SENSITIVITY ANALYSIS IN METROLOGY : STUDY AND COMPARISON OF DIFFERENT INDICES FOR MEASUREMENT UNCERTAINTY

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Outline

- Context of sensitivity analysis in metrology
- Presentation of different indices to perform sensitivity analysis
- Illustration based on « classical » examples in the literature
- Discussion and recommendations
- Conclusion and perspectives

Prescriptions for sensitivity analysis

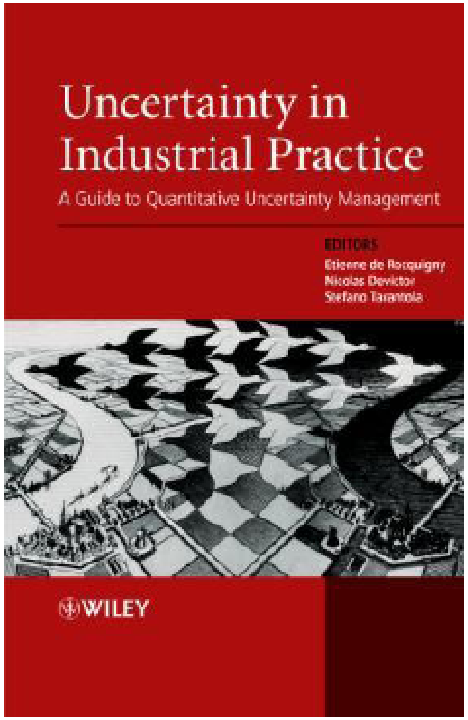
"A good sensitivity analysis should conduct analyses over the full range of plausible values of key parameters and their interactions, to assess how impacts change in response to changes in key parameters".

European Commission (JRC) Guidelines
for extended impact assessment of Directives

Context - Goals

- To understand the influence or to rank the importance of uncertainties, hence to guide any additional measurement, modelling or R&D efforts

- In Metrology
  - ✓ To provide an "uncertainty budget" when performing MCM. This may be useful to identify the dominant terms contributing to $u^2(y)$
  - ✓ To provide a quantitative tool, that fully describes the decomposition of the variance of the measurand



Sensitivity analysis according to the GUM

- In the GUM, sensitivity coefficient and contribution for each input quantity to the uncertainty associated with the estimate of the measurand are defined:
  - ✓ Sensitivity coefficient : $c_i = \left(\dfrac{\partial f}{\partial x_i} \right)$
  - ✓ Contribution to the variance: $c_i^2 u^2(x_i)$
  - ✓ Ratio in the "uncertainty budget": $\dfrac{c_i^2 u^2(x_i)}{u^2(y)}$
- Terms of second order in the Taylor series expansion (when used) provide interaction effects between two input quantities: $\left[\dfrac{1}{2} \left[\dfrac{\partial^2 f}{\partial x_i \partial x_j} \right]^2 + \dfrac{\partial f}{\partial x_i} \dfrac{\partial^2 f}{\partial x_i \partial x_j^2} \right] u^2(x_i) u^2(x_j)$

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Regression based approach to sensitivity analysis

- **Least square can be used to construct the regression model :**

$$Y = b_0 + \sum_{i=1}^{p} b_i x_i$$

- **The coefficients $b_i \hat{s}_i / \hat{s}$ are called the Standardized Regression Coefficients SRC and are often used as measures of variable importance**

$$SRC = \rho_{x,Y} = \frac{\sum_{j=1}^{n} \left(x_j - \bar{x}\right)\left(y_j - \bar{y}\right)}{\sqrt{\sum_{j=1}^{n} \left(x_j - \bar{x}\right)^2 \sum_{j=1}^{n} \left(y_j - \bar{y}\right)^2}}$$

- **We used the normalized indices in order to assess the relative contribution of x_i :**

$$\frac{SRC_i^{\,2}}{\sum_i SRC_i^{\,2}}$$

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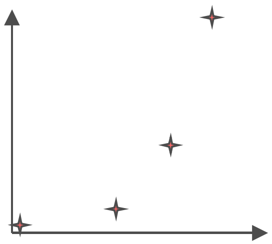
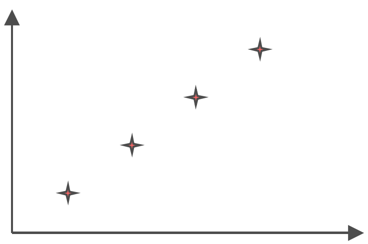
Rank transformation

- If the linear hypothesis is not valid while one assume a monotonic relationship *f*, the rank transformation can be performed to linearize the relationships



$$\begin{pmatrix} x & z \\ 4 & 4 \\ 0 & 0 \\ 5 & 10 \\ 3 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} r_x & r_z \\ 3 & 3 \\ 1 & 1 \\ 4 & 4 \\ 2 & 2 \end{pmatrix}$$



- The usual regression and correlation procedures are performed on these ranks
- The rank-transformed data provide others sensitivity indices, **SRRC Standardized Rank Regression Coefficients**

$$SRRC(r_x; r_y) = \frac{\sum_{j=1}^{n} \left(r_{x_j} - \bar{r}_x\right)\left(r_{y_j} - \bar{r}_y\right)}{\sqrt{\sum_{j=1}^{n} \left(r_{x_j} - \bar{r}_x\right)^2 \sum_{j=1}^{n} \left(r_{y_j} - \bar{r}_y\right)^2}}$$

"One factor At a time" (OAT)

- The GUM Supplement 1(Annex B) recommends an approach, known as **OAT (One factor At a time)** for sensitivity analysis

- Principle: holding all input quantities but one fixed at their best estimates while performing MCM. This provides the pdf for the output quantity having just that input quantity as a variable

- Generalization of the partial-derivative approach
  - ✓ Sensitivity coefficient : $c_i = \dfrac{u_i(y)}{u(x_i)}$
  - ✓ Contribution to the variance: $c_i^2 u^2(x_i)$
  - ✓ Ratio in the "uncertainty budget": $\dfrac{u_i^{\,2}(y)}{u^2(y)}$

Variance-based method

- Decomposition of the model function *f* into summands of increasing dimensionality

$$f(x) = f_0 + \sum_{i=1}^{k} f_i(x_i) + \sum_i \sum_{j>i} f_{ij}(x_i, x_j) + \ldots + f_{1,2,\ldots,k}(x_1, x_2, \ldots, x_k)$$

- If each term is chosen with a zero mean, the decomposition has the following properties :
  - ✓ f_0 is the mean of the function $f(x)$
  - ✓ the summands are orthogonal

Variance-based method

- **Being the terms orthogonal we can square and integrate the equation and decompose the variance of *f(x)* into terms of increasing dimensionality**

$$V(Y) = \sum_{i=1}^{k} V_i + \sum_i \sum_j V_{ij} + \sum_i \sum_j \sum_k V_{ijk} \dots + V_{1,2,\dots,k}$$

$$V_i = \int f_i^2(x_i)dx_i \qquad V_{i_1,i_2,\dots i_s} = \int f^2{}_{i_1,\dots,i_s} dx_{i_1} dx_{i_2} \dots dx_{i_s}$$

$$1 = \sum_{i=1}^{k} S_i + \sum_i \sum_j S_{ij} + \sum_i \sum_j \sum_k S_{ijk} \dots + S_{1,2,\dots,k}$$

Measures of importance

$$1 = \sum_{i=1}^{k} S_i + \sum_{i<j} S_{ij} + \sum_{i<j<l} S_{ijl} + \ldots + S_{1,2,\ldots,k}$$

first order or main effect of x_i

second order index. It measures the effect of pure interaction between any pair of variables on the output.

… higher-order indices ...

- If $\sum_i S_i = 1$ **the model is additive**
- If $\sum_i S_i < 1$ **presence of interactions**

Measures of importance

- Decomposition of the variance of *Y*:

$$V(Y) = V\left(E\left[Y|X_i\right]\right) + E\left[V\left(Y|X_i\right)\right]$$

  - ✓ Variance of the conditional expectation of *Y*, suitable measure of the importance of x_i: $V_i = V\left(E\left[Y|X_i\right]\right)$
  - ✓ First order sensitivity indices $S_i = \frac{V\left(E\left[Y|X_i\right]\right)}{V(Y)}$
  - ✓ As all input are assumed to be independent

$$V_{ij} = V\left(E\left[Y|X_i, X_j\right]\right) - V_i - V_j$$

$$V_{ijk} = V\left(E\left[Y|X_i, X_j, X_k\right]\right) - V_{ij} - V_{ik} - V_{jk} - V_i - V_j - V_k$$

$$\ldots$$

$$V_{1\ldots p} = V(Y) - \sum_{i=1}^{p} V_i - V_j - V_k$$

  - ✓ Leads to second order sensitivity indices, suitable measures of the importance of the interactions x_i,x_j

$$S_{ij} = \frac{V_{ij}}{V(Y)}$$

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The method of Sobol

- The VCE needs computation of many integrals, too complex to estimate
- Idea : to transform the many integrals (dimension *k*) in the integrals of the products of *f(x)* and *f(x')* (dimension 2k-1)

$$Var[E(Y \mid x_i)] = \int E^2(Y \mid x_i) dx_i - E^2(Y)$$

$$Var[E(Y \mid x_i)] =$$

$$= \int \int \cdots \int f(x_1, x_2, \ldots, x_i, \ldots, x_k) f(x_1^{'}, x_2^{'}, \ldots, x_i, \ldots, x_k^{'}) \; d\Omega \cdot d\Omega^{'} / dx_i^{'} - E^2(Y)$$

- Performing *N* Monte Carlo trials, this means to compute:

$$Var\left[E\left(Y \mid x_i\right)\right] = \frac{1}{N-1} \sum_{r=1}^{N} f\left(x_{r1}, x_{r2}, \ldots, x_{rk}\right) f\left(x'_{r1}, x'_{r2}, \ldots, x'_{r(i-1)}, x_{ri}, x'_{r(i+1)}, \ldots, x'_{rk}\right) - E^2(Y)$$

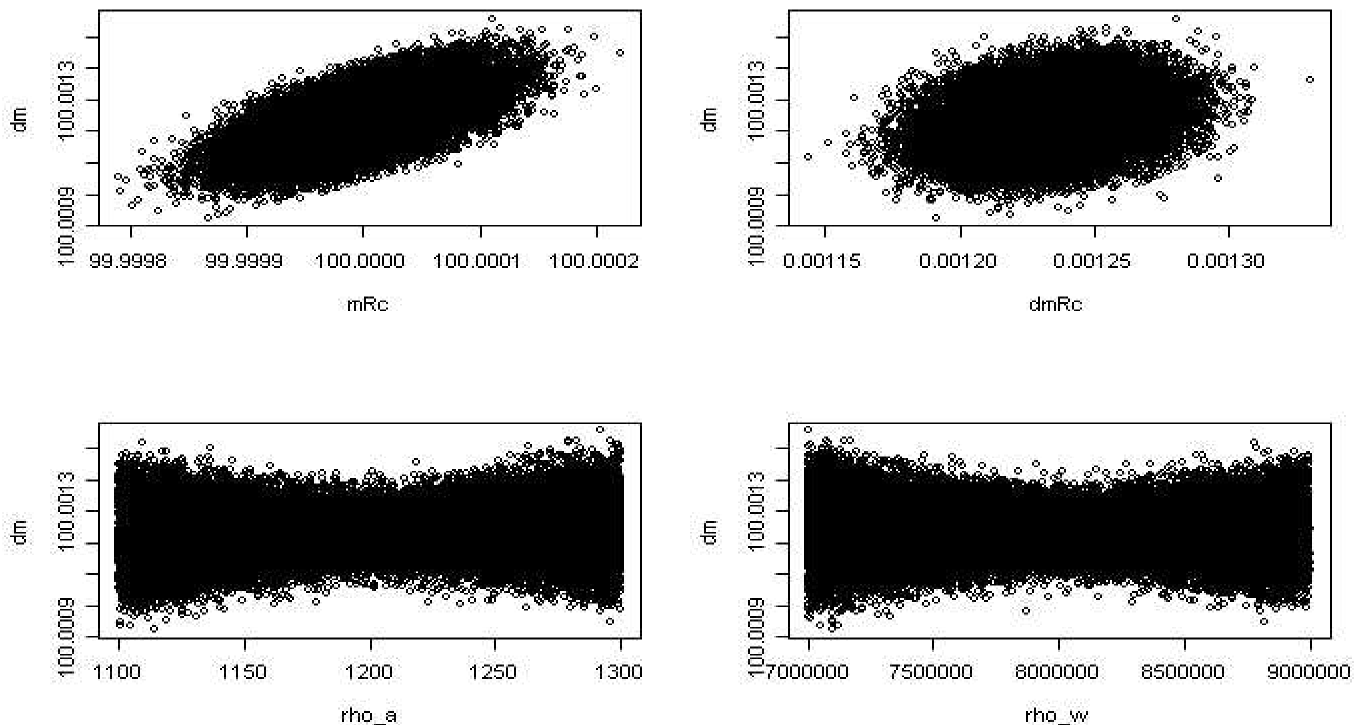
Linear model (GUM – S1 9.2.4)

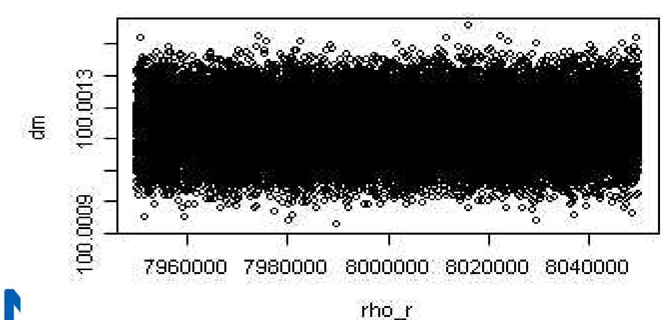
Variable	PDF
X1	U[- SQRT(3);SQRT(3)]
X2	U[-SQRT(3);SQRT(3)]
X3	U[-SQRT(3);SQRT(3)]
X4	U[-10*SQRT(3);10*SQRT(3)]

$$Y = X_1 + X_2 + X_3 + X_4$$

SENSIBILITY INDICES					
Variable	Partial derivatives LPU	OAT GUM S1	Rank	Sobol Matlab	Sobol R
X1	0,010	0,010	0,009	0,012	0,010
X2	0,010	0,010	0,009	0,012	0,010
X3	0,010	0,010	0,009	0,012	0,010
X4	0,973	0,971	0,973	0,971	0,971

Mass calibration (GUM-S1 9.3) - scatterplot





$$Y = (mrc - dmrc)\left(1 + (a - 1200000)\left(\frac{1}{rhow} - \frac{1}{rhor}\right)\right)$$

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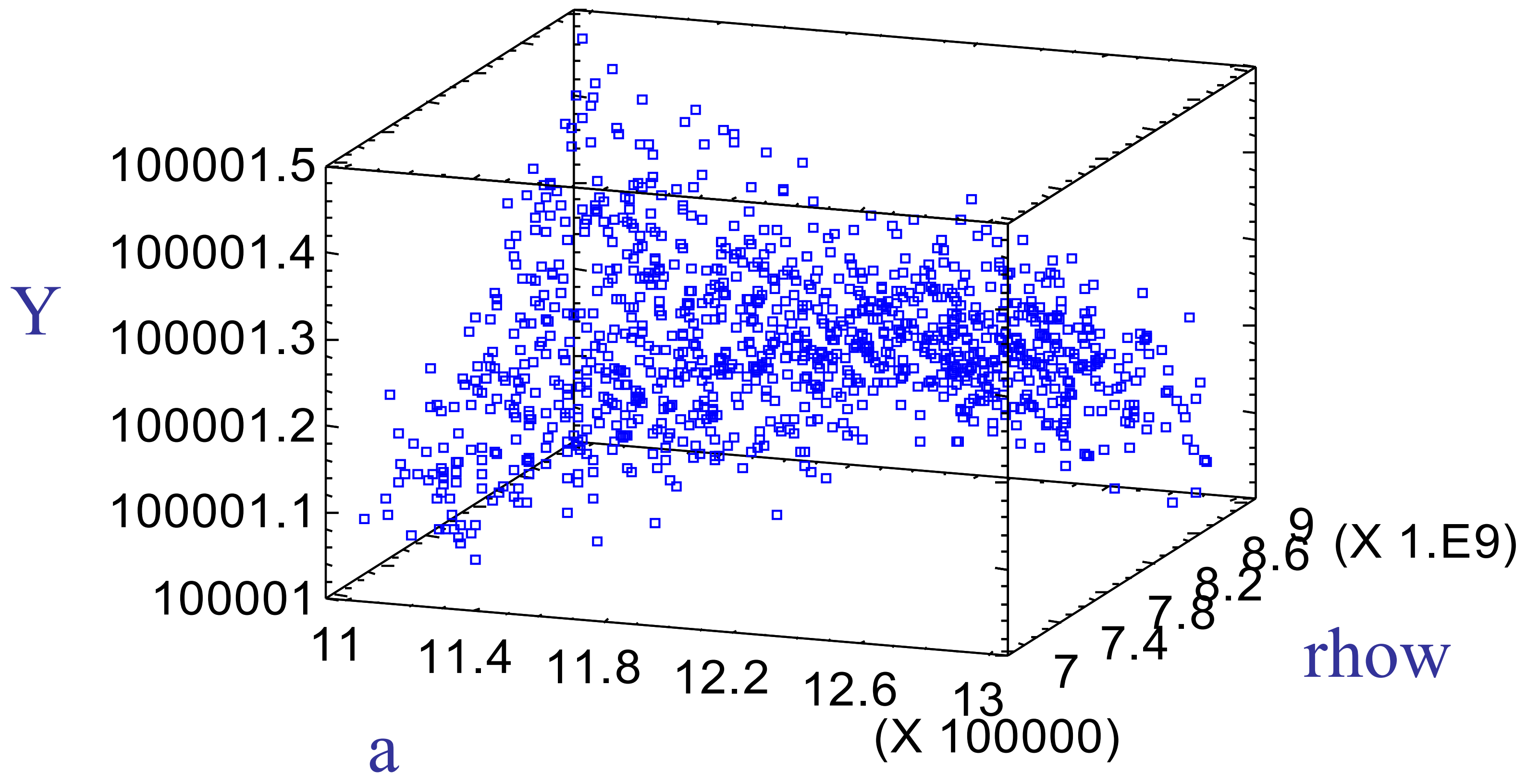
Mass calibration – 3D

Effect of interaction *a,rhow*



Mass calibration (GUM S1)

Variable	PDF
X1 - mrc	N(100 000;0.05)
X2 - dmrc	N(1.234;0.02
X3 - a	U[1 100 000;1 300 000]
X4 - rhow	U[7 000 000 000;9 000 000 000]
X5 - rhor	U[7 950 000 000;8 050 000 000]

Non linear model

$$Y = (mrc - dmrc)\left(1 + (a - 1200000)\left(\frac{1}{rhow} - \frac{1}{rhor}\right)\right)$$

SENSIBILITY INDICES						
Variable	LPU 1st order	LPU 2nd order	OAT GUM S1	Rank	Sobol Matlab	Sobol R
X1	0,862	0,445	0,860	0,862	0,439	0,439
X2	0,138	0,071	0,140	0,135	0,068	0,071
X3	0,000	0,000	0,000	0,003	0,000	0,003
X4	0,000	0,000	0,000	0,000	0,000	0,001
X5	0,000	0,000	0,000	0,000	0,000	0,000
Interaction X3-X4	-	0,483	-	-	0,489	0,485
Interaction X3-X5	-	0,001	-	-	0,004	0,001

Ishigami function

Variable	PDF
X1	U([-0.314;0.314])
X2	U([-0.314;0.314])
X3	U([-0.314;0.314])

Non monotonic function

$$Y = \sin(X_1) + 7(\sin(X_2))^2 + 0.1X_3^4 \sin(X_1)$$

SENSIBILITY INDICES					
Variable	LPU 1st order	OAT	Rank	Sobol - Matlab	Sobol - R
X1	1,000	0,448	1	0,445	0,442
X2	0,000	0,552	0	0,555	0,548
X3	0,000	0,000	0	0,000	0,000

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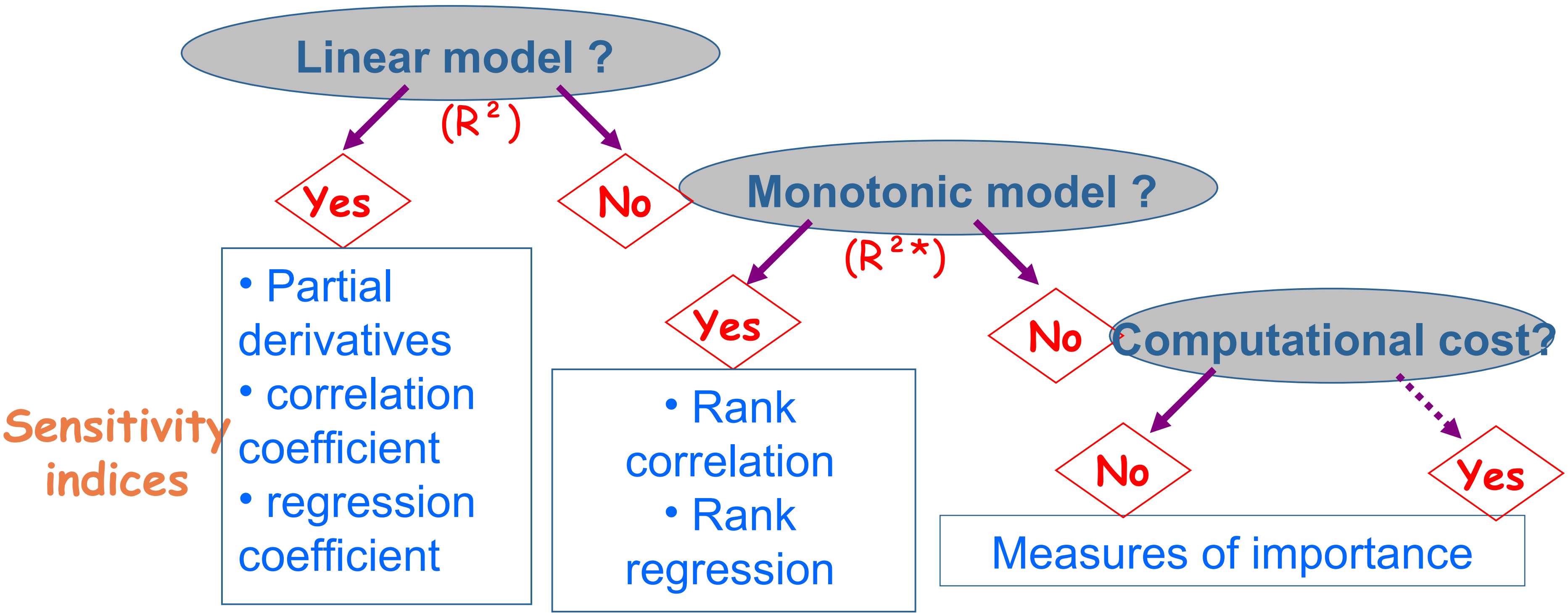
Discussion

- Estimators such as the SRC or based on partial derivatives are easy to implement and intuitive. However they have the limit of being as good as the regression on which they are based
- The rank version SRRC is also easy to implement (Crystal Ball..). Doesn’t provide interaction effect and need the assumption of monotonic model
- The computational execution time of the model is a major concern when using complex codes. OAT method implies *N* times more runs of MC simulations for each sensitivity coefficient to compute
- OAT and partial derivatives methods provide local sensitivity indices
- The Sobol’s theory offers the ideal theoretical background to the problem. It allows the computation of interaction effects simultaneously as the propagation of uncertainty

In conclusion

Decision tree for the choice of the appropriate framework to perform sensitivity analysis



We recommend

SA methods should be able to :

- ✓ deal with a model regardless of assumptions about model's linearity and additivity;
- ✓ consider effects of interaction among model input uncertainties
- ✓ evaluate the effect of a given input while all other inputs are allowed to vary as well

→ **Sobol indices**

Perspectives

- To adapt and compute the Sobol indices to applications that use complex codes

- Application of the Sobol indices for correlated quantities to some metrological examples

- Related topic:
  - ✓ To investigate the sensitivity of the output variable to the choice of the input variables pdfs

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Thank you for your attention