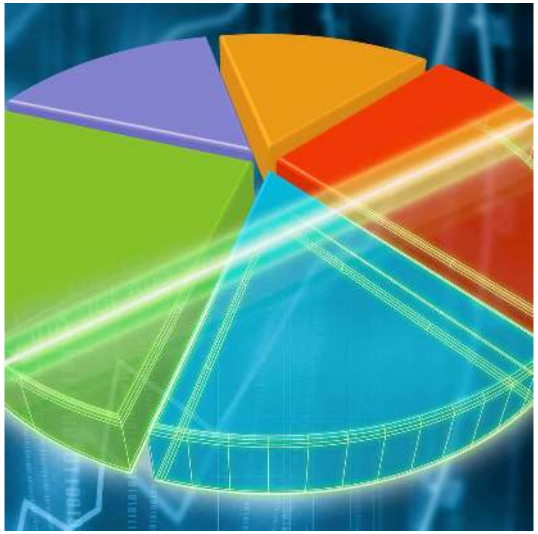
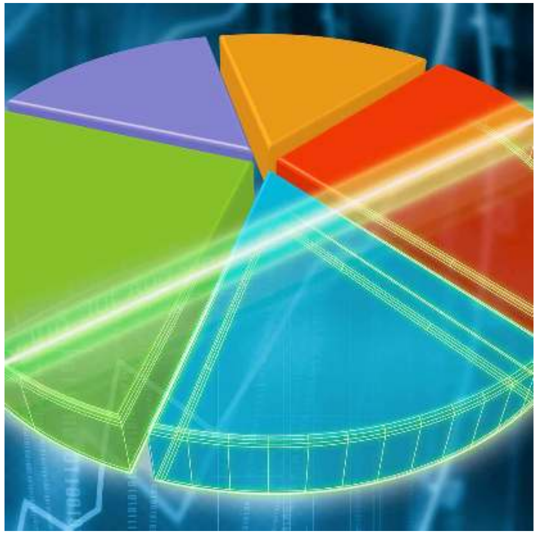


Innovative SA methods

Stefano Tarantola

Joint Research Centre
of the European Commission

Cadarache
January, 12 2010



Sobol's formula for first order indices

Classic Sobol' formula (1993) $x = (y, z)$

$$V_y = \int f(x) f(y, z') dx dz' - f_0^2$$

$$S_y = V_y / V$$

For the r-th MC trial two independent random points x_r and x'_r are used:

$$f_0 \approx \frac{1}{N} \sum_{r=1}^{N} f(x_r)$$

$$V \approx \frac{1}{N} \sum_{r=1}^{N} f^2(x_r) - f_0^2$$

$$V_y \approx \frac{1}{N} \sum_{r=1}^{N} f(x_r) f(y_r, z'_r) - f_0^2$$

When $V_y \ll f_0^2$ can loose accuracy

Sobol', Tara, Gatelli, Kuche (2007) $x = (y, z)$

$$f_0^2 = \int f(x) f(x') dx dx'$$ ← Saltelli (2002)

$$V_y = \int f(x) f(y, z') dx dz' - f_0^2$$

$$V_y = \int f(x) \left[f(y, z') - f(x') \right] dx dx'$$

The MC algorithm:

$$V_y \approx \frac{1}{N} \sum_{r=1}^{N} f(x_r) \left[f(y_r, z'_r) - f(x'_r) \right]$$

More stable than the original algorithm

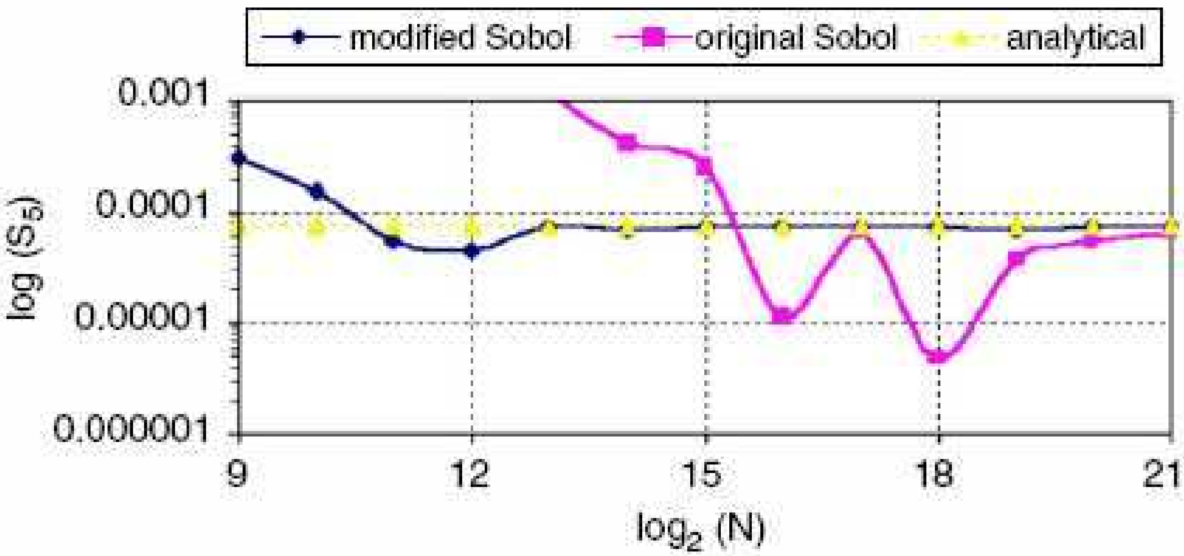
Classic Sobol' (1993)

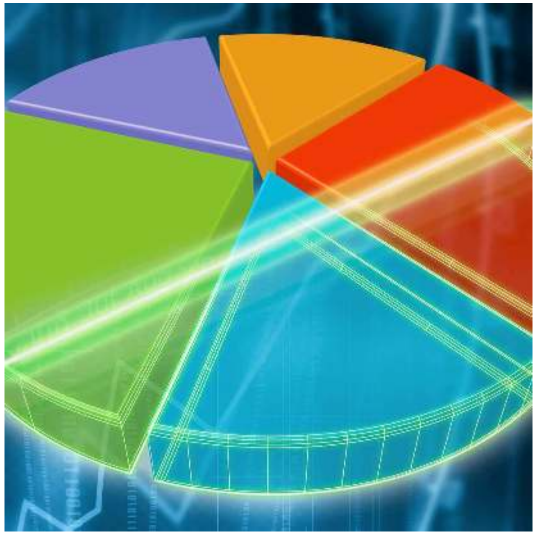
$$V_y \approx \frac{1}{N}\sum_{r=1}^{N} f(x_r) f(y_r, z'_r) - f_0^2$$

$$f_0 \approx \frac{1}{N}\sum_{r=1}^{N} f(x_r)$$

Sobol', Tara, Gatelli, Kuche (2007)

$$V_y \approx \frac{1}{N}\sum_{r=1}^{N} f(x_r)\left[f(y_r, z'_r) - f(x'_r)\right]$$





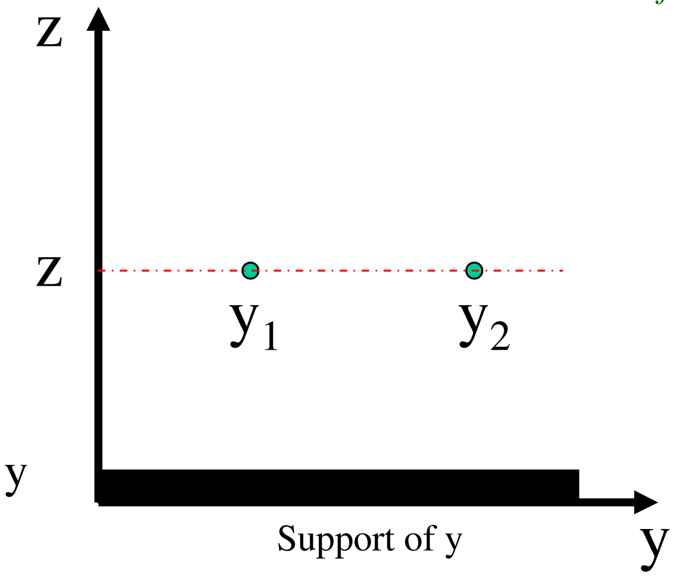
Jansen's formula for total indices

Jansen's formula

$$f(x) = f(y, z) \qquad S_{Ty} = \frac{E_z\left[Var_y(f \mid z)\right]}{Var_x(f)}$$

$$d \equiv f(y_1, z) - f(y_2, z)$$

y_1, y_2 are two independent realizations of y



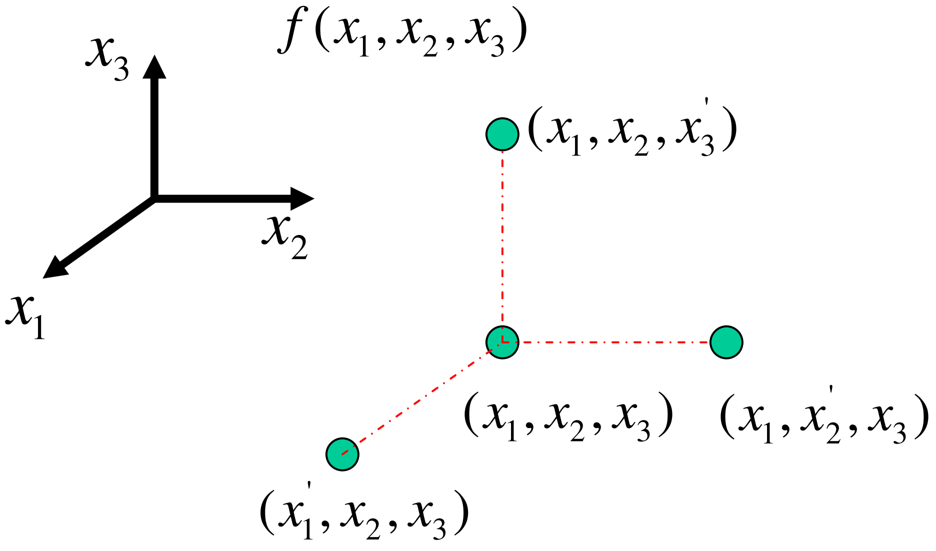
$$E_y(f(y_1, z)) = E_y(f(y_2, z)) \Rightarrow E_y(d) = 0$$

$$Var(d) = E(d^2) = 2Var_y(f \mid z)$$

$$\tfrac{1}{2} E_z E_y(d^2) = E_z[Var(f \mid z)]$$

$$E_z[Var(f \mid z)] = \tfrac{1}{2} E(d^2)$$

$$E_z[Var(f \mid z)] \approx \frac{1}{2N} \sum_{r=1}^{N} \left[f(y_r, z_r) - f(y_r^{'}, z_r)\right]^2$$



$$S_{T1} = \frac{E[Var(f \mid x_2, x_3)]}{Var(y)}$$

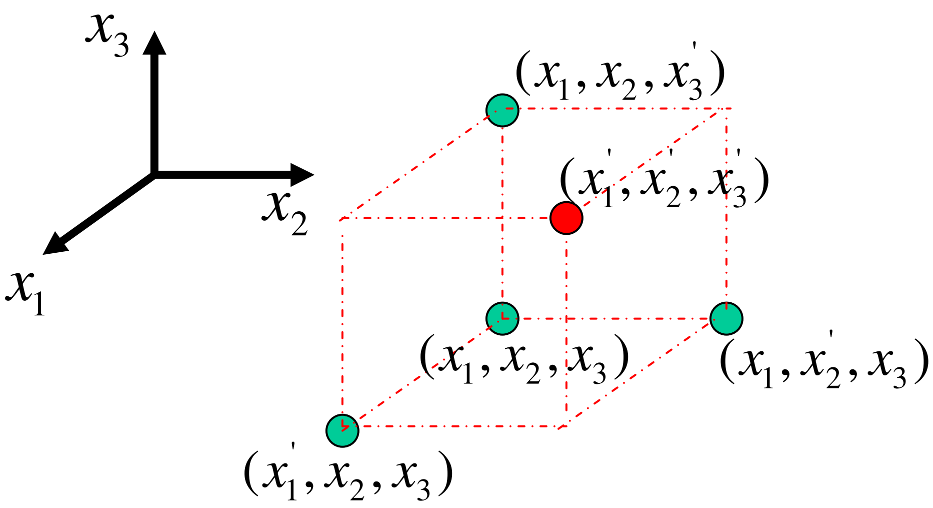
$$S_{T2} = \frac{E[Var(f \mid x_1, x_3)]}{Var(y)}$$

$$S_{T3} = \frac{E[Var(f \mid x_1, x_2)]}{Var(y)}$$

$$E[Var(f \mid x_2, x_3)] = \frac{1}{2(N-1)} \sum_{r=1}^{N} \left[f(x_{r1}, x_{r2}, x_{r3}) - f(x'_{r1}, x_{r2}, x_{r3}) \right]^2$$

$$E[Var(f \mid x_1, x_3)] = \frac{1}{2(N-1)} \sum_{r=1}^{N} \left[f(x_{r1}, x_{r2}, x_{r3}) - f(x_{r1}, x'_{r2}, x_{r3}) \right]^2$$

$$E[Var(f \mid x_1, x_2)] = \frac{1}{2(N-1)} \sum_{r=1}^{N} \left[f(x_{r1}, x_{r2}, x_{r3}) - f(x_{r1}, x_{r2}, x'_{r3}) \right]^2$$



$$S_1 = \frac{Var[E(f \mid x_1)]}{Var(f)}$$

$$S_2 = \frac{Var[E(f \mid x_2)]}{Var(f)}$$

$$S_3 = \frac{Var[E(f \mid x_3)]}{Var(f)}$$

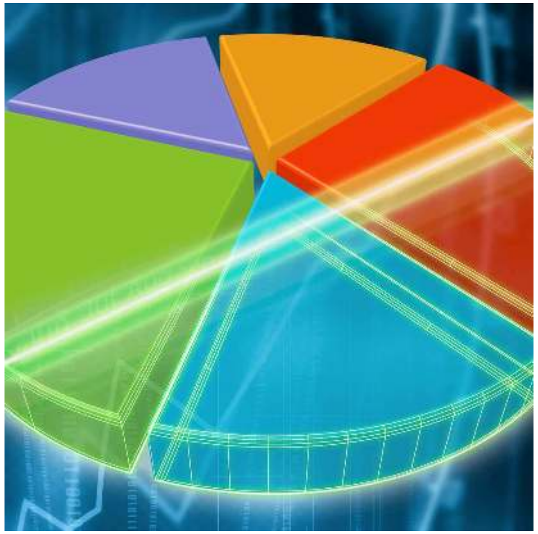
$$Var[E(f \mid x_1)] = \frac{1}{N-1}\sum_{r=1}^{N} f(x_{r1}, x_{r2}, x_{r3})[f(x_{r1}, x'_{r2}, x'_{r3}) - f(x'_{r1}, x'_{r2}, x'_{r3})]$$

? ?

Swap x with x’

$$Var[E(f \mid x_1)] = \frac{1}{N-1}\sum_{r=1}^{N} f(x'_{r1}, x'_{r2}, x'_{r3})[f(x'_{r1}, x_{r2}, x_{r3}) - f(x_{r1}, x_{r2}, x_{r3})]$$

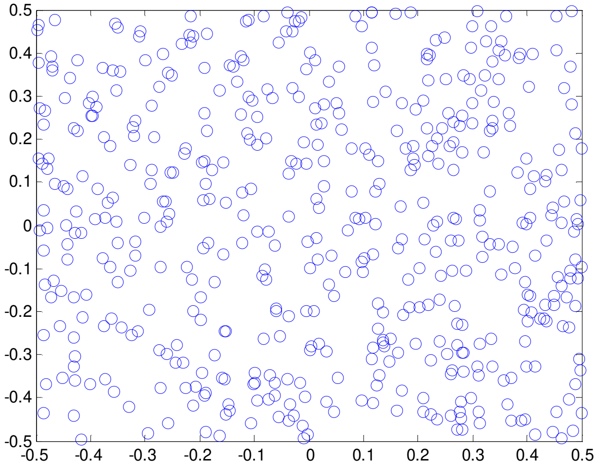
?



Sampling strategies

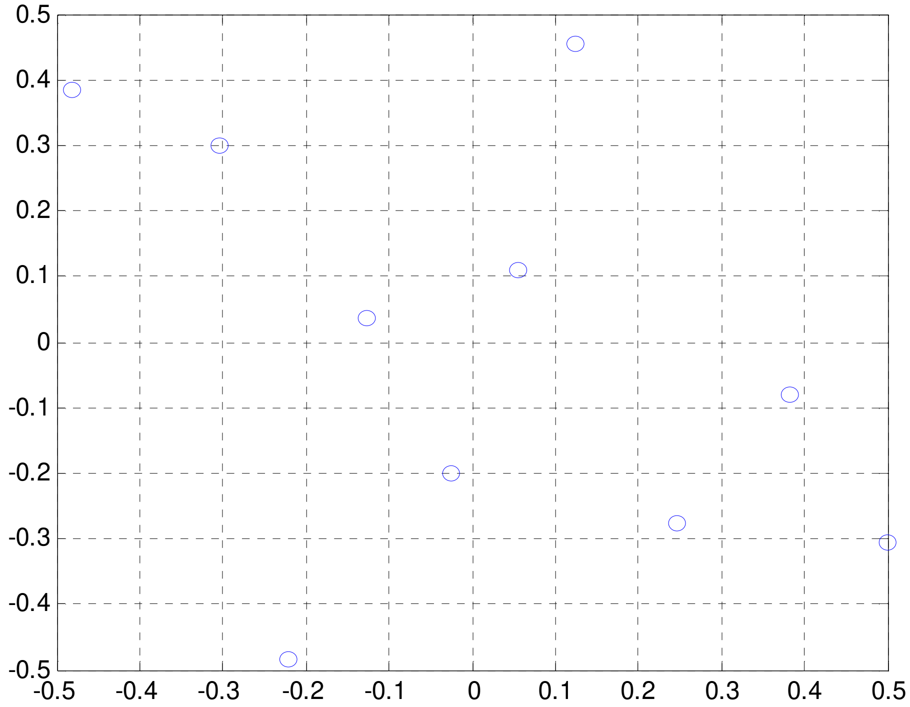
Sampling strategies

Different strategies can be used to generate the input sample



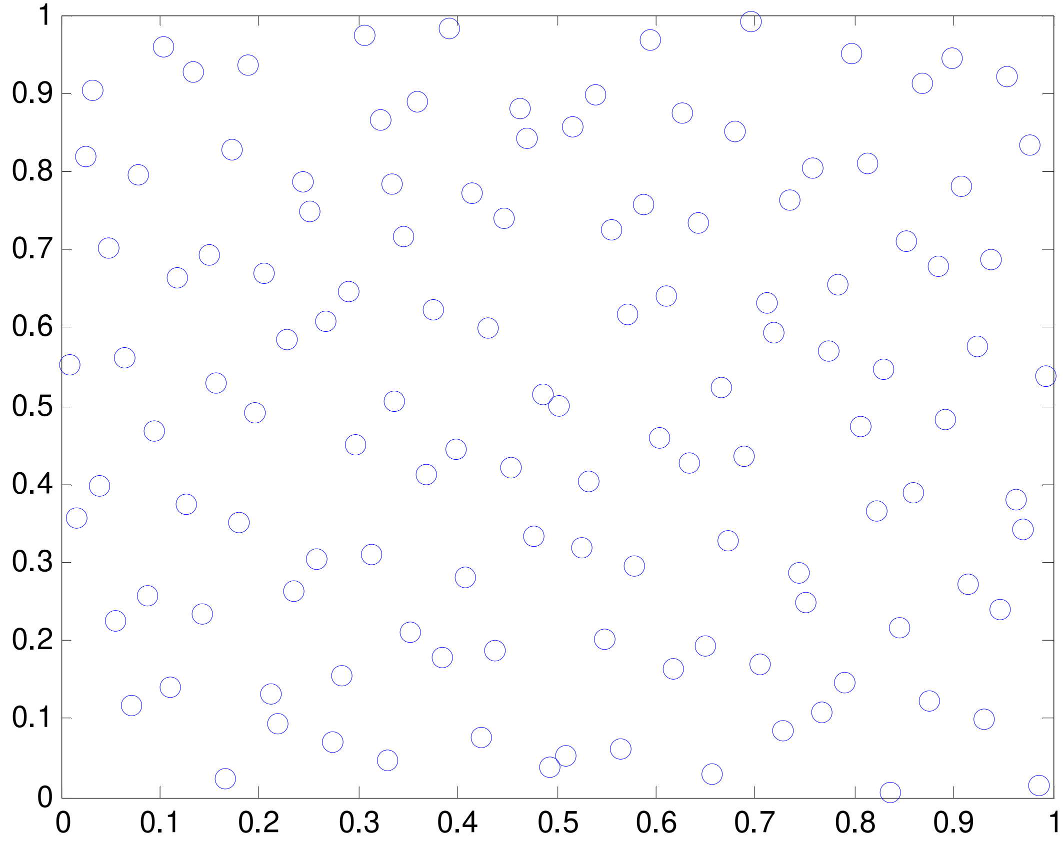
Pure random

Latin Hypercube

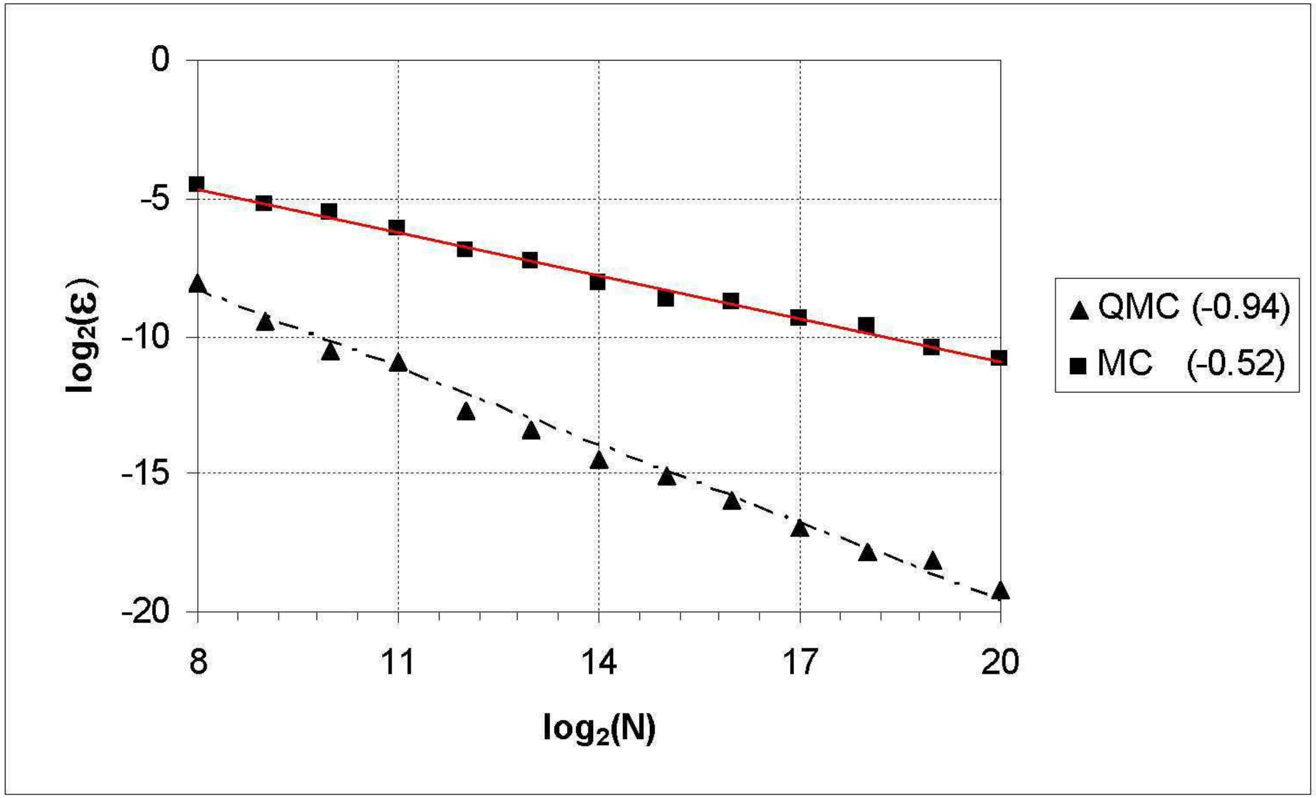


Sampling strategies

…or quasi random sequences

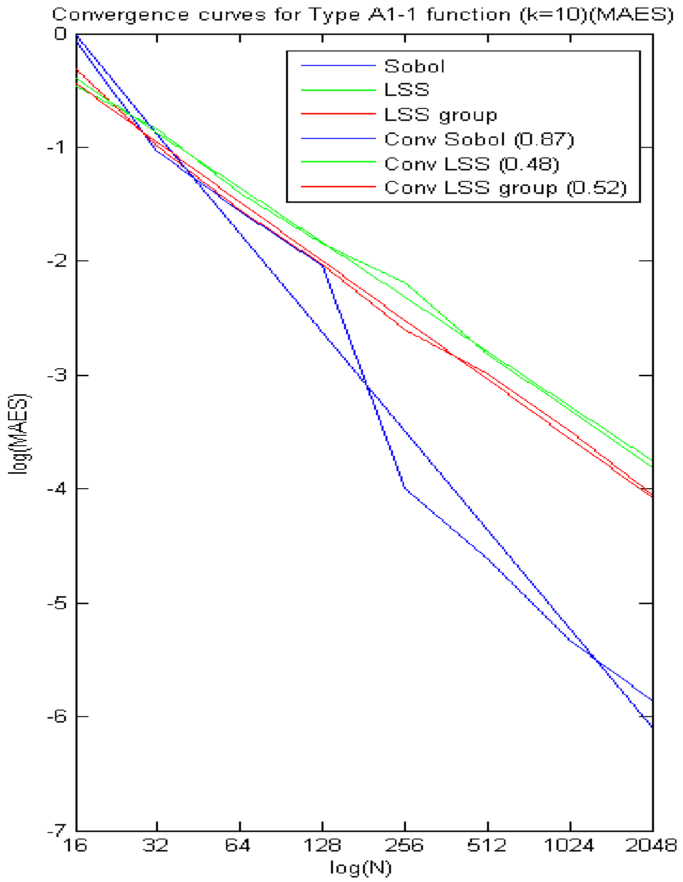


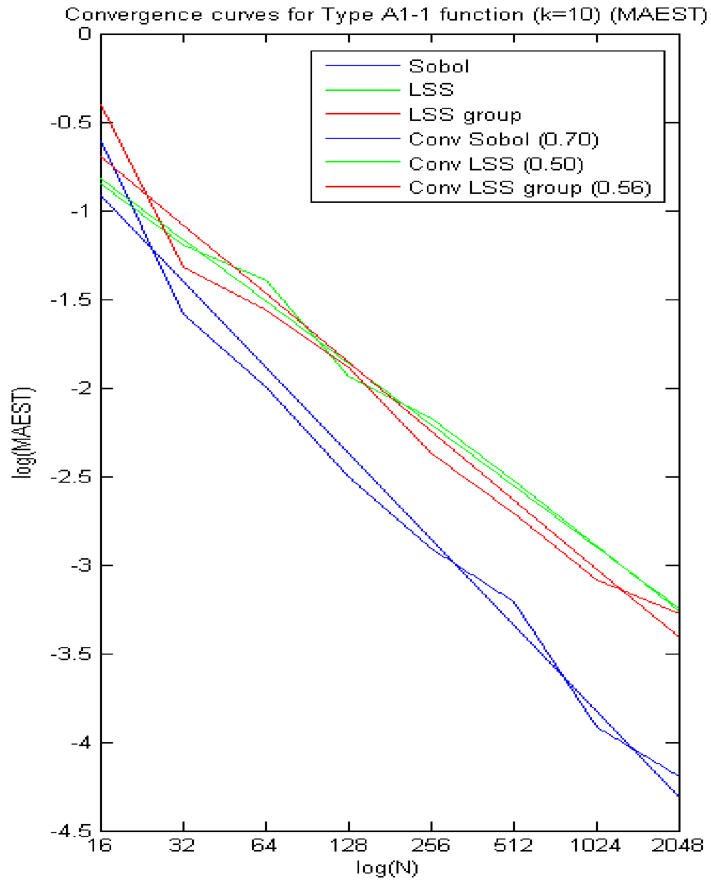
Convergence properties



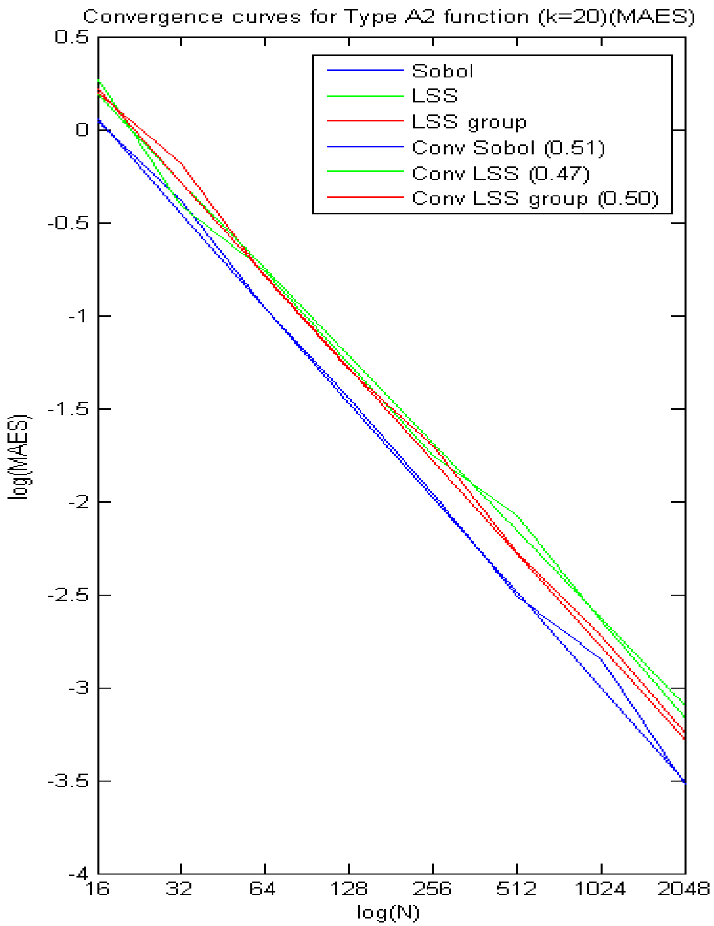
Source: Mauntz and Kucherenko, 2005

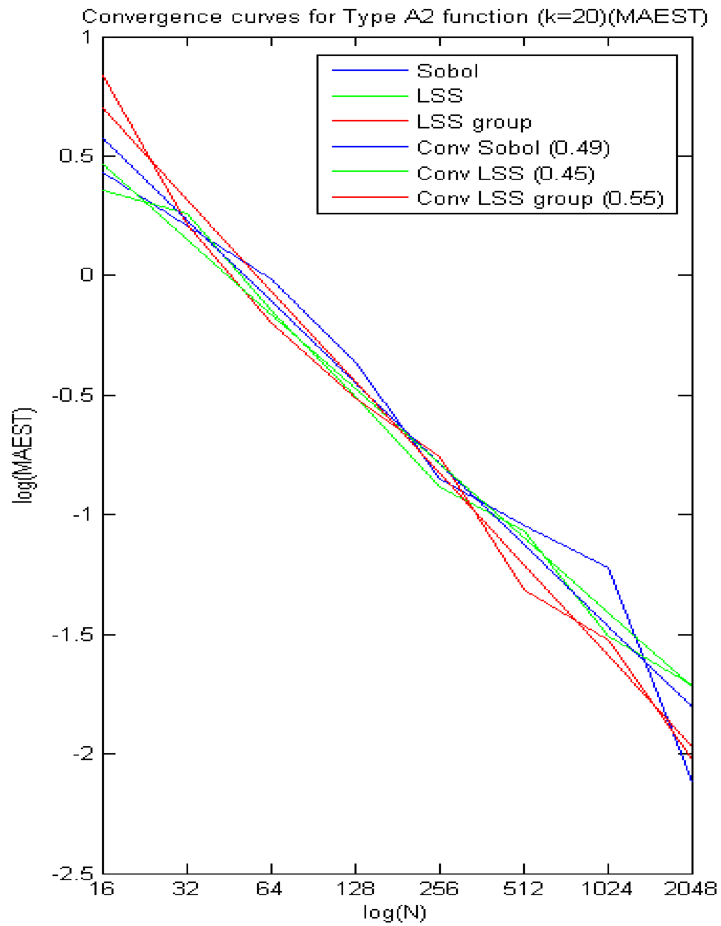
Convergence properties

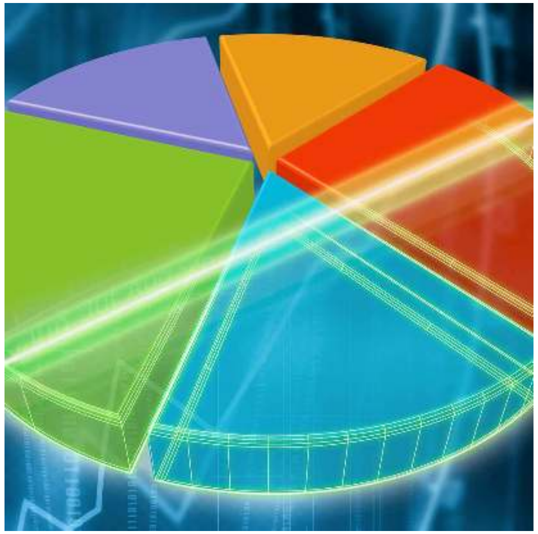




Convergence properties







Screening methods

Joint Research Centre

Screening designs “highlight” few important inputs among many (hundreds, thousands)

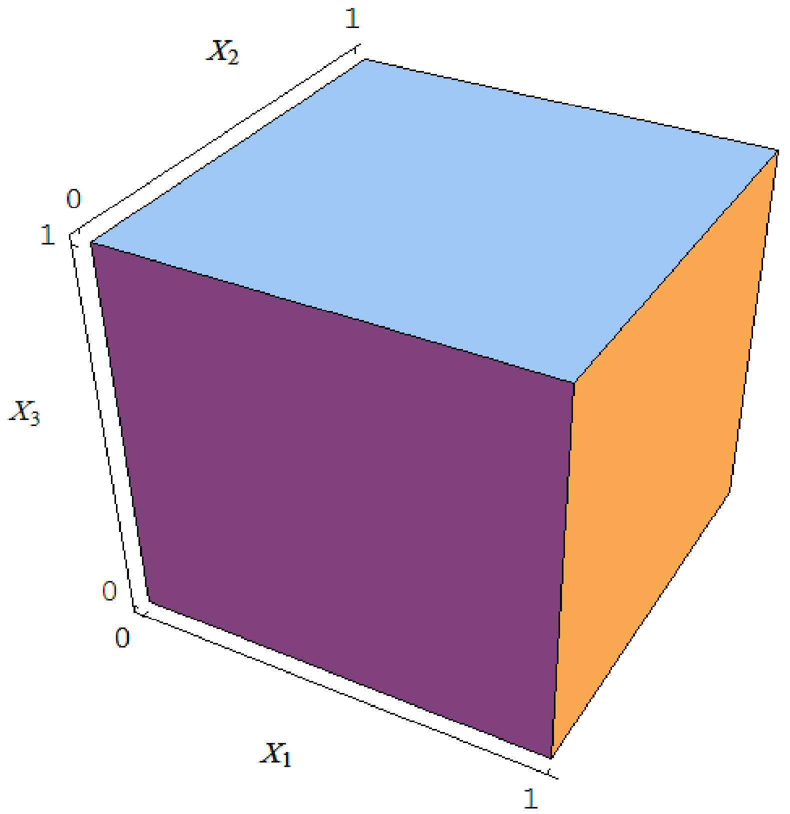
Goal: Model simplification

Screening designs derive from
Design of Experiments (DOE)

The Full Factorial Design

A 2-Level Full Factorial Design for 3 parameters

X_1	X_2	X_3
1	1	1
-1	1	1
1	-1	1
-1	-1	1
1	1	-1
-1	1	-1
1	-1	-1
-1	-1	-1



The full design requires an enormous number of points to get all combinations of levels.

Using 2 levels: 10 parameters $\rightarrow$ $2^{10} = 1024$ points

20 parameters $\rightarrow$ more than a million!!

Solution

Select only a sub-set of these points to generate a smaller design that can still produce useful results

A Fractional Factorial design can be generated using Hadamard matrices.

Def. A Hadamard matrix is a matrix of 1's and –1's that is orthogonal such that:

$$H_n H_n^T = nI_n$$

$$H_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \qquad H_2 H_2^T = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} = 2I_2$$

A $2^k \times 2^k$ Hadamard matrix can be generated recursively. For example, for k=2:

$$H_4 = \left[\begin{array}{c|c} H_2 & H_2 \\ \hline H_2 & -H_2 \end{array}\right] = \left[\begin{array}{cc|cc} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ \hline 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{array}\right]$$

Removing the first column, a Hadamard matrix makes a balanced Fractional Factorial design. Indeed …

A Hadamard matrix makes a design of Resolution III:
any 2 columns are such that the 4 combinations
(1, 1), (1, –1), (–1, 1) and (–1, –1) appear equally often in those columns

$$\left[\begin{array}{c|cc} 1 & 1 & 1 \\ -1 & 1 & -1 \\ \hline 1 & -1 & -1 \\ -1 & -1 & 1 \end{array}\right]$$

[It is possible to make Resolution IV designs where any 3 columns are such that the 8 combinations:
(1, 1, 1), (1, 1, –1), (1, –1, 1), (1, –1, –1), (–1, 1, 1), (–1, 1, –1), (–1, –1, 1) and (–1, –1, –1) appear equally often in those columns]

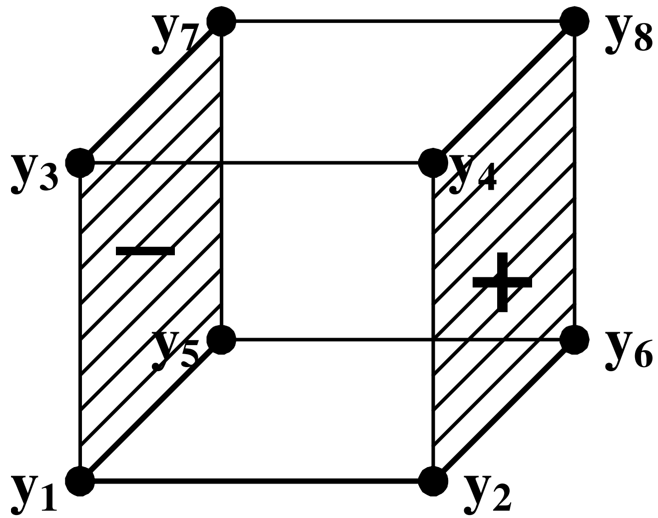
$$H_8 = \left[\begin{array}{c|c} H_4 & H_4 \\ \hline H_4 & -H_4 \end{array} \right]$$

Resolution III design with 7 factors (H_8):

X_1	X_2	X_3	X_4	X_5	X_6	X_7
1	1	1	1	1	1	1
–1	1	–1	1	–1	1	–1
1	–1	–1	1	1	–1	–1
–1	–1	1	1	–1	–1	1
1	1	1	–1	–1	–1	–1
–1	1	–1	–1	1	–1	1
1	–1	–1	–1	–1	1	1
–1	–1	1	–1	1	1	–1

The main effect of factor X_i on Y in a FF design:

$$ME_i(y) = \frac{1}{2n}\left(\sum_{x_{ji}=1} y_j - \sum_{x_{ji}=-1} y_j\right)$$



For a 2-level FF design, the variance explained by parameter X_i alone is just $\hat{V}_i(y) = \left(ME_i(y)\right)^2$

(orthogonality of the Hadamard matrix)

Method of elementary effects: is able to “screen” a subset of few important inputs among the many (tenths, hundreds) often contained in models

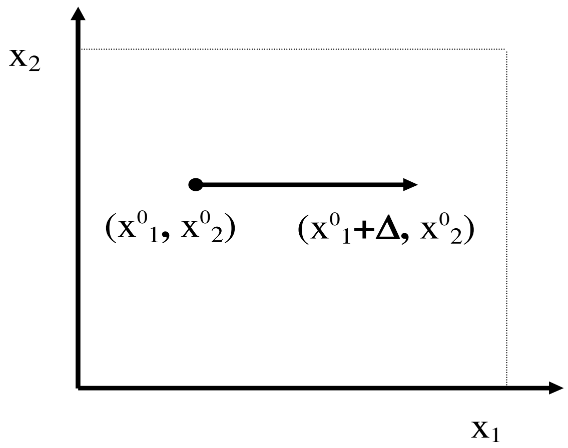
The method of elementary effects is simply a derivative (in the form of incremental ratios) computed at different points in the space of the input and averaged over the same space.

(Morris, 1991)

Model $y = y(x_1,..., x_k)$

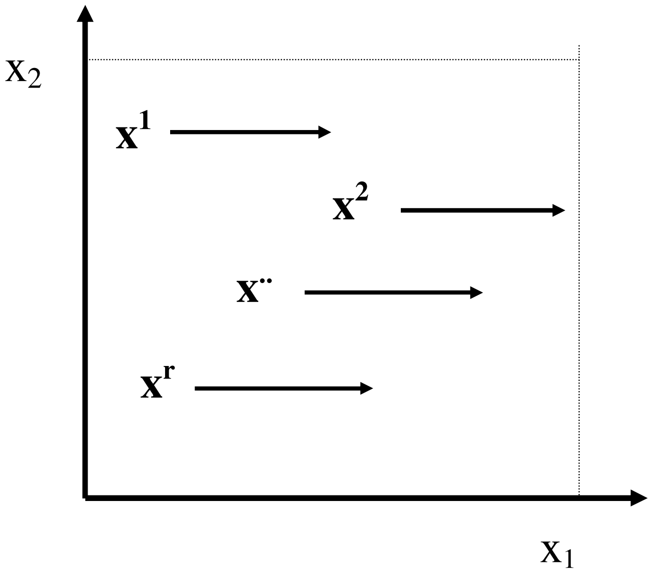
Elementary Effect for the i-th input in a point X°

$$EE_i(x_1^0,..., x_k^0) = \frac{y(x_1^0, x_2^0,..., x_{i-1}^0, x_i^0 + \Delta, x_{i+1}^0,..., x_k^0) - y(x_1^0,..., x_k^0)}{\Delta}$$



Δ is larger than in local methods

The average of several EE_i is taken.

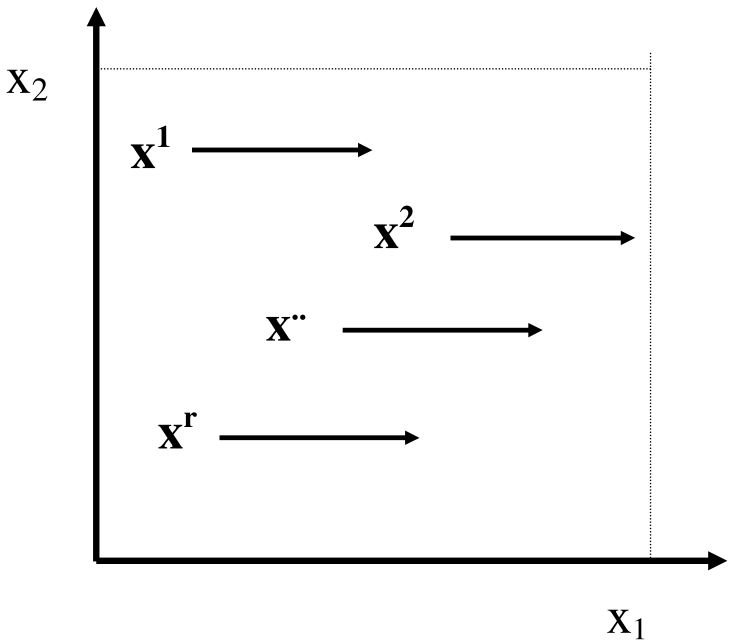


r elementary effects EE^1_i EE^2_i … EE^r_i are computed at X_1 , … , X_r

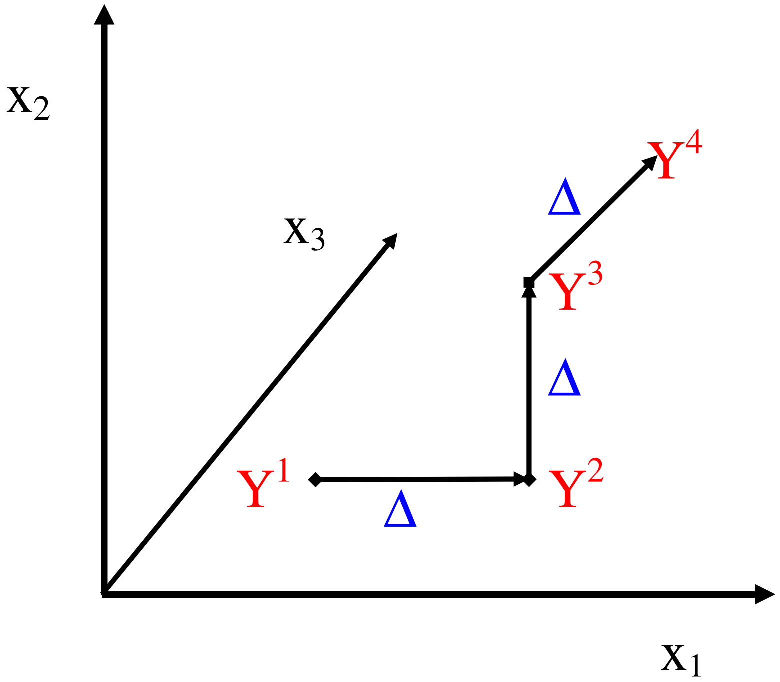
Average of $|EE_i|$'s $\rightarrow$ $\mu^*(x_i)$

$\mu^*(x_i)$ is useful to identify inputs that are not responsible for output variation

The standard deviation σ of the EE's is a measure of the sum of all interactions of x_i with other inputs



A clever sample design is used to build r trajectories of (k+1) sample points each providing one EE per input. The total cost of the screening is (k+1)r instead of 2kr.

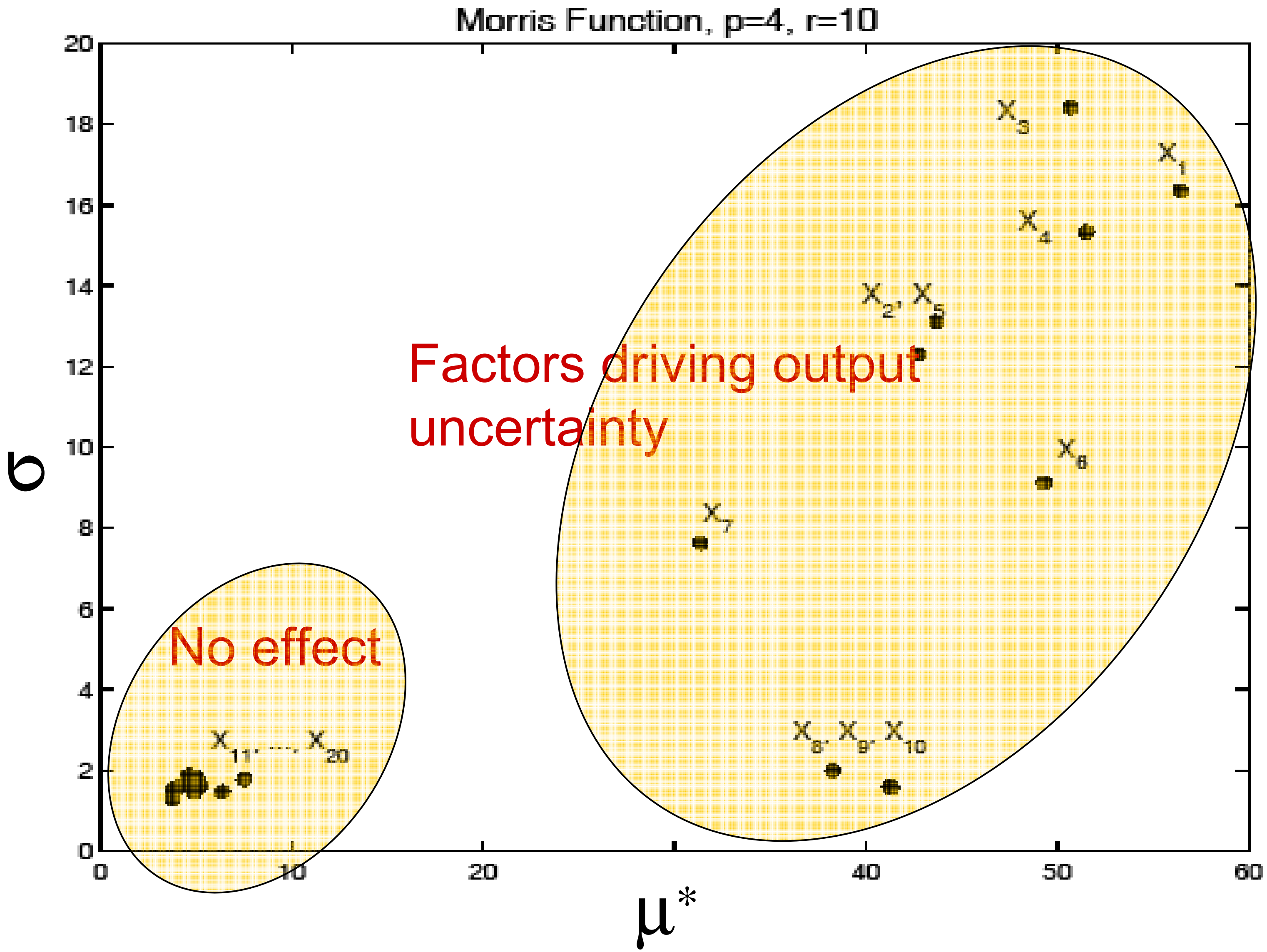


$$EE^1_1 = (Y^2 - Y^1) / \Delta$$

$$EE^1_2 = (Y^3 - Y^2) / \Delta$$

$$EE^1_3 = (Y^4 - Y^3) / \Delta$$

A graphical representation of results



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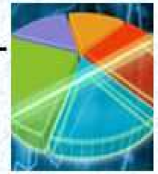
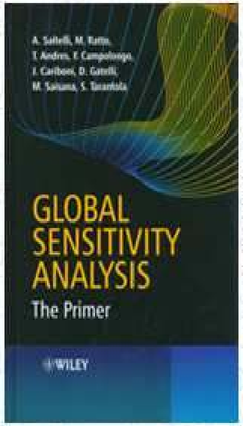
http://sensitivity-analysis.jrc.ec.europa.eu/



Sensitivity Analysis



Global Sensitivity Analysis **The Primer**
Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D. Saisana, M., and Tarantola, S., 2008, John Wiley & Sons (ISBN: 978-0-470-05997-5)

Who needs Sensitivity Analysis

Tutorial on Sensitivity Analysis

SimLab Software for Sensitivity Analysis

What's New

- Sixth **International Conference** on Sensitivity Analysis of Model Output, Bocconi University of Milan, 19-22 July 2010
- Sixth **Summer School** on Sensitivity Analysis of Model Output, Villa La Stella, Fiesole - Florence, 21-24 September 2010

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