Computing first-order sensitivity indices with contribution to the sample mean plot

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Kopustinskas, V. [2] Bolado-Lavin, R. [3]

SAMO 2013 - Nice, July 1-4

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[3] *Joint Research Center of the European Commission, Petten, Netherlands*

Sensitivity analysis from **given data**

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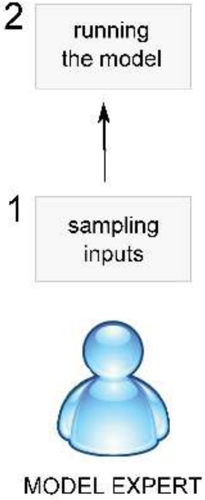

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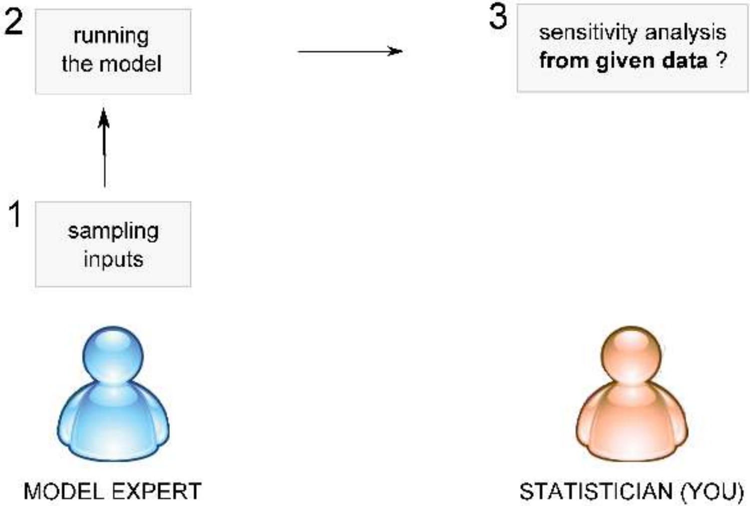

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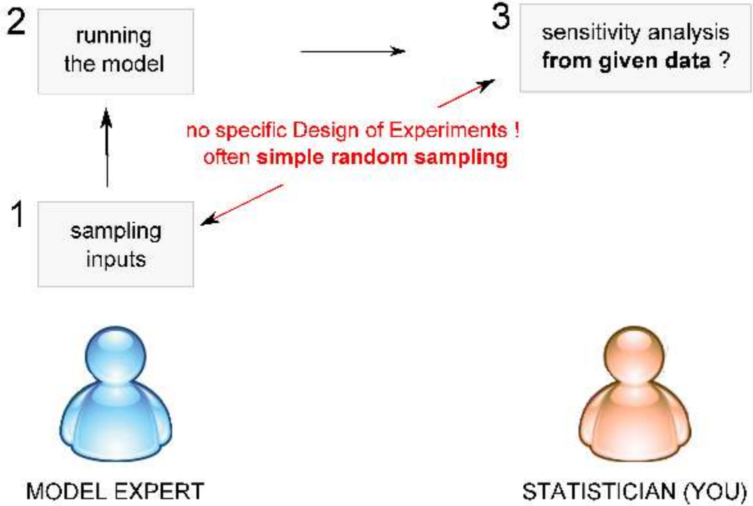

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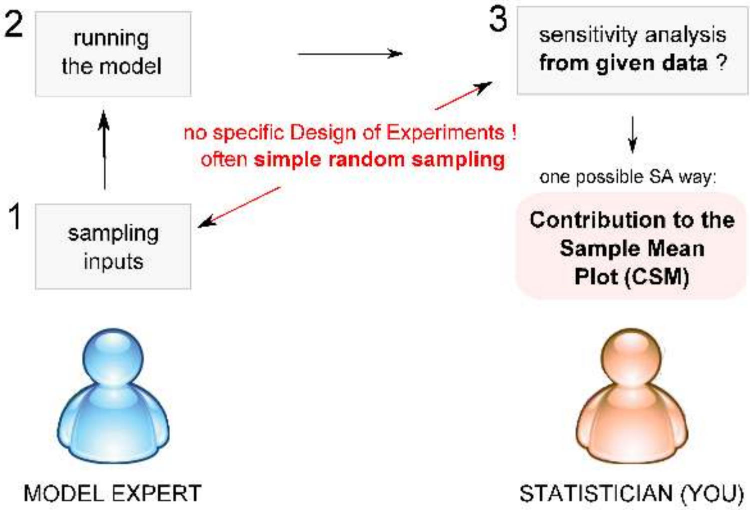

Contribution to the Sample Mean (CSM)

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- Model $Y = G(X_1, \dots, X_m)$
- $X_1, \dots, X_m$ independent random variables, pdf p_j, cdf F_j
- The **Contribution to the Sample Mean** (CSM) **for $\mathbf{X_j}$** is:

$\forall q \in [0; 1]$,

$$C_j(q) = \frac{\int_{-\infty}^{F_j^{-1}(q)} \left(\int_{\mathbb{R}^{m-1}} G(x) p_{X_{\sim j}}(x_{\sim j}) dx_{\sim j} \right) p_j(x_j) dx_j}{\int_{\mathbb{R}^m} G(x) p_X(x) dx} \tag{1}$$

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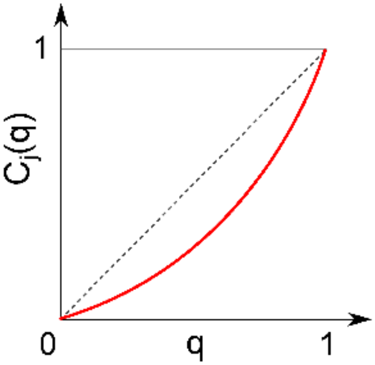
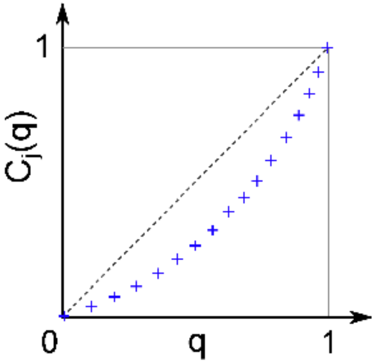


$C_j(q)$ represents the **fraction of the output mean** due to the **fraction** q **of smallest values of** X_j.

Contribution to the Sample Mean (CSM)

Procedure to approximate CSM plot from a set of n model runs.
input sample $(x_{ij})_{i=1\dots n, j=1\dots m}$ and output vector $(y_i)_{i=1\dots n}$



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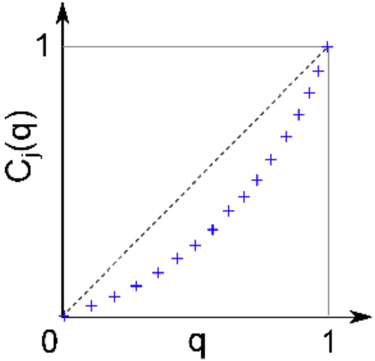

1. compute the output mean $\hat{\mu}$
2. **sort increasingly** the n random realisations of X_j:

$$x_{\pi(1)j} \leq \dots \leq x_{\pi(n)j}$$

3. compute $(c_1, \dots, c_n)$:

$$c_i = \frac{1}{n\hat{\mu}} \sum_{s=1}^{i} y_{\pi(s)}$$

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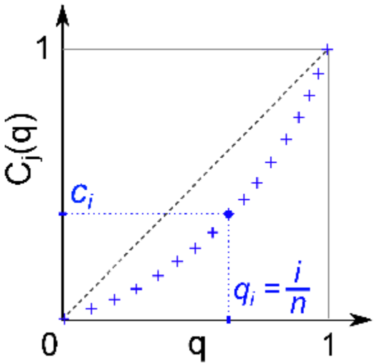

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4. plot $(c_1, \dots, c_n)$ against $(q_1, \dots, q_n)$ with $q_i = i/n$

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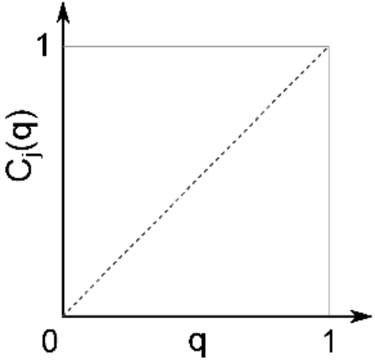

CSM and first-order effects

X_j with **low first-order effect**

$\sim$

CSM line **close to the diagonal**

(Bolado-Lavin *et al.*, 2009)

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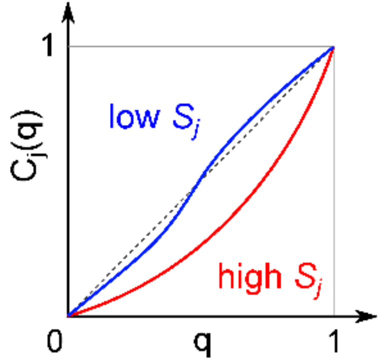

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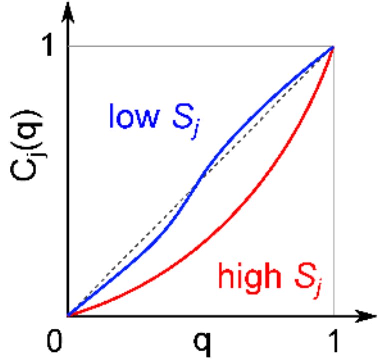

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2 research questions

1. what relationship between CSM plot and S_j ?
2. is it possible to compute S_j from a CSM plot ?

1st question

What relation between CSM plot and first-order sensitivity indices S_j?

Relation between CSM and first-order indices S_j

Property

Let denote $c_v = \sigma(Y)/\mathbf{E}(Y)$.

For any input X_j we have:

$$S_j = \frac{1}{c_v^2} \cdot \int_0^1 \left[\frac{d}{dq} \left(C_j(q) - q \right) \right]^2 dq \qquad (2)$$

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Elements of proof

Elements of proof

CSM expression using conditional expectation

$$\forall q \in [0;1], \quad C_j(q) = \frac{1}{\mathbf{E}(Y)} \int_{-\infty}^{F_j^{-1}(q)} \mathbf{E}\left[Y \mid X_j = x_j\right] p_j(x_j) dx_j$$

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CSM derivative

Using $\frac{d}{dq}(F_j^{-1}(q)) = 1/p_j\left(F_j^{-1}(q)\right)$:

$$\forall q \in [0;1], \quad \frac{d}{dq} C_j(q) = \frac{\mathbf{E}\left[Y \mid X_j = F_j^{-1}(q)\right]}{\mathbf{E}(Y)}$$

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2nd question

Computing first-order effects S_j from a CSM plot?

Computing S_j from a CSM plot

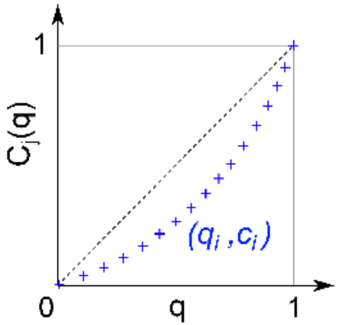
Start from a sample of n CSM points $(q_i, c_i)_{i=1,\ldots,n}$.

A. Polynomial regression

- fit a polynomial model on CSM points (q_i, c_i)
- exact formula for S_j from the regression coefficients

B. Spline smoothing

- fit a spline model on the CSM points
- approximate CSM derivative
- compute S_j using Eqn.(2)



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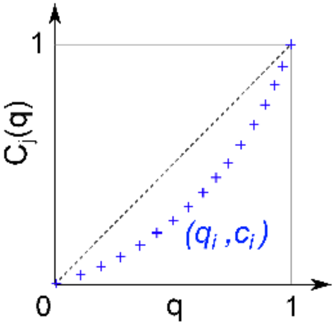

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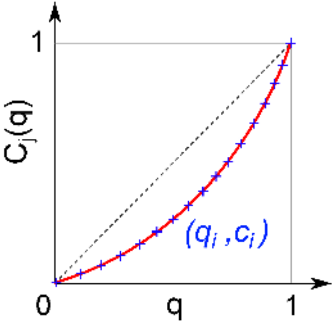

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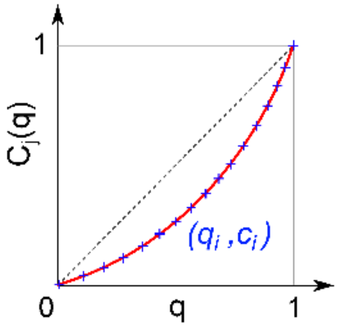

Polynomial regression

Polynomial regression

- expansion of CSM using **shifted Legendre polynomials** $(P_k)_{k\in\mathbb{N}}$ which are orthogonal on $[0,1]$

$$\forall i = 1\dots n, \quad c_i = \sum_{k=0}^{d} \alpha_k P_k(q_i) + \epsilon_i$$

Polynomial regression

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$$\forall i = 1 \dots n, \quad c_i = \sum_{k=0}^{d} \alpha_k P_k(q_i) + \epsilon_i$$

- **selecting max order d*** by minimizing AICc information criterion

$$d^\star = \underset{d\in\mathbb{N}}{\operatorname{argmin}} \left[\frac{n}{2} \cdot \log\left(\frac{2\pi}{n} \sum_{i=1}^{n} \epsilon_i(d)^2 \right) + \frac{n}{2} + \frac{n\cdot(d+2)}{n-d-3} \right]$$

Polynomial regression

- **explicit formula for $\mathbf{S_j}$** derived from Eqn.(2) using P_k properties

with :

$$\tilde{\alpha}_k = \begin{cases} \alpha_k & \text{if} \quad k > 1, \\ \alpha_k - \frac{1}{2} & \text{if} \quad k = 1 \end{cases}$$

we obtain:

$$\hat{S}_j = \frac{2}{\hat{c_v}^2} \sum_{\substack{k,l=1 \\ k+l \in 2\mathbb{Z}}}^{d} \tilde{\alpha}_k \tilde{\alpha}_l \cdot \min(k,l)\left[1 + \min(k,l)\right] \qquad (3)$$

3[rd] point

Numerical test cases

Test cases

1. Ishigami function
   - X_1 to X_3 i.i.d $\sim U[-\pi, \pi]$

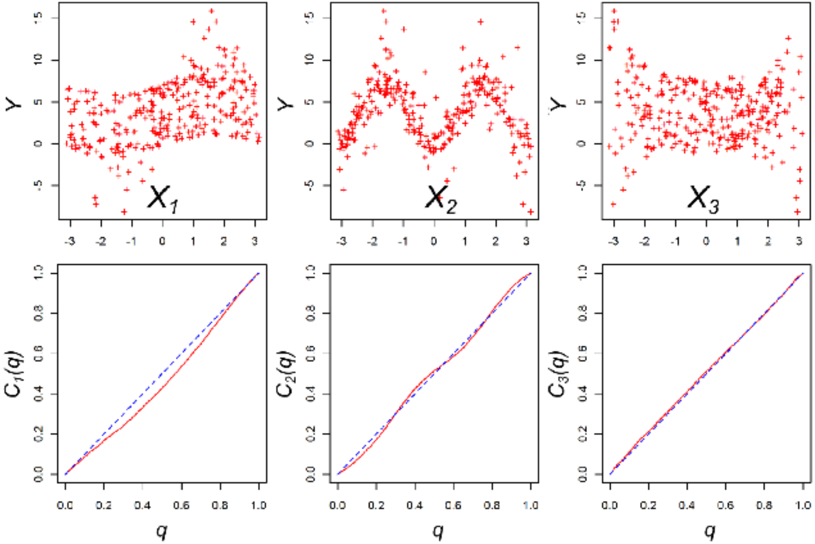
$$Y = \sin(X_1) + a \cdot \sin(X_2)^2 + b \cdot X_3^4 \cdot \sin(X_1)$$

2. G-Sobol function
   - X_1 to X_8 i.i.d $\sim U[0, 1]$
   - fixed parameter vector $a = (0, 1, 4.5, 9, 99, 99, 99, 99)$:

$$Y = \prod_{j=1}^{8} \frac{|4X_j - 2| + a_j}{1 + a_j}$$

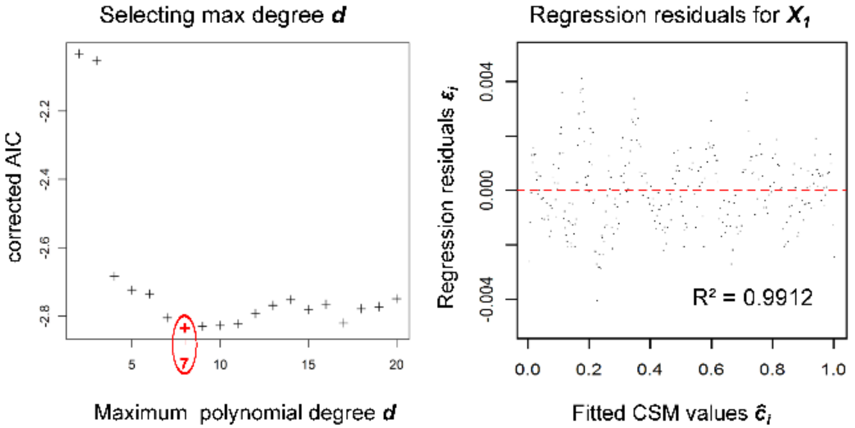
Scatterplots and CSM plots

sample size $n = 300$ (simple random sample)



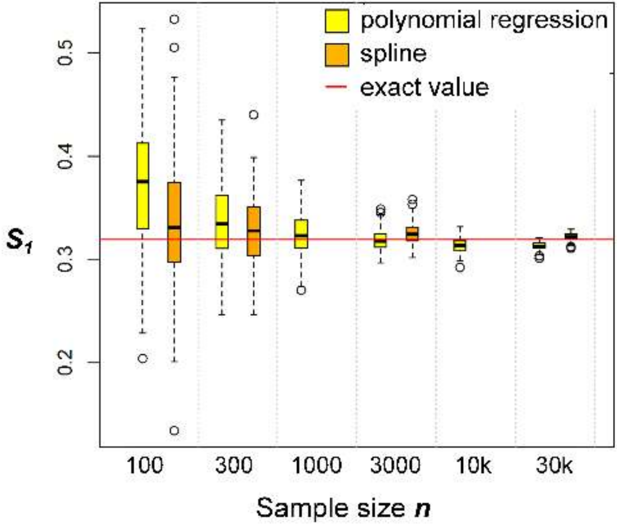
Polynomial fit for input X_1

sample size $n = 300$ (simple random sample)



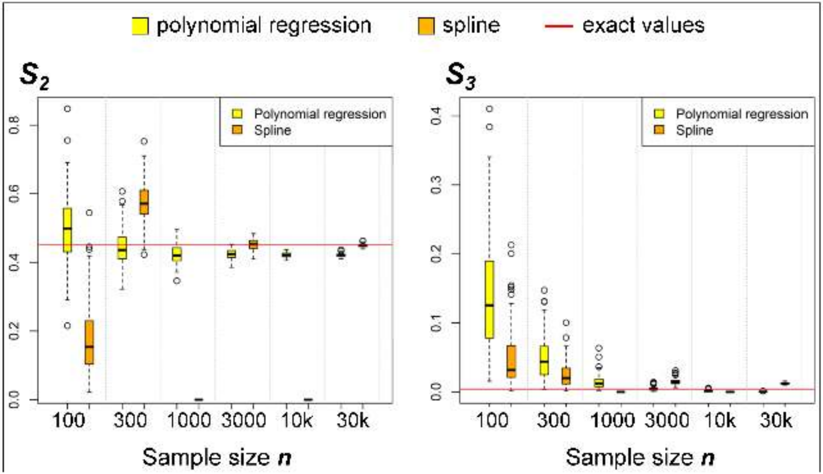
Estimation of first-order effects

Convergence of $\hat{S}_1$ for increasing sample size n



Estimation of first-order effects

Convergence of $\hat{S}_2$ and $\hat{S}_3$ for increasing sample size n



Conclusion

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+ Results

- explicit formula **linking $\mathbf{S_j}$ and CSM (derivative)**
- $\hat{S}_j$ estimator based on **polynomial expansion of the CSM plot** (explicit formula from regression coefficients)

  $\longrightarrow$ computation of S_j from **given data**

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  $\longrightarrow$ computation of S_j from **given data**

− Limits

- minimum sample size $n \sim 1000$
- $\hat{S}_j$ **does not compare well** with other estimators based on given data such as EASI (Plischke, 2010)
- why ? because it requires **approximating derivatives**

Conclusion

⟶ Further research

- Total-order effects ?
  - Contribution to the Sample Variance (CSV plot)
  - first attempts were unsuccessful but...

Tarantola S., V. Kopustinskas, R. Bolado-Lavin, A. Kaliatka, E. Uspuras, M. Vaisnoras
Sensitivity analysis using contribution to sample variance plot: Application to a water hammer model
Reliab. Eng. Syst. Saf., 2012, 99, 62-73.

Thank you for your attention !

Funding (6 weeks stay in JRC, Ispra, Italy):

PEER
Partnership for European Environmental Research

Groupement de Recherche
MASCOT-NUM
Méthodes d'Analyse Stochastique pour les COdes et Traitements NUMériques

Appendix

References

References

Bolado-Lavin, R., Castaings, W., & Tarantola, S.

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Abramowitz, M. & Segun, I. (eds.)

Handbook of mathematical functions with Formulas, Graphs, and Mathematical Tables

1972, New York: Dover Publications

Elements of proof (2)

First-order variance-based sensitivity indices

$$S_j = \frac{\mathrm{Var}_{X_j}\left(\mathbf{E}_{X_{\sim j}}\left[Y \mid X_j\right]\right)}{\mathbf{V}(Y)} \quad \text{(Saltelli et al., 2008)}$$

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\end{aligned}
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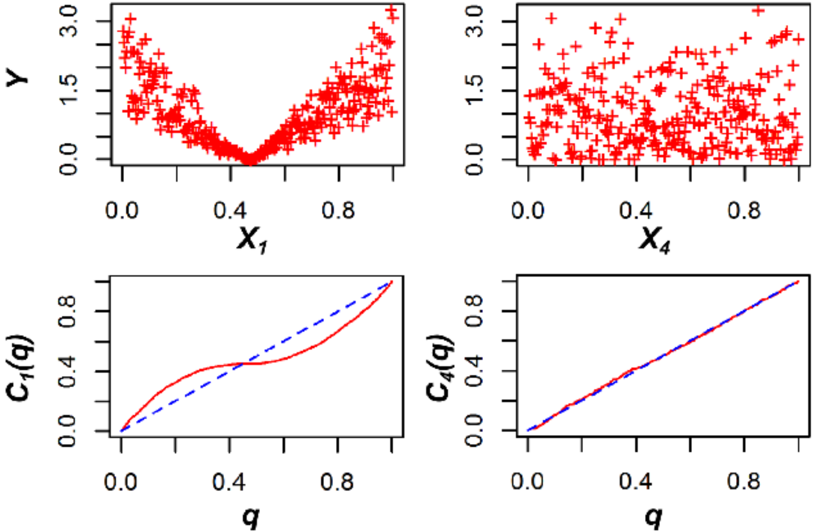
&= \frac{1}{c_v^2} \int_0^1 \left[\frac{d}{dq}\left(C_j(q) - q\right)\right]^2 dq
\end{aligned}
$$

G-Sobol test case $(n = 300)$

Scatterplots and CSM plots



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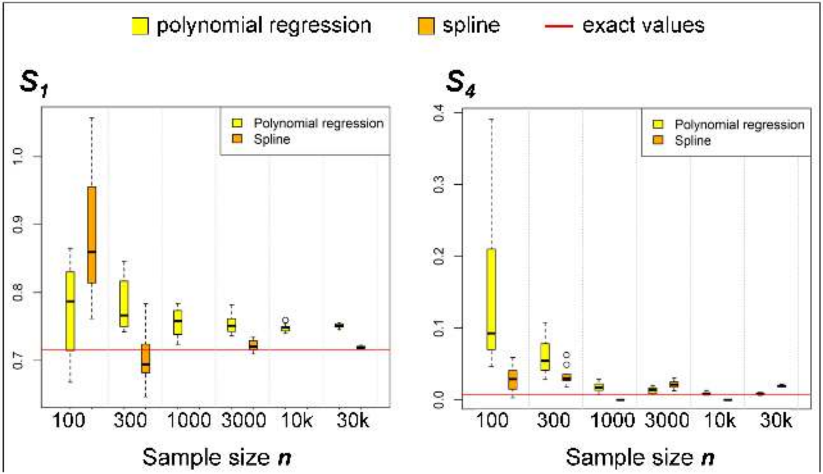
Convergence of $\hat{S}_1$ and $\hat{S}_4$ for increasing sample size n



Estimation of the coefficient of variation

Set of CSM points $(q_i, c_i)_{i=1\ldots n}$

Coefficient of variation $c_v = \sigma(Y)/E(Y)$

Using $c_i - c_{i-1} = y_{\pi(i)}/(n\hat{\mu})$ we get:

$$\hat{c}_v = n\sqrt{\sum_{i=1}^{n-1}(c_{i+1} - c_i - \frac{1}{n})^2} \qquad (4)$$

Shifted Legendre polynomials

Shifted Legendre polynomial P_k are defined by
$P_k(q) = P_k^{(s)}(2q - 1)$
with $P_k^{(s)}$ the standardized Legendre polynomials,
which are given by the Rodrigue's formula [2, p.785, Eqn. 22.11.5]
:

$$\forall k \in \mathbb{N}, \forall q \in [-1, 1], \quad P_k^{(s)}(q) = \frac{(-1)^k}{2^k \cdot k!} \frac{d^k}{dq^k} \left[(q^2 - 1)^k \right]$$

Detailed proof for Eqn.(3)

Using the approximation $C(q) \approx \sum_k \alpha_k P_k(q)$, we get an approximation of the integral $I = \int_0^1 \frac{d}{dq}\left(C(q) - q\right)^2 dq$:

$$\hat{I} = \int_0^1 \left[\left(\sum_{k=1}^{d} \alpha_k P_k'(q) \right) - 1 \right]^2 dq \tag{5}$$

We use the fact that $P_1'(q) = 2$ to define modified coefficients $(\tilde{\alpha}_k)_{k=1,\dots,d}$ as equal to coefficients $(\alpha_k)_{k=1,\dots,d}$ except for $\tilde{\alpha}_1 = \alpha_1 - \frac{1}{2}$, :

$$\begin{aligned} \hat{I} &= \int_0^1 \left[\sum_{k=1}^{d} \tilde{\alpha}_k P_k'(q) \right]^2 dq \\ &= \sum_{k,l=1}^{d} \tilde{\alpha}_k \tilde{\alpha}_l \int_0^1 P_k'(q) P_l'(q) dq \\ &= \sum_{k,l=1}^{d} \tilde{\alpha}_k \tilde{\alpha}_l I_{kl} \end{aligned} \tag{6}$$

Detailed proof for Eqn.(3)

Using the approximation $C(q) \approx \sum_k \alpha_k P_k(q)$, we get an approximation of the integral $I = \int_0^1 \frac{d}{dq}\left(C(q) - q\right)^2 dq$:

$$\hat{I} = \int_0^1 \left[\left(\sum_{k=1}^{d} \alpha_k P_k'(q) \right) - 1 \right]^2 dq \tag{5}$$

We use the fact that $P_1'(q) = 2$ to define modified coefficients $(\tilde{\alpha}_k)_{k=1,\dots,d}$ as equal to coefficients $(\alpha_k)_{k=1,\dots,d}$ except for $\tilde{\alpha}_1 = \alpha_1 - \frac{1}{2}$, :

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Detailed proof for Eqn.(3)

Let assume that $k \leq n$.
Using an integration by parts we have :

$$I_{k,l} = \left[P'_k(q)P_l(q)\right]_0^1 - \int_0^1 P''_k(q)P_l(q)dq \quad (7)$$

P''_k is a polynom of degree $k-2$: it can be decomposed on the finite orthogonal basis $(P_i)_{i=1,\dots,k-2}$. As $k-2 < l$, using the orthogonality of shifted Legendre polynomials $(P_k)_{k\in\mathbb{N}}$ on $[0,1]$, we find that the integral $\int_0^1 P''_k(q)P_l(q)dq$ is equal to 0. Hence :

$$I_{k,l} = P'_k(1)P_l(1) - P'_k(0)P_l(0) \quad (8)$$

Detailed proof for Eqn.(3)

The values of $P_k(q)$ and its derivative $P'_k(q)$ at $q = 0$ and $q = 1$ can be found from the corresponding values of non-shifted Legendre polynomial $P_k^{(s)}(q)$ at $q = -1$ and $q = 1$, which are given in [2, p.777], Eqn.(22.4.6), (22.5.37) and (22.4.2). Using the relations $P_k(q) = P_k^{(s)}(2q-1)$ and $P'_k(q) = 2(P_k^{(s)})'(2q-1)$ we have:

$$\forall k \in \mathbb{N} \quad \begin{cases} P_k(1) & = & 1 \\ P'_k(1) & = & k(k+1) \\ P_k(0) & = & (-1)^k \\ P'_k(0) & = & (-1)^{k-1} k(k+1) \end{cases} \tag{9}$$

We finally obtain:

$$\begin{aligned} &\forall (k,l) \in \mathbb{N}^2, k \leq l, \\ &I_{k,l} = k(k+1)[1 + (-1)^{k+l}] \end{aligned} \tag{10}$$

which we can also write this way:

$$\begin{aligned} &\forall (k,l) \in \mathbb{N}^2, \\ &I_{kl} = 2\min(k,l)\,[1 + \min(k,l)]\,\mathbf{1}_{\{(k+l)\,\in\,2\mathbb{N}\}} \end{aligned} \tag{11}$$

Detailed proof for Eqn.(3)

The values of $P_k(q)$ and its derivative $P'_k(q)$ at $q = 0$ and $q = 1$ can be found from the corresponding values of non-shifted Legendre polynomial $P_k^{(s)}(q)$ at $q = -1$ and $q = 1$, which are given in [2, p.777], Eqn.(22.4.6), (22.5.37) and (22.4.2). Using the relations $P_k(q) = P_k^{(s)}(2q-1)$ and $P'_k(q) = 2(P_k^{(s)})'(2q-1)$ we have:

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Contribution to the Sample Variance

Contribution to the sample variance for input parameter X_j at quantile q is given by:

$$D_j(q) = \frac{1}{\mathbf{V}(Y)} \int_{-\infty}^{F_j^{-1}(q)} \mathbf{E}\left[(Y - \mathbf{E}(Y))^2 \mid X_j = x_j\right] p(x_j) dx_j \tag{12}$$

Contribution to the Sample Variance

Slope of the CSV plot

The slope of the CSV plot between the two points $(q_1, D(q_1))$ and $(q_2, D(q_2))$ is given by:

$$\frac{D(q_2) - D(q_1)}{q_2 - q_1} = \frac{\mathbf{V}(Y^{\star[z_1,z_2]})}{\mathbf{V}(Y)} \qquad (13)$$

with variance $\mathbf{V}(Y^{\star[z_1,z_2]})$, defined as the variance of the model output when the range of the parameter X_j is reduced to $[z_1, z_2]$, but with respect to constant mean $\mathbf{E}(Y)$ over the full range of all parameters:

$$\mathbf{V}(Y^{\star\{z\}}) = \mathbf{E}\left[(Y - \mathbf{E}(Y))^2 \mid X_j = z\right]$$

Contribution to the Sample Variance

Relation with total order sensitivity indices?

Total order sensitivity indices:

$$ST_j = 1 - \frac{\mathbf{E}_{X_j}\left[\mathrm{Var}_{X_{\sim j}}\left(Y \mid X_j\right)\right]}{\mathbf{V}(Y)}$$

$$= 1 - \frac{\mathbf{E}_{X_j}\left(\mathbf{E}_{X_{\sim j}}\left[\left(Y - \mathbf{E}\left[Y \mid X_j\right]\right)^2 \mid X_j = x_j\right]\right)}{\mathbf{V}(Y)}$$

Let denote by $\mathbf{V}(Y^{\circ\{x_j\}})$ the quantity $\mathbf{E}_{X_{\sim j}}\left[\left(Y - \mathbf{E}\left[Y \mid X_j\right]\right)^2 \mid X_j = x_j\right]$. It is the variance of model output when model input X_j is fixed to the value x_j, but with respect to the conditional mean $\mathbf{E}\left[Y \mid X_j = x_j\right]$. We then have:

$$ST_j = \int_0^1 \left[1 - \frac{\mathbf{V}(Y^{\circ\left\{F_j^{-1}(q)\right\}})}{\mathbf{V}(Y)}\right] dq \qquad (14)$$

Contribution to the Sample Variance

Relation with total order sensitivity indices?

Trouble is that the two variances $\mathbf{V}(Y^{\circ\{z\}})$ and $\mathbf{V}(Y^{\star\{z\}})$ are not equal, as they are not computed with respect to the same mean value.

- constant mean $\mathbf{E}(Y)$ for $\mathbf{V}(Y^{\star\{z\}})$
- conditionnal mean $\mathbf{E}\left[Y \mid X_j = z\right]$ for $\mathbf{V}(Y^{\circ\{z\}}))$