Moment Independent Sensitivity Analysis: an Introduction and some Recent Results

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Part I

Overview and Principles

Summary

- Overview of Sensitivity Analysis
- Brief Review of Variance Based Sensitivity
- Motivation of Moment Independent Sensitivity
- Definition of the $\delta-$importance measure
- Properties
- Analytical Results and New Findings

Sensitivity Analysis

- Fürbinger (1996): "*Sensitivity Analysis for Modellers: Would You go to an Orthopaedist who didn't use X-ray?*"
- US EPA, 2009: "*recommends best practices to help determine when a model, despite its uncertainties, can be appropriately used to inform a decision. Specifically, it recommends that model developers and users ... perform sensitivity and uncertainty analyses. Sensitivity analysis evaluates the effect of changes in input values or assumptions on a model's results*"

Sensitivity Analysis

- White House, 2002: "*Sensitivity analysis is generally considered a minimum, necessary component of a quality risk assessment report*"
- Florida Commission on Hurricane Loss Projection Methodology (FCHLPM) "*has established a professional team to perform onsite (confidential) audits of computer models . . . an important part of the auditing process requires uncertainty and sensitivity analyses to be performed with the applicant's proprietary model [Iman et al (2005)a].*"

Sensitivity Analysis Research Evolution

The research on sensitivity analysis has evolved in the quest of finding sensitivity measures increasingly capable of reflecting a decision-maker's degree of belief on the problem at hand.
From local to global [overview in Borgonovo (2006)].

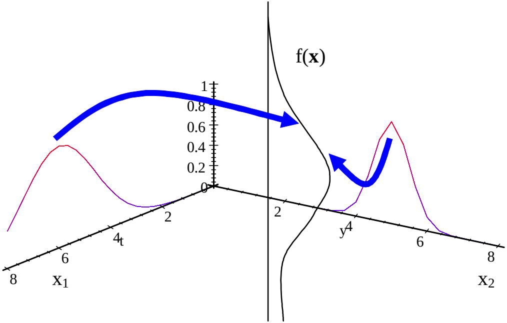


Figure: A visual representation of global SA.

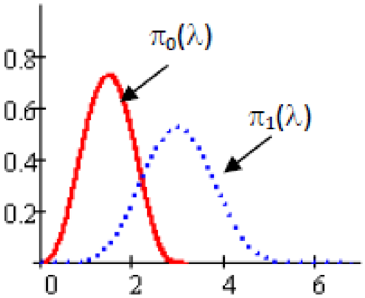
The decision-making viewpoint

- Probability is, by the subjective school, defined as (loosely speaking) that function that reflects a decision-maker's degree of belief about trhe occurrence of an event.
- Decision-theory, intrinsically linked to Statistics by the works of Savage, de Finetti etc.
- Problem: how should a decision-maker select among uncertain quantities

Degree of belief

Initially, your degree of belief is represented by density $\pi_0(\lambda|E)$.
Then you receive information on evidence E. New view, $\pi_1(\lambda|E)$ by Bayes Theorem.

$$\pi_1(\lambda|E) = \frac{L(E|\lambda)\pi_0(\lambda|E)}{\int L(E|\lambda)\pi_0(\lambda|E)\mathrm{d}\lambda} \quad (1)$$



Variance Based Sensitivity in General

- Information: $E = \{X_i = x_i\}$

Variance Based Sensitivity in General

- Information: $E = \{X_i = x_i\}$
- Setting: identifying 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)].

$$S_i = \frac{V_Y - \mathbb{E}_{X_i}[V_{Y|X_i}]}{V_Y} = \frac{V_{X_i}[\mathbb{E}_{Y|X_i}]}{V_Y} \tag{2}$$

Variance Based Sensitivity with Uncorrelated Inputs

$$S_{i_1,i_2,\ldots,i_k} = \frac{V_{i_1,i_2,\ldots,i_k}}{V_Y} \tag{3}$$

where

$$V_{i_1,i_2,\ldots,i_k} = \int t^2_{i_1,i_2,\ldots,i_k} \mathrm{d}\mu_{i_1} \mathrm{d}\mu_{i_2} \ldots \mathrm{d}\mu_{i_k} \tag{4}$$

and

$$t = t_0 + \sum_{s=1}^{n} \sum_{k=1}^{s} t_{i_1,i_2,\ldots,i_k}(x_{i_1}, x_{i_2}, \ldots, x_{i_k}) \tag{5}$$

Variance and Information

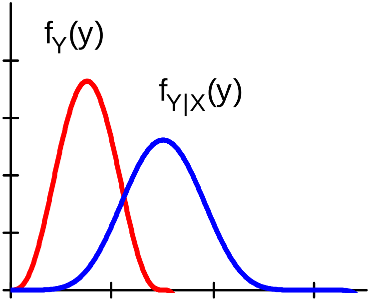
Several works have pointed out that Variance is not fully reflective of a decision-maker's belief in the problem at hand. Consider

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

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 $X_2 = 1$. $V_{Y|X_2=1} = 12.58 > V_Y$. Paradox.

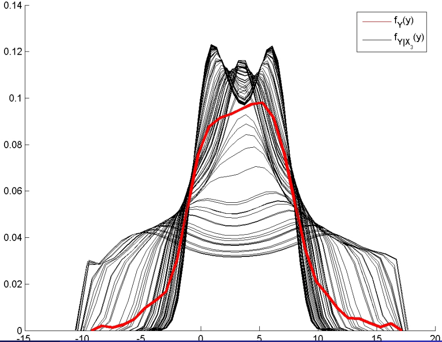
Effect of getting to know a parameter

- $y = t(x)$,
  $t : X \subseteq \mathbb{R}^n \rightarrow \mathbb{R}$
- $f_Y(y)$ unconditional model output density (continuous).
- You know that $X_j = x_j^*$
- $f_{Y|X_j=x_j^*}(y)$ (dashed).



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

$\mathbb{E}_{Y|X_3}$ independent of X_3. Therefore, $V_{X_3}\left[\mathbb{E}_{Y|X_3}\right] = 0$. Nonetheless, Figure 2 shows that fixing X_3 changes the decision-maker's degree of belief on Y. The effect of X_3 is captured, instead, by measuring the shift in the distribution of Y, from $f_Y(y)$ to $f_{Y|X_i}(y)$.



Measuring density separation

$$s(X_I) = \int \left| f_Y(y) - f_{Y|X_I}(y) \right| dy \qquad (8)$$

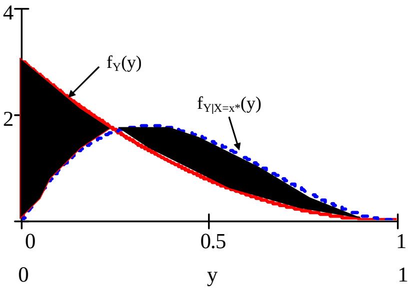


Figure: $f_Y(y)$ (continuous) and $f_{Y|X_I=x_I^*}(y)$ (dashed). The shift between the two densities is measured by Minkowski-Hellinger's distance of order 1.

Moment Independent Sensitivity Analysis

Moment independent approaches to sensitivity analysis start with the works by Parks and Ahn (1994), Chun et al (2000).

Parks and Ahn (1994): Kullback-Leibler ill-defined for global SA

Chun et al (2000): only one sensitivity case.

Limitations in these works are solved by Borgonovo (2006) and Borgonovo (2007) which introduces the δ importance measure.

The Importance of XI

Definition

$$\delta_I := \frac{1}{2}\mathbb{E}_{X_I}[s_I(X_I)] \tag{9}$$

with

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

Fact

Corresponding setting: "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)]."

Part II

Properties

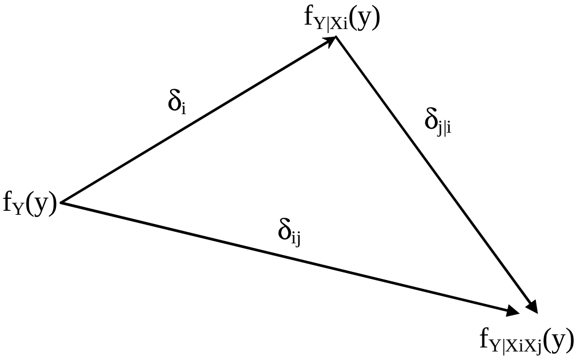
Properties

Table: Summary of the delta importance measure properties.

Nr.	Property
1	$0 \leq \delta_i \leq 1$. $\delta_i = 0$, if Y is independent of Ω_i
2	$\delta_i \leq \delta_{ij} \leq \delta_i + \delta_{j\|i}$. $\delta_{ij} = \delta_i$, if Y is independent of Ω_j
3	$\delta_{1,2,\ldots,n} = 1$
4	$\delta_i = \mathbb{E}_{X_i}[F_Y(Y_+^{x_i}) - F_{Y\|X_i}(Y_+^{x_i})]$
5	δ_i is invariant for monotonic transformation

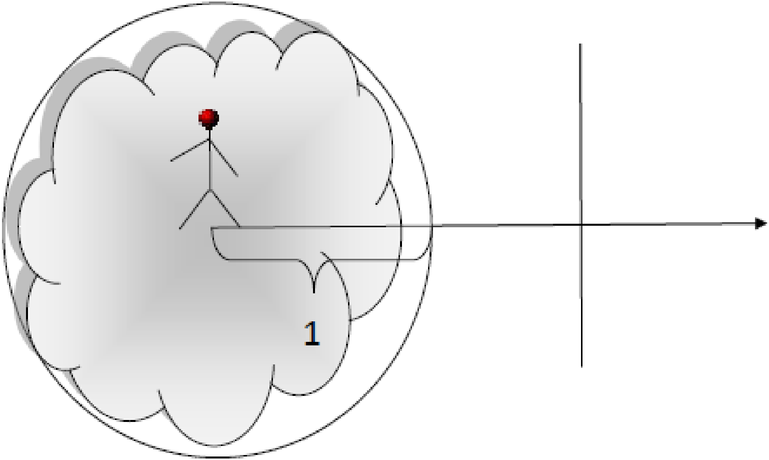
Properties (2)

Property 1 states normalization and independence.
Property 2



Property 3

Fixing all parameters at **x***, no more uncertainty.



Property 4

A bit more general.
We let $(\Omega, \mathcal{B}(\Omega), \mu)$ be a measure space, with $\Omega \subseteq \mathbb{R}$ an open interval.
Denoting by $f, g : \Omega \to \mathbb{R}^+$ any two densities with respect of μ, we let

$$\|f\|_\mu = \int |f| \, \mathrm{d}\mu(\omega) \tag{11}$$

and

$$\|f - g\|_\mu = \int |f - g| \, \mathrm{d}\mu(\omega), \tag{12}$$

Property 4 (cont): delta and F

Lemma

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

where $\Omega_+ = \{\omega \in \Omega : f(\omega) \geq g(\omega)\}$ *and* $\Omega_- = \Omega \backslash \Omega_+$.

Corollary

Let f be a generic density. Then,

$$\left\| f - \delta^{Dirac} \right\|_{\mu} = 2 \qquad (14)$$

Property 5: Monotonic Invariance

Lemma

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:*

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

Fact

If h, l *are any two measurable functions, then* $|h|, |l| \in \mathcal{L}(\Omega, \mathcal{B}(\Omega), \mu)$. *The normalized functions* $f = \frac{|h|}{\int_\Omega |h| \, d\mu}$ *and* $g = \frac{|l|}{\int_\Omega |l| \, d\mu}$ *possess the positivity and normalization properties of density functions. Therefore, these properties hold for the distance of all positive measurable functions, but for a normalization factor.*

Part III

Analytical Results

Procedure

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

Step nr	**Head**
1	Identification of $f_Y(y)$ and $f_{Y\|X_i}(y)$
2	Identification of $Y_+^{x_i}$ and $Y_-^{x_i}$
3	Evaluation of $s_i(X_i)$ by Property 4
4	Evaluation of δ_i

Additive Y and Independent Uniform X

Unconditional Density

$$u_Y^n(y) = \begin{cases} \frac{1}{(n-1)!}(y)^{n-1} & \text{if} \quad 0 \leq y < 1 \\ \cdots & \cdots \quad \cdots \\ \sum_{l=0}^{n-1}(-1)^l \binom{n}{l} \frac{1}{(n-1)!}(y-l)^{n-1} & \text{if} \quad n-1 \leq y < n \\ 0 & \quad \textit{otherwise} \end{cases} \tag{16}$$

Cumulative:

$$U_Y^n(y) = \begin{aligned} &\sum_{m=0}^{k^*-2}(\sum_{l=0}^{m}(\frac{(-1)^l}{l!(n-l)!}((m+1-l)^n-(m-l)^n)+ \\ &+\sum_{l=0}^{k^*-1}\frac{(-1)^l}{l!(n-l)!}((y-l)^n-(k^*-1-l)^n) \end{aligned} \tag{17}$$

Additive Y and Independent Uniform X

Proposition

1. $$F_Y = U_Y^n(y) \quad and \quad F_{Y|X_i=x_i} \sim U_Y^{n-1}(y - x_i) \tag{18}$$

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

$$u_Y^{n-1}(y - x_i) = u_Y^n(y) \tag{19}$$

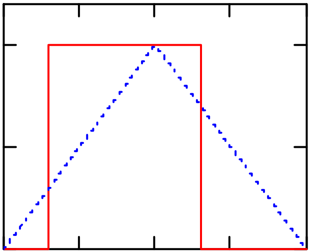
3. $$s_i(x_i) = 2[U_Y^n(a_i^n(x_i)) - U_{Y|X_i}^{n-1}(a_i^n(x_i)) + U_{Y|X_i}^{n-1}(b_i^n(x_i)) - U_Y^{n-1}(b_i^n(x_i))] \tag{20}$$

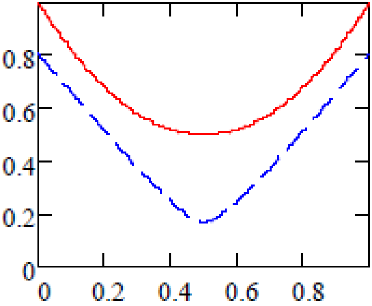
4. $$\delta_i = \int_0^1 \left[U_Y^n(a_i^n(s)) - U_{Y|X_i}^{n-1}(a_i^n(s)) + U_{Y|X_i}^{n-1}(b_i^n(s)) - U_Y^{n-1}(b_i^n(s))\right] ds \tag{21}$$

Additive Y and Independent Uniform X: n=2

$$\delta_i = \frac{1}{2}\int_0^1 s_i(v)dv = \frac{1}{3} \quad (22)$$

$$s_i(x_i) = 2x_i^2 - 2x_i + 1 \quad (23)$$

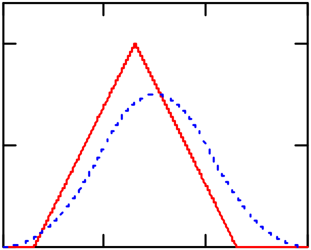


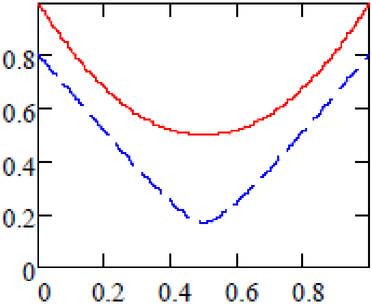


Additive Y and Independent Uniform X: n=3

$$\delta_i = 0.228 \qquad (24)$$

$$s_i(x_i) = \begin{cases} (-x_i + \frac{1}{\sqrt{2}} + 1 - \sqrt{2}x_i) \\ (2x_i - \frac{1}{\sqrt{2}} - 1 + \sqrt{2}x_i) \end{cases} \qquad (25)$$





Additive Y and Independent Additive X

Table: Moment Independent and Variance-Based Importance Measures for the uniform-additive case, with different model dimensions

n	2	3	4	5	6	10	100
δ analytical	0.333	0.228	0.186	0.166	0.149	0.113	0.032
δ normal approx.	0.306	0.224	0.185	0.160	0.144	0.107	0.032
S	0.5	0.333	0.25	0.2	0.167	0.1	0.01

Additive Y and Dependent Normal X

Theorem

Let $\mathbf{X} \in \mathbb{R}^n$, $\mathbf{X} \sim N(\mathbf{x}, \mathbf{m}, \Sigma)$, $(x_i = \mathbb{E}[X_i]$, $\det \Sigma \neq 0)$. $Y = \boldsymbol{\phi}\mathbf{x}$.

1.

$$F_{PV}(y) = N(y; PV, \sigma^2_{PV}) \text{ and } F_{Y|X_i}(y) = N(y; m_{Y|X_i}, V_{Y|X_i}) \tag{26}$$

where

$$\sigma^2_{PV} = \boldsymbol{\phi}\Sigma\boldsymbol{\phi}^T \quad \text{and} \quad \sigma^2_{PV|X_i} = \boldsymbol{\phi}\Sigma_{Y|X_i}\boldsymbol{\phi}^T \tag{27}$$

$$m_{Y|X_i} = \sum_{s=0, s\neq i}^{T} \phi_s \left[m_s + (x_i - \widetilde{x}_i)\frac{\sigma_{s,i}}{\sigma_i} \right], \quad i = 1, 2, ..., T \tag{28}$$

and

$$\Sigma_{Y|X_i} = \left[\sigma_{j,s} - \frac{\sigma_{j,i} \cdot \sigma_{i,s}}{\sigma_i}, \;\; j, s, i = 1, 2, ..., n \right] \tag{29}$$

Theorem

- $$s_i(X_i) = 2[N(y_1; m_Y, V_Y) + N(y_2; m_{Y|X_i}, V_{Y|X_i}) - N(y_2; m_Y, V_Y) - N(y_1; m_{Y|X_i}, V_{Y|X_i})] \quad (30)$$

  with

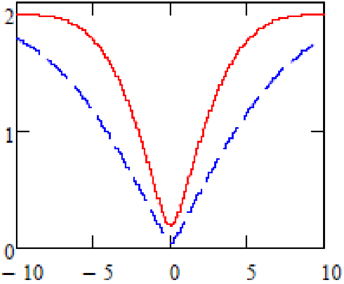
  $$y_{1,2} = \frac{1}{\sigma^2_{PV} - \sigma^2_{PV|X_i}} \left(\sigma^2_{PV} m_{Y|X_i} - \sigma^2_{PV|X_i} m_Y \pm \sqrt{\sigma^2_{PV}\sigma^2_{PV|X_i} \left[(\phi_i x_i)^2 + (\sigma^2_{PV} - \sigma^2_{PV|X_i}) \ln(\frac{\sigma^2}{\sigma^2_{P}} \right.} \right. \quad (31)$$

- $$\delta_i = \frac{1}{2}\mathbb{E}_{X_i}[\; N(y_1; m_Y, \sigma^2_{PV}) + N(u_2; m_{Y|X_i}, \sigma^2_{PV|X_i}) - N(u_2; m_Y, \sigma^2_{PV}) - N(u_1; m_{Y|X_i}, \sigma^2_{PV|X_i}) \;] \quad (32)$$

Zoom on si(xi)

Corollary

- *It is* $\lim_{X_i \to \pm\infty} s_i(X_i) = 2 \quad \forall \mathbf{a}, \mathbf{m}, \Sigma$
- *Symmetric*
- *The minimum is reached at* $\mathbb{E}[X_i]$



Results for Models of Increasing Dimensions

Table: Moment Independent and Variance-Based Importance Measures for the normal-additive case, with different model dimensions

n	2	3	4	5	10	100
δ	0.306	0.224	0.185	0.160	0.107	0.032
S	0.5	0.333	0.25	0.2	0.10	0.01

Multiplicative Y and Lognormal Xi

$$Y = \prod_{i=1}^{n} X_i^{a_i} \tag{33}$$

with $X_i \in (0, \infty)$ independent lognormally distributed random variables. We denote the lognormal distribution of X_i by $LN(x_i; \eta_i, \xi_i)$. For clarity, we report the density function of **X**:

$$\mu_{\mathbf{X}}(\mathbf{x}; \boldsymbol{\eta}, \boldsymbol{\xi}) = \prod_{i=1}^{k} \mu_i(x_i; \eta_i, \xi_i) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\xi_i x_i} e^{-\frac{1}{2}\left[\frac{\ln(x_i)-\eta_i}{\xi_i}\right]^2} \tag{34}$$

Results

- $S_i(x_i)$ no more symmetric, symmetric on a log scale
- Still, minimum at $\mathbb{E}[X_i]$
- Values same as for the normal-additive case, by invariance property

Table: Moment Independent and Variance-Based Importance Measures for the lognormal-multiplicative case, with different model dimensions

n	2	3	4	5	6	100
δ	0.306	0.224	0.185	0.160	0.144	0.032
S	0.268	0.090	0.032	0.012	$4.27E-3$	$2.52E-29$

$$S_i = 1 - \frac{\left(e^{\xi_Y^2} - e^{\xi_i^2}\right)}{\left(e^{\xi_Y^2} - 1\right)} \tag{35}$$

Some Remarks

- Importance of knowing one out of n variables decreases with n, in accordance with intuition
- Difference in δ_i and S_i in the case of interactive model variables

Unconditional density of the sum of independent rv's

Let $Y = \sum X_i$. Let $\mathbf{X}$ be a random vector with density $f_{\mathbf{X}}(\mathbf{x}) = \prod_{i=1}^{n} f_i(x_i)$.

Then, the random variable

$$Y = \mathbf{1V} \tag{36}$$

has density

$$f_Y(y) = f_n * f_{n-1} * ... * f_1 \tag{37}$$

where $f_n * f_{n-1}$ means the convolution integral of f_n and f_{n-1}.

Conditional density of the sum of independent rv's

Lemma

$$f_{Z|X_i}(z) = f_n * f_{n-1} * \ldots * \delta^{Dirac}(x - x_i) * \ldots * f_1$$

General result

Theorem

Let $Y_i \in \mathbb{R}$. Then,

$$d_I(X_I) = \int \left| \mathcal{F}^{-1}\left\{\prod_{j=1}^{n} \mathcal{F}_j; y\right\} - \mathcal{F}^{-1}\left\{e^{-iX_I} \prod_{j=1, j\neq i}^{n} \mathcal{F}_j; y\right\}\right| dy \quad (38)$$

$$\delta_I = \frac{1}{2}\mathbb{E}_{X_I}\left[\int \left| \mathcal{F}^{-1}\left\{\prod_{j=1}^{n} \mathcal{F}_j; y\right\} - \mathcal{F}^{-1}\left\{e^{-iX_I} \prod_{j=1, j\neq i}^{n} \mathcal{F}_j; y\right\}\right| dy\right] \quad (39)$$

$\mathcal{F}$ replaced by $\mathcal{L}$ if $Y_i \in \mathbb{R}^+$.

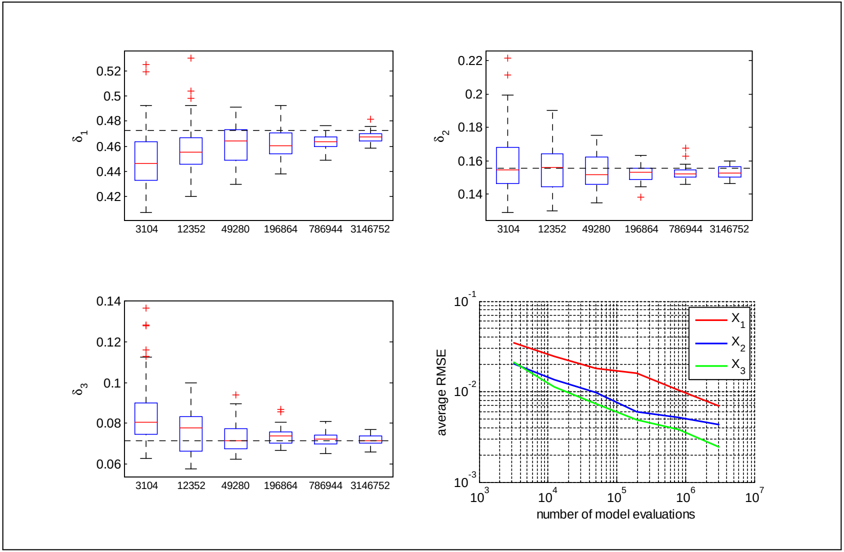
Part IV

Numerical Estimation

Numerical vs Analytical Results

- The multi-dimensional integral in eq. (9) is resolved by using Monte Carlo methods.
- Unconditional sample of size N characterising the input-output mapping $X_i = \left(x_i^{(1)}, \ldots, x_i^{(N)}\right)$, $\forall i = 1, \ldots, k$ and $Y = \left(y^{(1)}, \ldots, y^{(N)}\right)$.
- Conditional samples: fix all elements of the i^{th} column to $x_i^{(j)}$; then, a) in the case of correlated model inputs, re-sample the other model input values from the conditional distribution of the model inputs, $F_{\mathbf{X}|X_i}$; b) in the case of uncorrelated inputs the conditional samples can be obtained without actual resampling, by fixing all elements of the i^{th} column to the same value $x_i^{(j)}$.
- The associated total number of model evaluations is, in both cases, $N(nN+1)$.
- To evaluate $s_i(X_i)$ kernel density estimation [non-parametric approach, [Parzen (1962)]] is used to fit the conditional and unconditional distributions.

Some results



Comparison of Moment Independent vs Variance Based

- δ_i measures the shift in decision-maker's degree of belief bypassing model structure (see the multiplicative case)
- $S_{i_1,i_2,..,i_k}$ provide information on model structure, given that the input are independent
- δ_i well defined also in the presence of correlations.
- δ_i well defined also for skewed distributions

Future Research

- Applications in various areas

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- Numerical experiments for computing $s_i(x_i)$ (Borgonovo, Castaings, Tarantola)

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- Numerical experiments for computing $s_i(x_i)$ (Borgonovo, Castaings, Tarantola)
- Numerical experiments for smoothing methods
- Numerical experiments for conditional moments (links to analytic properties in Functional ANOVA)
- Moment Independent Sensitivity and Emulators

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