expected value of the random inputs. Furthermore, it is $lim_{x_i \to \infty} s_i(x_i) = 2$ and also $lim_{x_i \to 0} s_i(x_i) = 2$, similarly to the lognormal case study.

The values of the importance measures for increasing values of α are reported in Table 2, lines $13 - 15$. One notes that X_1 and X_2 have the same importance, both when ranked using moment independent and variance based sensitivity measures. The value of the global sensitivity indices (S), however, indicates the presence of a slight interaction effect, provoked by the non-additive structure of the model. By inspecting the values of S in row 15 of Table 2, one observes that the relevance of interactions decreases with α. Interactions are not felt for high values of α. As far as moment independent sensitivity measures are concerned, δ_i decreases with α, showing that it becomes less relevant to get to know a model input as α increases, in accordance with our previous discussion (when α increases, the distribution becomes more concentrated on $\mathbb{E}[y]$.)

The present and the previous three sections have formulated analytical test cases for moment independent importance measures. In the next section, we discuss numerical experiments.

8 Using the Analytical Test Cases to Perform Numerical Experiments

In this section, we discuss the numerical estimation of moment independent sensitivity measures in connection with the four test cases developed in the previous sections.

The computation of δ requires the quantification of the two integrals in eq. (9). The internal integral estimates $s_i(X_i)$. The external integral carries out the expectation over the distribution of X_i.

We utilize the following estimation procedure. Latin hypercube [McKay et al (1979)] is used to generate the unconditional model input sample of size N. This is represented by a matrix $X = [x_{i,j}, \begin{array}{c} i = 1, 2, ..., N \\ j = 1, 2, ..., n \end{array}]$, whose rows are a possible realization of the n input values, and whose columns represent the values of input X_i generated across the N Monte Carlo samples. We denote a column by $\widehat{X}_i = \left(x_i^{(1)}, \ldots, x_i^{(N)}\right)^T$, $\forall i = 1, \ldots, n$. By the corresponding N model runs, one obtains the unconditional model output sample, $\widehat{Y} = \left(y^{(1)}, \ldots, y^{(N)}\right)$. The unconditional model output sample is then utilized to estimate the unconditional model output density, $f_Y(y)$. In this respect, we make use of kernel density estimation [non-parametric approach, Parzen (1962)] to fit unconditional distribution. For obtaining the conditional density, we proceed as follows. First, the conditional model input sample is obtained. To condition on, say, X_r one fixes all elements of the r^{th} column of matrix $\widehat{X}$ to one of the values sampled, say, $\widehat{x}_{r,i}$. Then, two alternatives are possible depending on whether the model inputs are correlated: a) in the presence of correlations, one needs to re-samples the remaining $n-1$ model inputs given that $X_r = \widehat{x}_{r,i}$; b) in the case of uncorrelated inputs, one can obtain the conditional samples without actual re-sampling, but by simply repeating the column substitution (substituted columns sampling plan). At each $\widehat{x}_{r,i}$, one then estimates $f_{Y|x_{r,s}}(y)$ by kernel density. One is, then, in a position to evaluate the separation $s_i(\widehat{x}_{r,i})$. Finally, the statistics $\sum_{r=1}^{N} \frac{s_i(\widehat{x}_{r,i})}{2N}$ provides an estimate of δ_i. The total number of model evaluations for this computational strategy is $nN^2 + N$, both in the case of correlated and uncorrelated model inputs.

In order to assess whether the envisioned strategy leads to a correct estimation of the sensitivity measures, one can utilize the analytical test cases developed in the previous sections as benchmarks. In this exercise, we use all the four case studies, with the following input data:

1. Model of Section 4, with three parameters ($n = 3$), equal weights ($\mathbf{a} = \mathbf{1}$), and parameters of the normal distributions $\boldsymbol{\mu} = \mathbf{1}$ and diagonal covariance matrix $\Sigma = diag(16, 4, 1)$;

2. Model of Section 5, with three parameters ($n = 3$), equal weights ($\mathbf{a} = \mathbf{1}$), and parameters of the lognormal distributions $\boldsymbol{\eta} = 1$, and $\xi_1 = 16, \xi_2 = 4$, and $\xi_3 = 1$;

3. Model of Section 6, with three uniformly distributed parameters;

4. Model of Section 7 with input parameter distributions $\alpha = \beta = 3$.

Based on these data, by Propositions 4, 5, 6, and 7, one obtains the following values of the sensitivity measures:

1. $\delta_1 = 0.472$, $\delta_2 = 0.155$ and $\delta_3 = 0.071$;

2. $\delta_1 = 0.472$, $\delta_2 = 0.155$ and $\delta_3 = 0.071$;

3. $\delta_1 = \delta_2 = \delta_3 = 0.228$;

4. $\delta_1 = \delta_2 = 0.315$.

Figures 7, 8, 9 and 10 report the results of numerical experiments showing both robustness (replicates at same sample size) and convergence (increasing the sample size) of the sensitivity measure estimates.

We start with describing the results of the third and fourth case studies (Figures 9 and 10). In these test cases, the model inputs are equally important. The dotted line shows the analytical value of the importance measures. The horizontal axis displays the number of model evaluations. The size of the base Latin hypercube sample (N) is varied from 8 to 128, leading to a number of model runs varying from 200 to 49280. In the first three (two) graphs Figures 9 and 10, respectively, the estimates of δ are displayed. The box-plots surrounding the values of the importance measures describe the accuracy in the estimation. The box-plots are obtained by 100 replicates of the estimation procedure at each sample size. In each box plot, the central mark is the median of the replicates, and the edges are the 25^{th} and 75^{th} percentiles, respectively. The dotted reference line marks the analytical value. The whiskers extend to the most extreme data points not considered outliers; outliers are plotted individually. Results show that: *i*) the numerical estimates monotonically converge towards the analytical values as N increases; *ii*) the analytical value is always contained in the uncertainty bounds provided by the replicates; *iii*) the dispersion is significantly and constantly reduced as the sample size increases. In this respect, the fourth (third) graph in 9 and 10 report the evolution of the average root mean square error (RMSE) (where the average is taken across the 100 replicates) in a loglog plot. RMSE decreases steadily with N. Besides receiving confirmation of the correctness of the estimation procedures, the graphs in Figures 9 and 10, can be utilized to gain additional insights on numerical convergence. In this respect, let us examine the results for the normal and lognormal test cases (Figures 7 and 8). In these two case studies, the model inputs have different importance. By considering the model input ranking instead of the importance measures values, one can identify the sample size that leads to consistent ranking. In our case, starting with $N = 784$, there is no more overlapping between the box plots of the model inputs. Given the monotonic convergence to the analytical estimates, this fact indicates that the ranking of the parameters is stable and is not going to change by increasing the sample size.

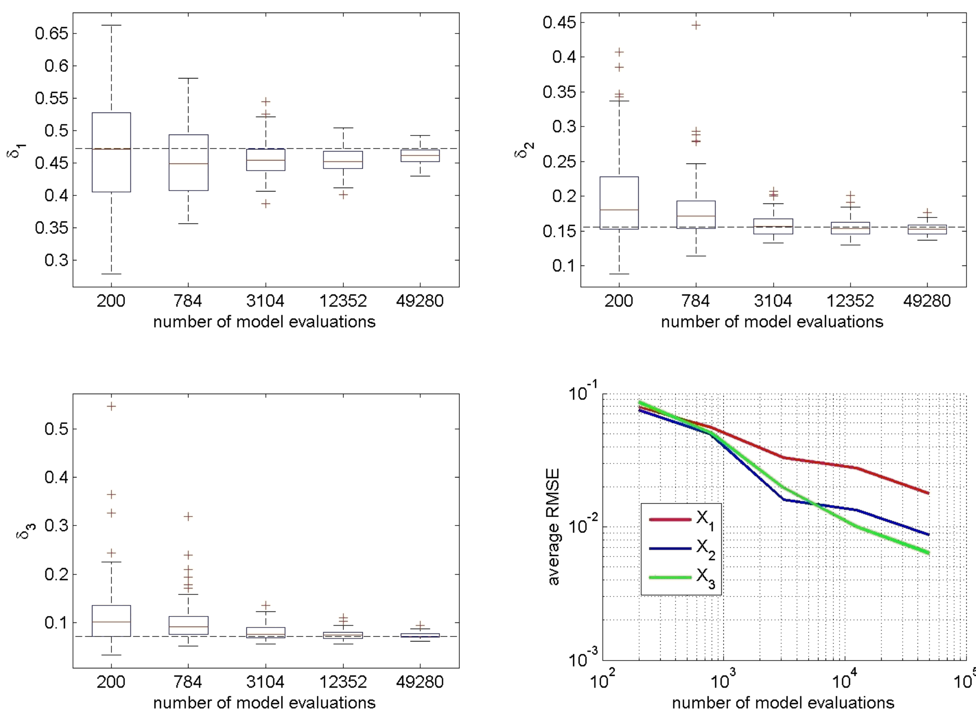

Figure 7: Numerical results for the additive model with normal input variables (i.e. model defined by eq. 21), $n = 3$, $\mathbf{a} = \mathbf{1}$ and $\Sigma = diag(16, 4, 1)$. Box edges are defined by the 25^{th} and 75^{th} percentiles, the reference values by dotted lines.

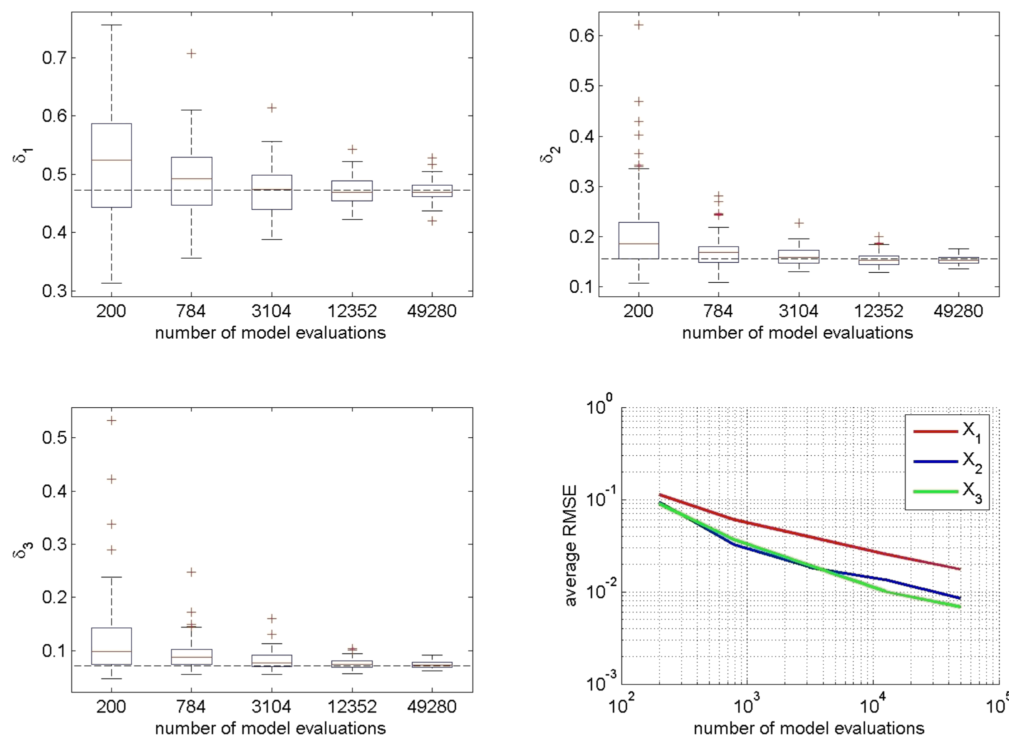

Figure 8: Numerical results for the multiplicative model with lognormal input variables (i.e. the case stufy defined in Section 5), for $n = 3$, $\mathbf{a} = \mathbf{1}$ and $\Sigma = diag(16, 4, 1)$. Box edges are defined by the 25^{th} and 75^{th} percentiles, the reference values by dotted lines.

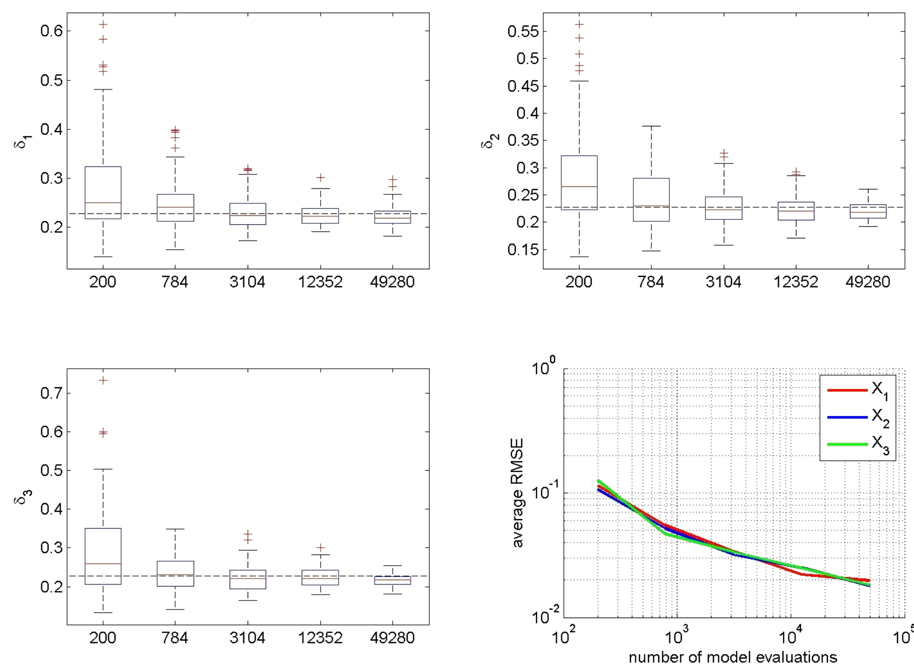

Figure 9: Numerical results for the additive model with uniform input variables (i.e., the test case defined in Section 6) for $n = 3$. Box edges are defined by the 25^{th} and 75^{th} percentiles, the reference values by dotted lines.

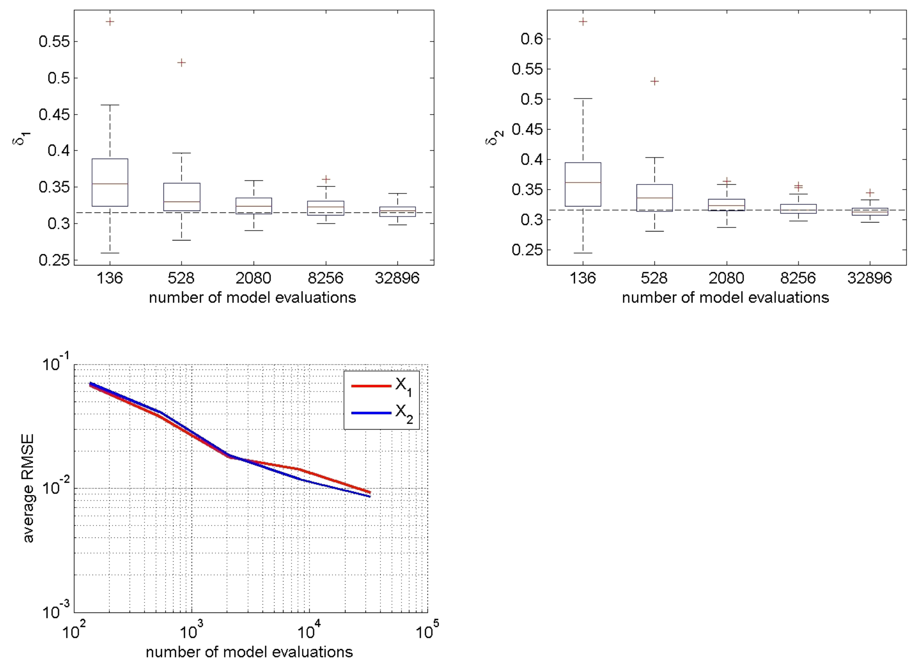

Figure 10: Non additive and non-multiplicative model with Gamma input variables (i.e. case study defined in Section 7}, for $\alpha = \beta = 3$. Box edges are defined by the 25^{th} and 75^{th} percentiles, the reference values by dotted lines.

9 Conclusions

Moment independent sensitivity measures have been developed along the lines of uncertainty and global SA works underlying the need for providing a thorough way of assessing the influence of an uncertain model input on the model output (decision criterion, risk metric). In particular, moment independent techniques avoid reliance on the assumption that variance is sufficient to characterize uncertainty. However, due to the lack of analytical test cases, works in moment independent SA rely on ad-hoc numerical strategies in estimating the sensitivity measures. This lack makes it impossible to assess the reliability of a given estimation strategy. Furthermore, the absence of benchmarks prevents one from comparing alternative estimation designs.

This paper has introduced a new methodology that allows one to obtain moment independent importance measures analytically. At the basis of the methodology is the establishment of the link between moment independent importance measures and the statistical theory of density separation. This link has enabled us to obtain two new properties for moment independent importance measures: *i*) invariance for monotonic transformation of the model output; *ii*) evaluation via cumulative distribution. The former property is relevant in numerical applications in which re-scaling is applied to the model output. The latter property has enabled us to formalize a four-step procedure for obtaining moment independent importance sensitivity measures analytically. We have illustrated the methodology via the formulation of four case studies: *i*) additive model with multivariate normal random inputs; *ii*) multiplicative model with lognormally iid random inputs; *iii*) additive model with uniformly distributed random variables; and *iv*) non-additive-non-multiplicative model with gamma distributed random variables. It has then been possible to analyze the behavior of moment independent importance measures for different combinations of model input support (finite, semi-infinite and infinite) and model structures (additive and interactive). For each test case, we have also obtained the corresponding values of the variance-based sensitivity measures. By comparing variance-based and moment-independent results, has enabled us to shed further light on the differences between these two global SA approaches and about the differences in insights they deliver to decision-makers. In particular, the complementary nature of the insights derived by the two methods emerges, with moment independent methods better capable of reflecting uncertainty and variance based of reflecting model structure.

Finally, we have demonstrated the use of the four case studies through numerical experiments.

We conclude with a note on future research. The analytical test cases developed in this work provide a benchmark for future studies aimed at comparing and improving the numerical sampling strategies, by testing combinations of sampling designs, on the one hand, and approaches to evaluate the shift between unconditional and conditional densities, on the other hand. The availability of analytical test cases with dependent inputs (Proposition 4) provides the benchmark for assessing the impact of the independence assumption that characterizes most of global SA studies to date. A further research direction is represented by the combination of emulators and moment independent techniques. Moment independent techniques, being global, potentially ask for a high number of model runs in numerical estimation. This might make their computation problematic for models requiring long computational times. The recent developments in the area of meta-modelling and emulators, however, suggest the combination of emulators — that reduce model complexity — and moment independent techniques as a promising way for obtaining importance measures that thoroughly reflect uncertainty, even in the presence of computationally intensive models.

10 Appendix A: Proofs

Proof of Proposition 1. Since $\Omega_+ \cap \Omega_- \cap \Sigma = \varnothing$, by additivity of the integral

$$\begin{aligned} &\int_\Omega |f-g|\mathrm{d}\mu(\omega) = \int_{\Omega_+}(f-g)\mathrm{d}\mu(\omega) + \int_{\Omega_-}(g-f)\mathrm{d}\mu(\omega) + \int_\Sigma 0\mathrm{d}\mu(\omega) \\ &= \int_{\Omega_+} f\mathrm{d}\mu(\omega) - \int_{\Omega_+} g\mathrm{d}\mu(\omega) + \int_{\Omega_-} g\mathrm{d}\mu(\omega) - \int_{\Omega_-} f\mathrm{d}\mu(\omega) \\ &= F(\Omega_+) - G(\Omega_+) + G(\Omega_-) - F(\Omega_-) \\ &= F(\Omega_+) - G(\Omega_+) + [1-G(\Omega_+)] - [1-F(\Omega_+)] \\ &= 2F(\Omega_+) - 2G(\Omega_+) \end{aligned} \tag{57}$$

and

$$\begin{aligned} &F(\Omega_+) - G(\Omega_+) + G(\Omega_-) - F(\Omega_-) \\ &= 1 - F(\Omega_-) - [1-G(\Omega_-)] + G(\Omega_-) - F(\Omega_-) \\ &= 2G(\Omega_-) - 2F(\Omega_-) \end{aligned} \tag{58}$$

■

Proof of Corollary 1. Let $\omega_0 \in \Omega$ the point such that, given a generic function $h(\omega)$

$$\int_\Omega h(\omega)\cdot\delta^{Dirac}\mathrm{d}\mu(\omega) = h(\omega_0) \tag{59}$$

In this case, $\Omega_+ = \Omega_+ - \{\omega_0\}$ and $\Omega_- = \{\omega_0\}$. Consequently, in eq. (13), $F(\Omega_+) = 1$ and $G^{Dirac}(\Omega_+) = 0$. Conversely, $G^{Dirac}(\Omega_-) = 1$ and $F(\Omega_-) = 0$. Inserting in eq. (13) completes the proof. ■

Proof of Proposition 2. By eq. (11),

$$\|f_Z - g_Z\| = \int_\Omega |f_Z(z(\omega)) - g_Z(z(\omega))|\mathrm{d}\mu(z(\omega)) \tag{60}$$

which, by positivity of $\mathrm{d}\mu(z(\omega))$ implied by the monotonicity of $z(\omega)$, can be rewritten as

$$\|f_Z - g_Z\| = \int_\Omega |f_Z(z(\omega))\mathrm{d}\mu(z(\omega)) - g_Z(z(\omega))\mathrm{d}\mu(z(\omega))| \tag{61}$$

By the change of variable rule, one obtains

$$f_Z(z)\mathrm{d}\mu(z) = f_\Omega(\omega)\mathrm{d}\mu(\omega) \tag{62}$$

and

$$g_Z(z)\mathrm{d}\mu(z) = g_\Omega(\omega)\mathrm{d}\mu(\omega) \tag{63}$$

whence

$$\begin{aligned}\|f_Z - g_Z\| = \int_\Omega |f_Z(z)\mathrm{d}\mu(z) - g_Z(z)\mathrm{d}\mu(z)| \\ = \int_\Omega |f_\Omega(\omega)\mathrm{d}\mu(\omega) - g_\Omega(\omega)\mathrm{d}\mu(\omega)| = \|f_\Omega - g_\Omega\|_\mu\end{aligned} \tag{64}$$

■

Proof of Proposition 3. Item 1. If $Z = z(Y)$ is a monotonically increasing transformation of the model output, by eq. (15), one has:

$$\left\|f_Y - f_{Y|x_i}\right\| = \left\|f_Z - f_{Z|x_i}\right\| \tag{65}$$

It follows that $\mathbb{E}_{X_i}[\left\|f_Y - f_{Y|x_i}\right\|] = \mathbb{E}_{X_i}[\left\|f_Z - f_{Z|x_i}\right\|]$.

Item 2. Since $f_{Y|X_1=x_1,X_2=x_2,\ldots,X_n=x_n} = \delta^{Dirac}(\mathbf{x})$ [see Appendix A in Borgonovo (2007)] then eq. (17) follows by Corollary 1.

Item 3. $s_i(X_i) = \left\|f_Y - f_{Y|x_i}\right\|$, by eqs. (11) and (10). Hence, eq. (19) follows by Proposition 1. Eq. (20), follows by eq.(9).

1. Given $X_i = x_i$, eq. (21) can be rewritten as

$$Y|x_i = \sum_{\substack{s=1 \\ s\neq i}}^{n} a_s X_s + a_i x_i \tag{66}$$

   with $a_i x_i$ being a constant term. $Y|x_i$ is then still normal. The conditional distribution of X_s, given $X_i = x_i$, is $N(m_s + (x_i - m_i)\frac{\sigma_{s,i}}{\sigma_i}, \sigma_{j,s} - \frac{\sigma_{j,i}\cdot\sigma_{i,s}}{\sigma_i})$. It follows that $Y|x_i \sim N(\sum_{s=1}^{n} a_s \left[m_s + (x_i - m_i)\frac{\sigma_{s,i}}{\sigma_i}\right], \mathbf{a}\Sigma_{Y|x_i}\mathbf{a}^T)$, with $\Sigma_{Y|x_i}$ in eq. (24).

2. Two normal densities intersect at the points determined by the equality

$$\frac{1}{\sqrt{2\pi V_Y}} e^{-\frac{(y-m_Y)^2}{2V_Y}} = \frac{1}{\sqrt{2\pi V_{Y|x_i}}} e^{-\frac{\left(y-m_{Y|x_i}\right)^2}{2V_{Y|x_i}}} \tag{67}$$

   By some manipulation, one obtains the quadratic equation

$$0 = \frac{(y-m_Y)^2}{2V_Y} - \frac{\left(y - m_{Y|x_i}\right)^2}{2V_{Y|x_i}} + \ln\frac{\sqrt{V_Y}}{\sqrt{V_{Y|x_i}}} \tag{68}$$

   The solution is represented by the two points given in eq. (25).

3. By applying Proposition 3, one obtains

$$F_Y(Y_+^{x_i}) = N(y_1; m_Y, V_Y) + (1 - N(y_2; m_Y, V_Y)) \tag{69}$$

$$F_{Y|x_i}(Y_+^{x_i}) = N(y_1; m_{Y|x_i}, V_{Y|x_i}) + (1 - N(y_2; m_{Y|x_i}, V_{Y|x_i}) \tag{70}$$

Then eq. (26) follows by eq. (19).

4. Eq. (27) follows by expectation of eq. (26).

■

Proof of Corollary 2. If $X_i \to +\infty$, then by eq. (25), $y_1 \to +\infty$ and $y_2 \to -\infty$. Consequently, in eq. (26), for the terms concerning the unconditional distribution, one has:

$$\begin{aligned} \lim_{x_i \to \infty} N(+\infty; m_Y, V_Y) = 1 \\ \lim_{x_i \to \infty} N(-\infty; m_Y, V_Y) = 0 \end{aligned} \tag{71}$$

The terms concerning the conditional distribution behave as follows. $a)$ $\lim_{X_i \to +\infty} N(y_2; m_Y, V_Y) = 0$, since $\lim_{r \to -\infty} \int_{-\infty}^{r} \frac{1}{\sqrt{2\pi\sigma}} e^{\frac{-(s - m_{Y|x_i})^2}{2V_{Y|x_i}}} \mathrm{d}s = 0$. $b)$ $N(+\infty; m_{Y|x_i}, V_{Y|x_i}) \to 0$. In fact, by eq. (23), $\lim_{X_i \to \infty} m_{Y|x_i} = +\infty$ and the Gaussian density tends to the null function as X_i increases. Therefore,

$$\lim_{X_i \to +\infty} s_i(x_i) = 2 \lim_{X_i \to \infty} N(+\infty; m_Y, V_Y) \tag{72}$$

This limit equals 2 by eq. (71). The result for $X_i \to -\infty$ is proven in a similar fashion, and follows by symmetry. ■

Proof of Proposition 5. By taking the logarithm of both sides of eq. (31), one obtains

$$\ln Y = \ln \prod_{i=1}^{k} X_i^{a_i} = \sum_{i=1}^{k} a_i \ln X_i$$

Hence, $\ln Y \sim N(\sum_{i=1}^{k} a_i \eta_i, \sum_{i=1}^{k} a_i^2 \xi_i^2)$. The first equality in eq. (33) then follows. The second equality (conditional density of Y given $X_i = x_i$) is found as follows. By eq. (31),

$$Y_{|x_i} = x_i^{a_i} \prod_{\substack{s=1 \\ s \neq i}}^{n} X_s^{a_s} \tag{73}$$

By taking the logarithm of both sides, one writes

$$\ln Y_{|x_i} = a_i \ln x_i + \sum_{\substack{s=1 \\ s \neq i}}^{n} a_s \ln X_s$$

Hence, $\ln Y_{|X_i = x_i}$ is normally distributed with parameters

$$\eta_{Y|x_i} = \sum_{\substack{s=1 \\ s \neq i}}^{k} a_s \eta_s + a_i \ln x_i = \eta_Y - a_i \eta_i + a_i \ln x_i \tag{74}$$

and

$$\xi^2_{Y|x_i} = \sum_{\substack{s=1 \\ s\neq i}}^{k} \xi^2_s$$

It follows that $Y_{|X_i=x_i}$ is lognormally distributed with parameters $\eta_{Y|x_i}$ and $\xi^2_{Y|x_i}$. For items 2, 3 and 4, one needs to note that $Z = \ln Y$ is a monotonic transformation of Y and that Z is normally distributed. By Proposition 2, the problem is transformed back to the problem of Proposition 4. Hence, items 2, 3 and 4 follow by Point 3 of Proposition 3 and by Proposition 4. ■

Proof of Proposition 6. Item 1 holds by the change of variable rule. Item 2 follows by the definitions of$Y^{x_i}_+$ and $Y^{x_i}_-$ in Proposition 3. Items 3 and 4 follow by Proposition 3. ■

Proof of eq. (31) . By the properties of variance,

$$V_Y = \mathbb{E}[(\prod_{i=1}^{k} X_i - \prod_{i=1}^{k} \mathbb{E}[X_i])^2] = \prod_{i=1}^{k} \mathbb{E}[X_i^2] - \prod_{i=1}^{k} \mathbb{E}[X_i]^2 \tag{75}$$

In the case of lognormally distributed random variables, $\mathbb{E}[X_i] = e^{\eta_i + \xi_i^2/2}$ and $V[X_i] = (e^{\xi_i^2} - 1)e^{2\eta_i + \xi_i^2}$. Hence

$$\mathbb{E}[X_i^2] = V[X_i^2] + \mathbb{E}[X_i]^2 = e^{2\eta_i + 2\xi_i^2} \tag{76}$$

Substituting into eq. (75), one obtains

$$V_Y = \prod_{i=1}^{k} e^{2\eta_i + 2\xi_i^2} - \prod_{i=1}^{k} (e^{2\eta_i + \xi_i^2}) \tag{77}$$

We then let $\eta_Y = \sum_{i=1}^{k} \eta_i$ and $\xi_Y^2 = \sum_{i=1}^{k} \xi_i^2$, to obtain

$$V_Y = e^{2\eta_Y + 2\xi_Y^2} - e^{2\eta_Y + 2\xi^2} = e^{2\eta_Y + \xi^2}(e^{\xi_Y^2} - 1) \tag{78}$$

The conditional variance is obtained as follows. If X_i is fixed at x_i, then

$$\xi^2_{Y|x_i} = \sum_{s=1, i\neq s}^{k} \xi_s^2 = \xi_Y^2 - \xi_i^2 \tag{79}$$

$\eta_{Y|x_i}$ is given in eq. (74). Therefore,

$$V_{Y|x_i} = e^{2\eta_{Y|x_i} + \xi^2_{Y|x_i}}(e^{\xi^2_{Y|x_i}} - 1) = e^{\xi_Y^2 - \xi_i^2 + 2\eta - 2\eta_i + 2\ln x_i}(e^{\xi^2_{Y|x_i}} - 1) = x_i^2 \frac{e^{\xi_Y^2 + 2\eta}}{e^{\xi_i^2 + 2\eta_i}}(e^{\xi_Y^2 - \xi_i^2} - 1) \tag{80}$$

The corresponding expected value is

$$\begin{aligned} \mathbb{E}_{X_i}\left\{V(Y|x_i)\right\} &= \mathbb{E}\left(X_i^2\right) \frac{e^{\xi_Y^2 + 2\eta}}{e^{\xi_i^2 + 2\eta_i}}(e_i^{\xi_Y^2 - \xi_i^2} - 1) = e^{2\eta_i + 2\xi_i^2} \frac{e^{\xi_Y^2 + 2\eta}}{e^{\xi_i^2 + 2\eta_i}}(e_i^{\xi_Y^2 - \xi_Y^2} - 1) \\ &= e^{\xi_i^2} e^{\xi_Y^2 + 2\eta}(e_i^{\xi_Y^2 - \xi_i^2} - 1) \end{aligned} \tag{81}$$

Whence,

$$S_i = \frac{V_Y - \mathbb{E}_{X_i}\{V(Y|x_i)\}}{V_Y} = 1 - \frac{e^{\xi_i^2} e^{\xi_Y^2+2\eta}(e_i^{\xi_Y^2-\xi_i^2} - 1)}{e^{2\eta+\xi_Y^2}(e^{\xi_Y^2} - 1)} = 1 - \frac{(e^{\xi_Y^2} - e^{\xi_i^2})}{(e^{\xi_Y^2} - 1)}$$

■

Proof of Lemma 1. We prove the expression for the cumulative distribution function of the sum and conditional sum of uniformly distributed random variables. Let $s \in [k^* - 1, k^*]$, $k^* = 1, 2, .., n$. Then, by integrating eq. (40), one obtains

$$G(s) = \int_0^s f(s)ds = \sum_{m=0}^{k^*-2} \int_m^{m+1} f_m(s)ds + \int_{k^*-1}^s f_{k^*-1}(s)ds \tag{82}$$

The first term in the right hand side of eq. (82), is given by:

$$\begin{aligned} \sum_{m=0}^{k^*-2} \textstyle\int_m^{m+1} f_m(s)ds &= \sum_{m=0}^{k^*-2} \textstyle\int_m^{m+1} \sum_{l=0}^{m} (-1)^l \binom{n}{l} \frac{1}{(n-1)!}(s-l)^{n-1}\mathrm{d}s \\ &= \sum_{m=0}^{k^*-2} \sum_{l=0}^{m} (-1)^l \binom{n}{l} \frac{1}{(n)!}(m+1-l)^n - (m-l) \end{aligned} \tag{83}$$

The second term in the right hand side of eq. (41), is given by:

$$\begin{aligned} \textstyle\int_{k^*-1}^s f_{k^*-1}(s)ds &= \textstyle\int_{k^*-1}^s \sum_{l=0}^{k^*-1} (-1)^l \binom{n}{l} \frac{1}{(n-1)!}(u-l)^{n-1}\mathrm{d}u \\ &= \sum_{l=0}^{k^*-1} (-1)^l \binom{n}{l} \frac{1}{n!}((s-l)^n - (k^*-1-l)^n) \end{aligned} \tag{84}$$

As a consequence eq.(82) equals eq. (41). ■

Proof of eq. (50). The unconditional and conditional densities become

$$u_Y^3(y) = \begin{cases} \frac{1}{2}y^2 & if\ 0 \le y < 1 \\ -y^2 + 3y - \frac{3}{2} & if\ 1 \le y < 2 \\ \frac{1}{2}(y-3)^2 & if\ 2 \le y < 3 \\ 0 & otherwise \end{cases} \tag{85}$$

and

$$u_{Y|x_i}^3(y) = \begin{cases} y - x_i & if \quad x_i \le y < x_i + 1 \\ 2 - y + x_i & if\ x_i + 1 \le y < 2 + x_i \\ 0 & otherwise \end{cases} \tag{86}$$

respectively. By some manipulation, the points $a_i^3(x_i)$ and $b_i^3(x_i)$ are:

$$a_i^3(x_i) = \begin{cases} 1-\sqrt{1-2x_i}\, if\, 0 \leq x_i < \frac{1}{2} \\ \sqrt{x_i - \frac{1}{2}} + 1\, if\, \frac{1}{2} \leq x_i \leq 1 \end{cases} \tag{87}$$

$$b_i^3(x_i) = \begin{cases} 2-\sqrt{\frac{1}{2} - x_i}\, if\, 0 \leq x_i < \frac{1}{2} \\ \sqrt{2x_i - 1} + 2\, if\, \frac{1}{2} \leq x_i \leq 1 \end{cases} \tag{88}$$

The next step is to evaluate $U_Y^n(y)$ and $U_{Y|x_i}^{n-1}(y)$ at $a(x_i)$ and $b(x_i)$, respectively. By Proposition 6, we have:

$$U_Y^n(a(x_i)) = \begin{cases} \frac{1}{6}(1-\sqrt{1-2x_i})^3 & if\, 0 \leq x_i < \frac{1}{2} \\ \frac{1}{2}x_i + \frac{1}{2}\sqrt{x_i - \frac{1}{2}} - \frac{1}{3}\left(x_i - \frac{1}{2}\right)^{\frac{3}{2}} - \frac{1}{12} & if\, \frac{1}{2} \leq x_i \leq 1 \end{cases}, \tag{89}$$

$$U_Y^n(b(x_i)) = \begin{cases} \frac{1}{2}x_i - \frac{1}{2}\sqrt{\frac{1}{2} - x_i} + \frac{1}{3}\left(\frac{1}{2} - x_i\right)^{\frac{3}{2}} + \frac{7}{12} & if\, 0 \leq x_i < \frac{1}{2} \\ \frac{1}{2}\sqrt{2x_i - 1} - x_i + \frac{1}{6}\left(2x_i - 1\right)^{\frac{3}{2}} + \frac{4}{3} & if\, \frac{1}{2} \leq x_i \leq 1 \end{cases}, \tag{90}$$

$$U_{Y|x_i}^{n-1}\left\{a(x_i)\right\} = \begin{cases} \frac{1}{2}(1-\sqrt{1-2x_i} - x_i)^2\, if\, 0 \leq x_i < \frac{1}{2} \\ \frac{1}{2}(\sqrt{x_i - \frac{1}{2}} + 1 - x_i)^2\, if\, \frac{1}{2} \leq x_i \leq 1 \end{cases}, \tag{91}$$

and

$$U_{Y|x_i}^{n-1}\left\{b(x_i)\right\} = \begin{cases} \frac{1}{2}x_i - \frac{1}{2}x_i^2 - \frac{1}{2}\sqrt{2}x_i\sqrt{1-2x_i} + \frac{3}{4}\, if\, 0 \leq x_i < \frac{1}{2} \\ x_i\sqrt{2x_i - 1} - x_i - \frac{1}{2}x_i^2 + \frac{3}{2} \quad if\, \frac{1}{2} \leq x_i \leq 1 \end{cases} \tag{92}$$

By inserting the above results into eq. (44), and simplifying, one obtains the explicit expression for $s_i(X_i)$ in eq. (50). ■

Proof of Proposition 7. The first step is the determination of the density of Y. In this respect, a well known result in statistical theory states that, under the above assumptions on the distributions of X_1 and X_2, $Y \in [0,1]$ follows a Beta(α, β) distribution with density

$$f_Y(y) = \frac{y^{\alpha-1}(1-y)^{\beta-1}}{\int_0^1 s^{\alpha-1}(1-s)^{\beta-1}\mathrm{d}s} \tag{93}$$

The conditional densities are found as follows. If one conditions on $X_1 = x_1$, then the model output becomes a random variable depending only on X_2:

$$Y_{|x_1} = g(X_2) = \frac{x_1}{x_1 + X_2} \tag{94}$$

The density $f_{Y|x_1}(y)$ is obtained by the change of variable formula, as follows.

$$f_{Y|x_1}(z)dz = f_{X_2}(x_2)dx_2 \tag{95}$$

$$f_{Y|x_1}(y) = f_{X_2}(x_2)\frac{1}{\left|\frac{\partial z}{\partial X_2}\right|} = f_{X_2}(x_2)\frac{1}{\frac{\partial}{\partial X_2}(\frac{x_1}{x_1+X_2})} \tag{96}$$

Let us work out the right hand side. One has: $\frac{\partial}{\partial X_2}(\frac{x_1}{x_1+X_2}) = -\frac{x_1}{(X_2+x_1)^2}$, hence

$$f_{X_2}(x_2)\frac{1}{\frac{\partial}{\partial X_2}(\frac{x_1}{x_1+X_2})} = X_2^{\beta-1}\frac{e^{-\frac{X_2}{\theta}}}{\theta^{\alpha}\Gamma(\beta)}\frac{(X_2+x_1)^2}{x_1} \tag{97}$$

Substituting for $X_2 = \frac{x_1}{y} - x_1$, one obtains:

$$f_{X_2}(x_2)\frac{1}{\frac{\partial}{\partial X_2}(\frac{x_1}{x_1+X_2})} = \left(\frac{x_1}{y} - x_1\right)^{\beta-1}\frac{e^{-\frac{X_2}{\theta}}}{\theta^{\beta}\Gamma(\beta)}\frac{x_1}{y^2} \tag{98}$$

$$f_{Y|x_1}(y) = \frac{(1-y)^{\beta-1}}{y^{\beta+1}}x_1^{\beta}\frac{e^{-\frac{x_1}{\theta}(\frac{1-y}{y})}}{\theta^{\beta}\Gamma(\beta)} \tag{99}$$

Proceeding in a similar fashion, one has

$$f_{Y|x_2}(y) = \frac{y^{\alpha-1}}{(1-y)^{\alpha+1}}x_2^{\alpha}\frac{e^{-\frac{x_2}{\theta}(\frac{y}{1-y})}}{\theta^{\alpha}\Gamma(\alpha)} \tag{100}$$

Hence, the points at which the two distributions intercept are found, for X_1:

$$\frac{y^{\alpha-1}(1-y)^{\beta-1}}{\int_0^1 s^{\alpha-1}(1-s)^{\beta-1}ds} = \frac{(1-y)^{\beta-1}}{y^{\beta+1}}x_1^{\beta}\frac{e^{-\frac{x_1}{\theta}(\frac{1-y}{y})}}{\theta^{\beta}\Gamma(\beta)} \tag{101}$$

Letting $C_{Beta} = \int_0^1 s^{\alpha-1}(1-s)^{\beta-1}ds$ and $C_{Gamma} = \theta^{\beta}\Gamma(\beta)$, one obtains, while conditioning on X_1,

$$y^{\alpha+\beta} = \frac{C_{Beta}}{C_{Gamma}}x_1^{\beta}e^{-\frac{x_1}{\theta}\left(\frac{1-y}{y}\right)} \tag{102}$$

and, while conditioning on X_2

$$(1-y)^{\beta+\alpha} = \frac{C_{Beta}}{C_{Gamma}} x_2^{\alpha} e^{-\frac{x_2}{\theta}\left(\frac{y}{1-y}\right)} \tag{103}$$

By eqs. (54) and Proposition 3, the remainder follows.

We note that, in particular, one can write

$$s_1(x_1) = \int_0^1 \left| \frac{y^{\alpha-1}(1-y)^{\beta-1}}{\int_0^1 s^{\alpha-1}(1-s)^{\beta-1}ds} - \frac{(1-y)^{\beta-1}}{y^{\beta+1}} x_1^{\beta} \frac{e^{-\frac{x_1}{\theta}\left(\frac{1-y}{y}\right)}}{\theta^{\beta}\Gamma(\beta)} \right| dy \tag{104}$$

and

$$s_2(x_2) = \int_0^1 \left| \frac{y^{\alpha-1}(1-y)^{\beta-1}}{\int_0^1 s^{\alpha-1}(1-s)^{\beta-1}ds} - \frac{y^{\alpha-1}}{(1-y)^{\alpha+1}} x_2^{\alpha} \frac{e^{-\frac{x_2}{\theta}\left(\frac{y}{1-y}\right)}}{\theta^{\alpha}\Gamma(\alpha)} \right| dy \tag{105}$$

One observes that for $\alpha = \beta$, $s_1(x_1) = s_2(x_2)$ and, therefore, $\delta_1 = \delta_2$. ■

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