

Probabilistic sensitivity analysis: contribution to the sample mean plot and moment-independent importance measures

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Contribution to the sample mean plot

- Contribution to the sample mean plot
- Statistical test for inputs prioritisation

Moment independent sensitivity analysis

- Moment-independent importance measures
- Numerical and computational aspects
- Application examples

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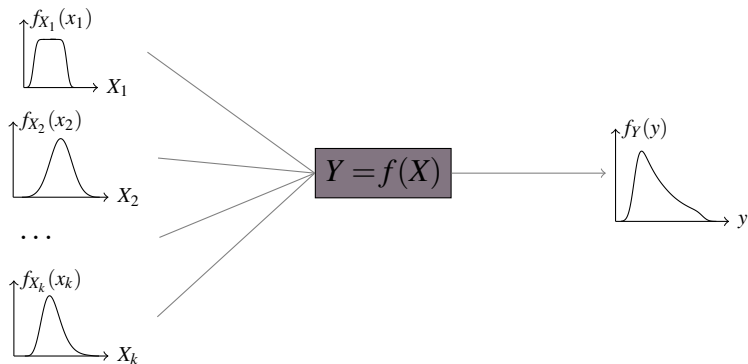
Contribution to the sample mean plot for graphical and numerical sensitivity analysis

R. Bolado

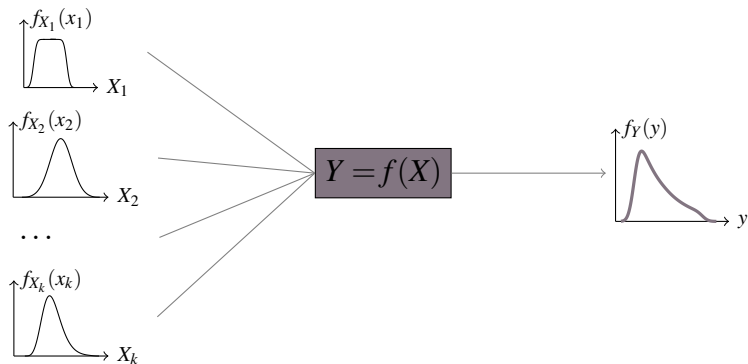
European Commission, Joint Research Centre (IE, Petten)

W. Castaings, S. Tarantola

European Commission, Joint Research Centre (IPSC, Ispra)



- f a deterministic scalar function
- $X = (X_1, \dots, X_k)$ and Y random variables
- $x = (x_1, \dots, x_k)$ realization of the model inputs X
- y realization of the model output Y



- **Objective:** understand the behaviour of the system with very few model runs

Context

- *Sinclair, (1993)* investigated how **finite changes** in inputs pdfs affect the **mean** and **variance** of the output
- **Contribution to the sample mean** (CSM) plot recognized as a general tool for sensitivity analysis

Objectives

- Revive and further develop CSM plot
- Exploit the full potential of this **graphical tool**
- CSM plot, primary building block of a **statistical test** for inputs prioritisation

Different steps for the construction of a CSM plot

- 1 realizations of X_i are sorted, generating $\{x_i^{(1)}, x_i^{(2)}, \dots, x_i^{(N)}\}$;
- 2 realizations of Y are sorted accordingly, generating $\{y^{(i,1)}, y^{(i,2)}, \dots, y^{(i,N)}\}$
- 3 new variable M_i defined by

$$m_i^{(q)} = \frac{1}{N} \sum_{j=1}^q y^{(i,j)} \quad q = 1, \dots, N$$

- 4 normalization of the M_i using the sample mean of Y ;
- 5 plot M_i against $F_{X_i}(x_i)$

Underlying features

- For both axes, values lie in the interval $[0, 1]$
- $(F_{X_i}(x_i^{(q)}), m_i^q)$: fraction of the output mean due to any given fraction of values of the input X_i .

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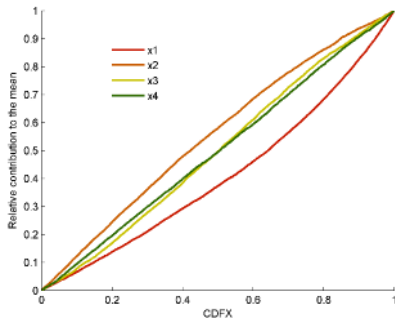
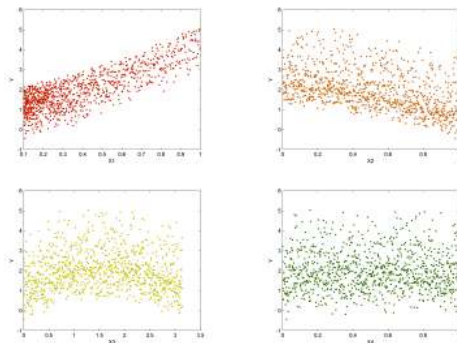
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Didactic example

All parameters, single output

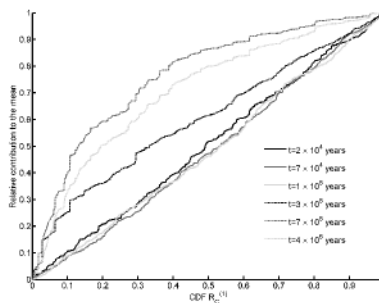
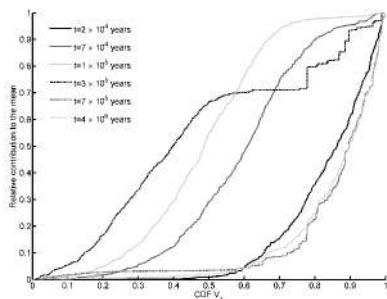


Analytic function

- $Y = 2 \exp(X_1) - \exp(X_2) + \sin(X_3)$
- $X_i, i = 1, 2, 4 \sim U(0, 1), X_3 \sim U(0, \pi)$

High-level waste repository model (LevelE)

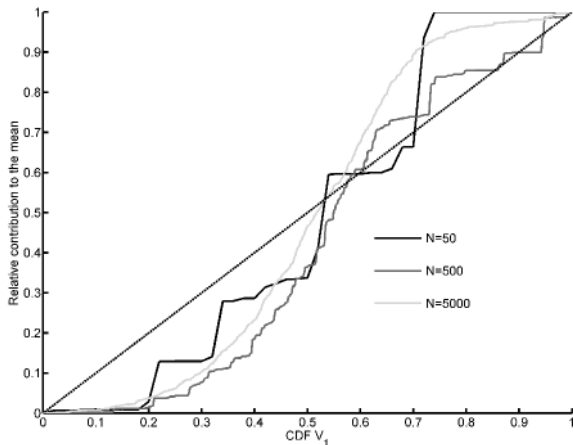
Single parameter, several outputs



Information provided by the plot

- Effects on the mean of the output of changes in the inputs pdfs
- Underlines the limitations of the sample size/design
- Global importance measures

CSM plot with increasing sample size



CSM plot

- If $F_{X_i}(x_i^{(q)}) \simeq m_i^q \forall q$, any quantile range of X_i has a similar influence on the output mean, i.e non-influent model input

Relation with VB

- Variance-based first-order effect

$$S_i = \frac{\text{Var}(E[Y|X_i])}{\text{Var}(Y)}$$

- CSM plot, variability of $E[Y|X_i < x_i^*]$ (rather than $E[Y|X_i = x_i^*]$) across the range

Features

- **Hypotheses** (null hypothesis H_0 and alternative hypothesis H_1):
 - $H_0: f_{Y|X_i}(y|x_i = x_i^*) = f_Y(y) \forall x_i^* \in R_i$ (R_i is the support of X_i);
 - $H_1: \exists x_i^*, x_i' \in R_i \ / \ f_{Y|X_i}(y|x_i = x_i^*) \neq f_{Y|X_i}(y|x_i = x_i')$.
- **Test statistic:** D_m , the **maximum distance** to the diagonal

Different steps

- 1 Empirical distribution of D_m
 - **Random permutations** of the inputs realizations
 - For each permutation, compute D_m from CSM plot
- 2 Compute $D_{m\alpha}$, value of the **test statistic** for the **critical level** α
- 3 Estimation of $D_{m_{X_i}} \forall i = 1, \dots, k$ from the *original* CSM plot
- 4 null hypothesis H_0 rejected if $D_{m_{X_i}} > D_{m\alpha}$ (i.e. X_i is an important input)

Features

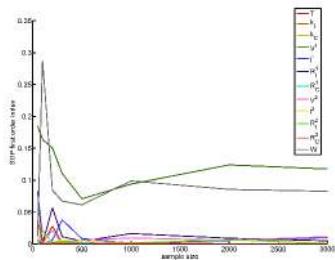
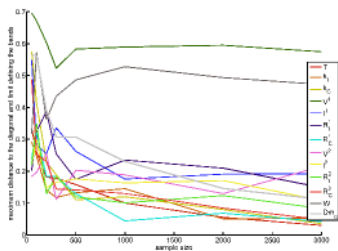
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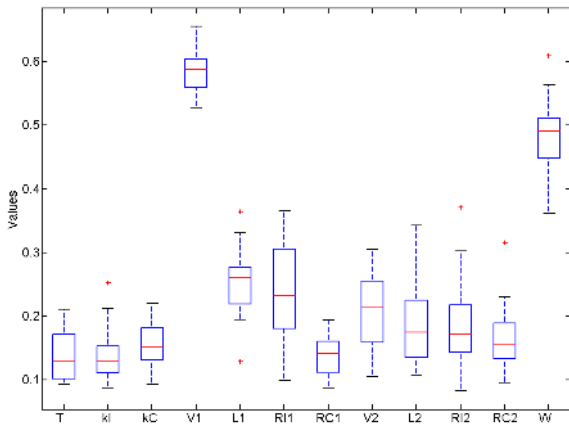
Convergence of importance measures

Test statistic and SDP (Ratto et al, 2007) first order indices (LHS samples 50-3000)



Robustness of importance measures

Test statistic across 20 LHS replicates of size 500



Conclusions

Potential

- CSM plot: simple, versatile and very informative **graphical tool**
- Statistical test: identifies **important model inputs** for very low sample size, no additional model run for robustness analysis

Limitations

- Inputs prioritisation assessment restricted to **first order effects**
- Statistical test prone to **type I error** (treating non-influential inputs as important)

To be done ...

- Systematic approach for **non-monotonic** mappings
- **Second order** interactions with surfaces
- Investigate the potential of the contribution to the sample variance (CSV) plot

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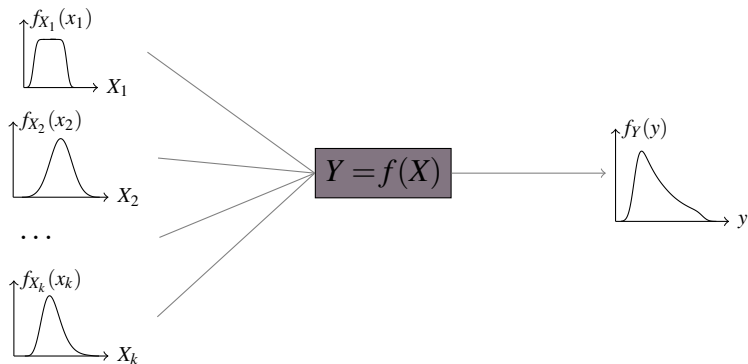
Relative importance of model inputs on the output probability distribution function

Emanuele Borgonovo

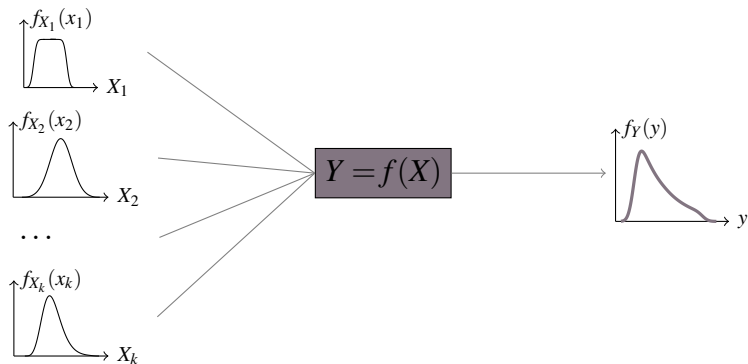
Bocconi University, Department of Decision Sciences (ELEUSI, Milan)

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- Variance not necessarily adapted to describe the output variability
- Analysis of the entire output distribution $f_Y(y)$ rather than $V(Y)$

- Conditional variance $V(Y|X_i)$ to be compared with $V(Y)$

$$S_i = \frac{V_i}{V(Y)}$$

$$V_i = V(E(Y|X_i)) = V(Y) - E(V(Y|X_i))$$

$$V(Y) = E(V(Y|X_i)) + V(E(Y|X_i))$$

- Conditional PDF $f_{Y|X_i}(y)$ to be compared with $f_Y(y)$

$$s(X_i) = \int |f_Y(y) - f_{Y|X_i}(y)| dy$$

$$\delta_i = \frac{1}{2} E_{X_i}[s(X_i)]$$

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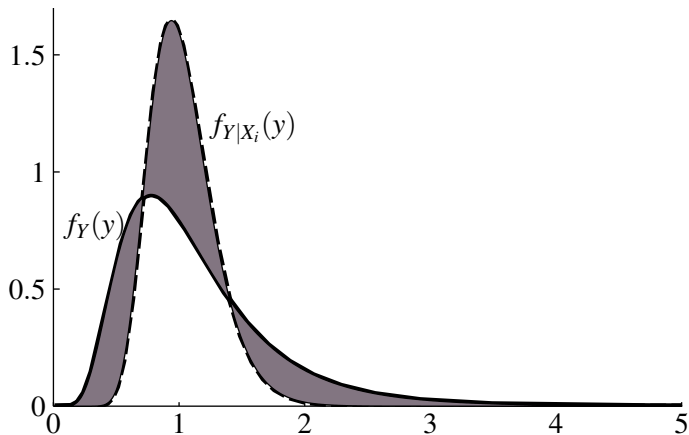
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- Other moment-independent important measures based on CDF (*Park et al, 1994; Chun et al, 2000*),
- The measures proposed by *Borgonovo, (2006)* have interesting normalization properties

✓ Individual importance

$$0 \leq \delta_i \leq 1$$

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Joint importance of X_i and X_j

$$\delta_{ij} = \frac{1}{2} \int f_{X_i, X_j}(x_i, x_j) \left[\int |f_Y(y) - f_{Y|X_i, X_j}(y)| dy \right] dx_i dx_j$$

$\delta_{ij} = \delta_i$ if Y is dependent on X_i but independent on X_j

☞ δ can be extended to any set of inputs (i.e. analysis by groups)

Essential properties

- ✓ Individual importance $0 \leq \delta_i \leq 1$
- ✓ Normalization of joint importance $\delta_{1,2,\dots,k} = 1$

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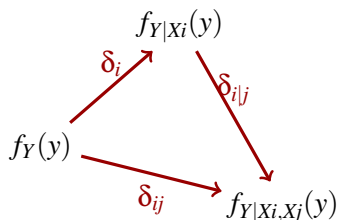
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✓ Normalization of joint importance

$$\delta_{1,2,\dots,k} = 1$$

✓ Subadditivity $\delta_i \leq \delta_{ij} \leq \delta_i + \delta_{j|i}$

$$\delta_{j|i} = \frac{1}{2} \int f_{X_i, X_j}(x_i, x_j) \times \left[\int |f_{Y|X_i}(y) - f_{Y|X_i, X_j}(y)| dy \right] dx_i dx_j$$



Essential properties

- ✓ Individual importance $0 \leq \delta_i \leq 1$
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- All properties hold for **dependent inputs**
- Proofs are provided in *Borgonovo, (2006; 2007)*

Essential aspects of the computational approach

- Focus on δ_i $i = 1, \dots, k$

$$\delta_i = \frac{1}{2} \int f_{X_i}(x_i) \left[\int |f_Y(y) - f_{Y|X_i}(y)| dy \right] dx_i$$

for i=1 to k *Loop on model inputs*

for j=1 to N *Loop on different values of X_i*

$$s(x_i) = \int |f_Y(y) - f_{Y|X_i}(y|X_i = x_i^{(j)})| dy$$

endfor

endfor

Key features

- 1 Sample generation
- 2 Evaluation of the area $s(X_i)$

1 Discrete model outputs

- Histograms are perfectly suited
- Zero width and number of bins calculated from the sample

2 Continuous model outputs

- Non-parametric estimation of PDFs (e.g. kernel density estimation)
- Monotonic transformations can be applied without altering δ properties
- Area calculated from CDFs (Liu and Homma, 2008)

Comparison with variance-based

- Approximation errors are potentially larger when dealing with the entire PDF
 - Shortcuts are more difficult to elaborate
- 1 Shift between $f_Y(y)$ and $f_{Y|X_i}(y)$ should be due to the fact that $X_i = x_i^*$
i.e. $\int |f_{Y|X_i} - f_Y(y)| dy < \epsilon$ if X_i is a dummy input
otherwise type I error (treating non influential inputs as important)
 - 2 A sufficient number of x_i^* should be explored for estimating $E_{X_i}[s(X_i)]$.

Sample generation for independent inputs

- Unconditional sample for $f_X(x)$ and $f_Y(y)$

$$\begin{pmatrix} x_1^{(1)} & x_2^{(1)} & \cdots & x_i^{(1)} & \cdots & x_k^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \cdots & x_i^{(2)} & \cdots & x_k^{(2)} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ x_1^{(N-1)} & x_2^{(N-1)} & \cdots & x_i^{(N-1)} & \cdots & x_k^{(N-1)} \\ x_1^{(N)} & x_2^{(N)} & \cdots & x_i^{(N)} & \cdots & x_k^{(N)} \end{pmatrix} = \begin{pmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N-1)} \\ y^{(N)} \end{pmatrix}$$

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- $X_{\sim i}$ not influenced by the fact that $X_i = x_i^{(j)}$
- Substituted column sampling can be applied

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- Ex. Conditional sample for $f_{X|X_i}(x|X_i = x_i^{(1)})$ and $f_{Y|X_i}(y|X_i = x_i^{(1)})$

$$\begin{pmatrix} x_1^{(1)} & x_2^{(1)} & \cdots & x_i^{(1)} & \cdots & x_k^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \cdots & x_i^{(1)} & \cdots & x_k^{(2)} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ x_1^{(N-1)} & x_2^{(N-1)} & \cdots & x_i^{(1)} & \cdots & x_k^{(N-1)} \\ x_1^{(N)} & x_2^{(N)} & \cdots & x_i^{(1)} & \cdots & x_k^{(N)} \end{pmatrix} = \begin{pmatrix} y^{(1')} \\ y^{(2')} \\ \vdots \\ y^{(N-1')} \\ y^{(N')} \end{pmatrix}$$

Sample generation for independent inputs

- N conditional samples of size N required for the calculation of δ_i
- Total number of model evaluations

$$COST = N(1 + kN)$$

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Slightly more efficient calculation strategy

- 1 Less than N sample points for approaching $f_X(x|X_i = x_i^*)$, i.e. $N_{int} < N$
- 2 Less than N different values x_i^* of X_i for approaching $E_{X_i}[s(X_i)]$, i.e. $N_{ext} < N$

Sample generation for independent inputs

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$$COST = N(1 + kN)$$

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- Reducing N_{int} can lead to type I error
- N_{ext} more likely to be reduced given the shape of $s(X_i)$,

Sample generation for independent inputs

- N conditional samples of size N

$$COST = N(1 + kN)$$

- N_{ext} conditional samples of size N_{int}

$$COST = N + kN_{int}N_{ext}$$

- No constraints for the design of the unconditional sample
- Efficient sampling strategies like Latin Hypercube Sampling (*McKay, 1979*) or Quasi-Random sampling (ex. *Sobol, 1976*) can be used

Sample generation for dependent inputs

- Unconditional correlated sample for $f_X(x)$ and $f_Y(y)$

$$\begin{pmatrix} x_1^{(1)} & x_2^{(1)} & \cdots & x_i^{(1)} & \cdots & x_k^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \cdots & x_i^{(2)} & \cdots & x_k^{(2)} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ x_1^{(N-1)} & x_2^{(N-1)} & \cdots & x_i^{(N-1)} & \cdots & x_k^{(N-1)} \\ x_1^{(N)} & x_2^{(N)} & \cdots & x_i^{(N)} & \cdots & x_k^{(N)} \end{pmatrix} = \begin{pmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N-1)} \\ y^{(N)} \end{pmatrix}$$

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- $X_{\sim i}$ influenced by the fact that $X_i = x_i^{(j)}$
- Generation of conditional correlated samples for $f_X|X_i(x)$
- Permuted columns sampling plans can be used

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- Replicated Latin Hypercube Sampling (*McKay, 1995*)
 - r matrices generated through column permutation
 - Correlations induced through permutations (*Iman et al, 1987; Stein et al, 1987*)

Approach based on rLHS

Tutorial example for sample generation

- $X_i \quad (i = 1, 2, 3) \sim U[-\pi - \pi]$
- rLHS sample, number of variables $k = 3$, base sample size $N = 4$, number of replicates $r = 2$

<i>Base sample</i>		
-2.11	-2.38	-2.18
0.79	-0.14	0.53
1.71	0.28	3.03
-0.39	3.09	-0.99
<i>1st Replicate</i>		
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Sorting replicates according to values of X_1

-2.11	3.09	-2.18
-2.11	0.28	0.53
-0.39	-0.1409	-0.99
-0.39	3.0980	-0.99
0.79	0.2820	3.03
0.79	-2.3887	-2.18
1.71	-2.38	0.53
1.71	-0.14	3.03

Approach based on rLHS

Tutorial example for sample generation

- $X_i \quad (i = 1, 2, 3) \sim U[-\pi - \pi]$
- rLHS sample, number of variables $k = 3$, base sample size $N = 4$, number of replicates $r = 2$

$f_X(x)$	(Base sample)	
-2.11	-2.38	-2.18
0.79	-0.14	0.53
1.71	0.28	3.03
-0.39	3.09	-0.99
1 st Replicate		
-2.11	3.09	-2.18
-0.39	-0.14	-0.99
0.79	0.28	3.03
1.71	-2.38	0.53
2 nd Replicate		
0.79	-2.38	-2.18
-0.39	3.09	-0.99
1.71	-0.14	3.03
-2.11	0.28	0.53

Conditional samples for $f_{X|X_1}(x)$

$f_{X X_1}(x X_1 = x_1^{(1)})$		
-2.11	3.09	-2.18
-2.11	0.28	0.53
$f_{X X_1}(x X_1 = x_1^{(2)})$		
-0.39	-0.1409	-0.99
-0.39	3.0980	-0.99
$f_{X X_1}(x X_1 = x_1^{(3)})$		
0.79	0.2820	3.03
0.79	-2.3887	-2.18
$f_{X X_1}(x X_1 = x_1^{(4)})$		
1.71	-2.38	0.53
1.71	-0.14	3.03

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	-2.11	-2.38	-2.18
	0.79	-0.14	0.53
	1.71	0.28	3.03
	-0.39	3.09	-0.99
<i>1st Replicate</i>			
	-2.11	3.09	-2.18
	-0.39	-0.14	-0.99
	0.79	0.28	3.03
	1.71	-2.38	0.53
<i>2nd Replicate</i>			
	0.79	-2.38	-2.18
	-0.39	3.09	-0.99
	1.71	-0.14	3.03
	-2.11	0.28	0.53

Sorting replicates according to values of X_2

	1.71	-2.38	0.53
	0.79	-2.38	-2.18
	-0.39	-0.14	-0.99
	1.71	-0.14	3.03
	0.79	0.28	3.03
	-2.11	0.28	0.53
	-2.11	3.09	-2.18
	-0.39	3.09	-0.99

Approach based on rLHS

Tutorial example for sample generation

- $X_i \quad (i = 1, 2, 3) \sim U[-\pi - \pi]$
- rLHS sample, number of variables $k = 3$, base sample size $N = 4$, number of replicates $r = 2$

$f_X(x)$ (Base sample)
-2.11 -2.38 -2.18
0.79 -0.14 0.53
1.71 0.28 3.03
-0.39 3.09 -0.99

1st Replicate

-2.11 3.09 -2.18
-0.39 -0.14 -0.99
0.79 0.28 3.03
1.71 -2.38 0.53

2nd Replicate

0.79 -2.38 -2.18
-0.39 3.09 -0.99
1.71 -0.14 3.03
-2.11 0.28 0.53

Conditional samples for $f_{X|X_2}(x)$

$f_{X X_2}(x X_2 = x_2^{(1)})$
1.71 -2.38 0.53
0.79 -2.38 -2.18

$f_{X|X_2}(x|X_2 = x_2^{(2)})$

-0.39 -0.14 -0.99
1.71 -0.14 3.03

$f_{X|X_2}(x|X_2 = x_2^{(3)})$

0.79 0.28 3.03
-2.11 0.28 0.53

$f_{X|X_2}(x|X_2 = x_2^{(4)})$

-2.11 3.09 -2.18
-0.39 3.09 -0.99

Approach based on rLHS

Tutorial example for sample generation

- $X_i \quad (i = 1, 2, 3) \sim U[-\pi - \pi]$
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$f_X(x)$	<i>(Base sample)</i>		
	-2.11	-2.38	-2.18
	0.79	-0.14	0.53
	1.71	0.28	3.03
	-0.39	3.09	-0.99
<i>1st Replicate</i>			
	-2.11	3.09	-2.18
	-0.39	-0.14	-0.99
	0.79	0.28	3.03
	1.71	-2.38	0.53
<i>2nd Replicate</i>			
	0.79	-2.38	-2.18
	-0.39	3.09	-0.99
	1.71	-0.14	3.03
	-2.11	0.28	0.53

Sorting replicates according to values of X_3

	-2.11	3.0980	-2.18
	0.79	-2.3887	-2.18
	-0.39	-0.1409	-0.99
	-0.39	3.0980	-0.99
	1.71	-2.3887	0.53
	-2.11	0.2820	0.53
	0.79	0.28	3.03
	1.71	-0.14	3.03

Approach based on rLHS

Tutorial example for sample generation

- $X_i \quad (i = 1, 2, 3) \sim U[-\pi - \pi]$
- rLHS sample, number of variables $k = 3$, base sample size $N = 4$, number of replicates $r = 2$

$f_X(x)$	<i>(Base sample)</i>		
	-2.11	-2.38	-2.18
	0.79	-0.14	0.53
	1.71	0.28	3.03
	-0.39	3.09	-0.99
<i>1st Replicate</i>			
	-2.11	3.09	-2.18
	-0.39	-0.14	-0.99
	0.79	0.28	3.03
	1.71	-2.38	0.53
<i>2nd Replicate</i>			
	0.79	-2.38	-2.18
	-0.39	3.09	-0.99
	1.71	-0.14	3.03
	-2.11	0.28	0.53

Conditional samples for $f_{X|X_3}(x)$

$f_{X X_3}(x X_3 = x_3^{(1)})$			
	-2.11	3.0980	-2.18
	0.79	-2.3887	-2.18
$f_{X X_3}(x X_3 = x_3^{(2)})$			
	-0.39	-0.1409	-0.99
	-0.39	3.0980	-0.99
$f_{X X_3}(x X_3 = x_3^{(3)})$			
	1.71	-2.3887	0.53
	-2.11	0.2820	0.53
$f_{X X_3}(x X_3 = x_3^{(4)})$			
	0.79	0.28	3.03
	1.71	-0.14	3.03

Sample generation for dependent inputs

- Replicated Latin Hypercube Sampling (*McKay, 1995*)
 - r matrices of size N generated through column permutation
 - Correlations induced through permutations (*Iman et al, 1987; Stein et al, 1987*)

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- Sample size used for approaching $f_{X|X_i}(x)$ (i.e. N_{int}) is given by the number of replicates r
- Number of values of x_i explored (i.e. N_{ext}) for estimation $E_{X_i}[s(X_i)]$ given by the base sample size N

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$$COST = r * N$$

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 - r matrices of size N generated through column permutation
 - Correlations induced through permutations (*Iman et al, 1987; Stein et al, 1987*)

$$COST = r * N$$

- r should be close to N in order to ensure that $\int |f_{Y|X_i} - f_Y(y)| dy < \epsilon$ if X_i is a dummy input

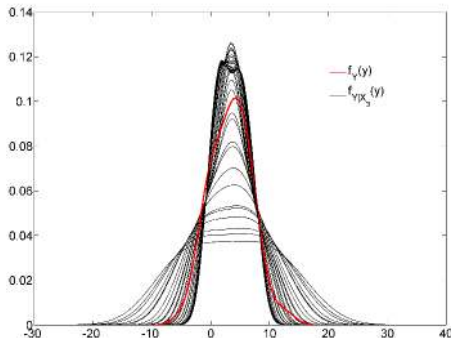
$$COST \sim N^2$$

☞ Number of model evaluations independent from k

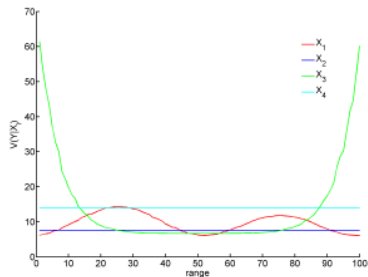
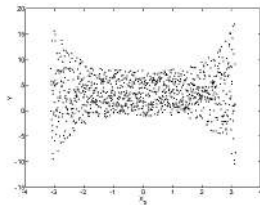
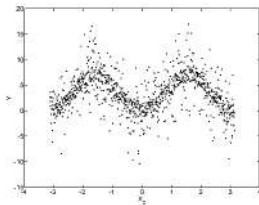
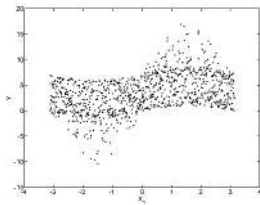
Brute force approach

- $X_i \quad (i = 1, \dots, 4) \sim U[-\pi - \pi]$
- Ishigami function $f(Y) = \sin X_1 + 7 \sin^2 X_2 + 0.1 X_3^4 \sin X_1$
- X_4 is a dummy input

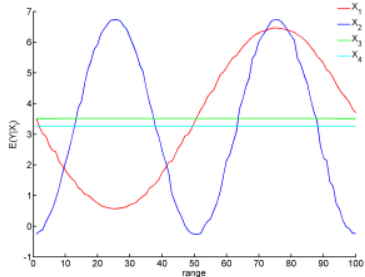
	X_1	X_2	X_3	X_4
S_i	0.3139	0.4424	0.	0.
δ_i	0.2110	0.4073	0.1568	0.



Brute force approach

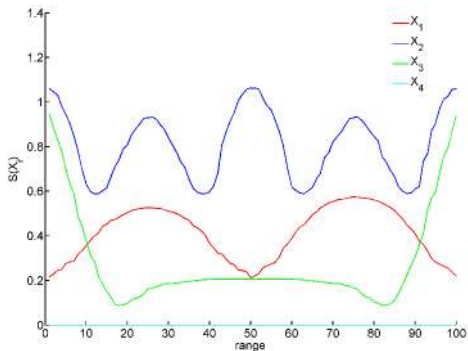
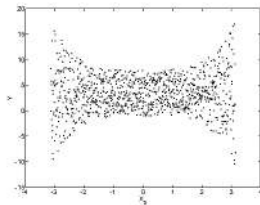
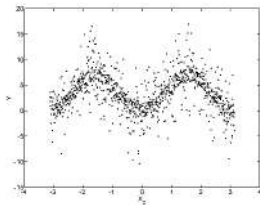
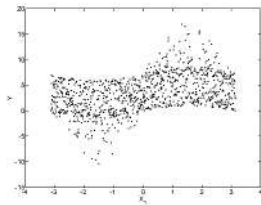


$V(Y|X_i)$



$E(Y|X_i)$

Brute force approach



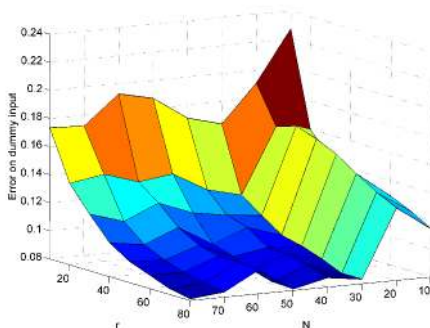
$s(X_i)$

rLHS approach

Validation for independent inputs

- Number of replicates essential in order to ensure that

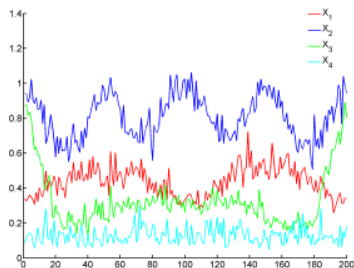
$$\int |f_{Y|X_i} - f_Y(y)| dy < \varepsilon \text{ for dummy input factors}$$



rLHS approach

Validation for independent inputs

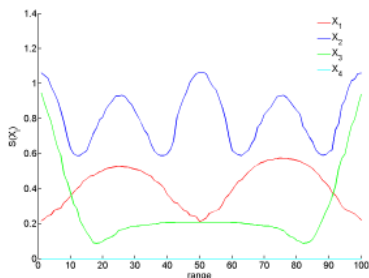
- Lack of correspondence for $X_{\sim i}$ lead to approximation error for $s(X_i)$
- Reasonable accuracy for δ_i estimates



rLHS approach

$$\delta_1 = 0.21, \delta_2 = 0.40$$

$$\delta_2 = 0.16, \delta_4 = 0.06$$



Brute force approach

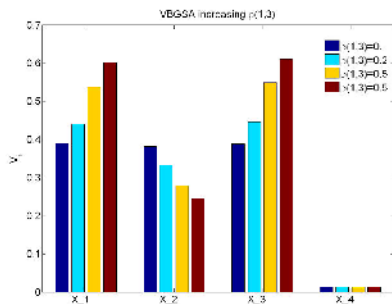
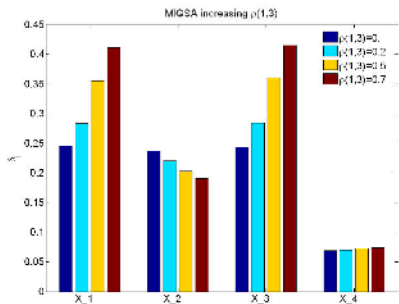
$$\delta_1 = 0.20, \delta_2 = 0.40$$

$$\delta_2 = 0.13, \delta_4 = 0.$$

rLHS approach

Effect of dependence among inputs

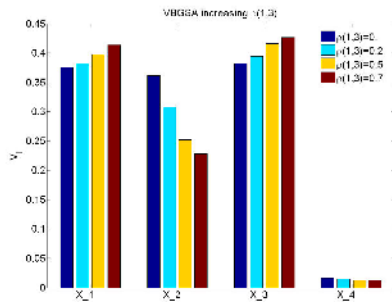
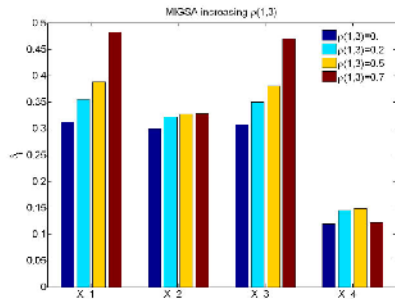
- $X_i \quad (i = 1, \dots, 4) \sim U[0,1]$
- $f(Y) = X_1 + X_2 + X_3$
- X_4 is a dummy input



rLHS approach

Effect of dependence among inputs

- $X_i \quad (i = 1, \dots, 4) \sim U[0,1]$
- $f(Y) = X_1.X_2.X_3$
- X_4 is a dummy input



- The presence of correlations or/and interactions increases the **approximation error**
- The **additional terms** generated by dependence create a non-null effect for a dummy factor
- Correlations increase the importance of the correlated parameters for both VB and MI
- In the presence of interactions, influence on other factors can be different

Conclusions

- Moment-independent importance measures with **interesting properties**
 - Any shortcut is prone to substantial **approximation errors** when dealing with the entire PDF
 - **Computationally intensive** assessment
 - Calculation methods for independent and dependent model inputs, other **sampling plans** to be investigated
- ☞ Rather than the entire PDF, a specific portion might be of interest

Ex. Focus on the variability of extremes

- Relative importance of model inputs in determining the variability of extremes

$$s(x_i) = \int |f_Y(y|Y > y^{90\%}) - f_{Y|X_i}(y|X_i, Y > y^{90\%})| dy$$

Monte Carlo Filtering

- Select the sample points verifying $Y > y^{90\%}$
- Induced correlation structure for $f_X(x|Y > y^{90\%})$
- Conditional samples generation (i.e. $f_{Y|X_i}(y|X_i, Y > y^{90\%})$) might be difficult

Adaptation of importance measure

- Restrict the area calculation to the targeted region of the model output

$$s(x_i) = \int_{\Omega} |f_Y(y) - f_{Y|X_i}(y|X_i)| dy$$

Merci de votre attention ...

Q?