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This abstract is submitted for the "keynote PSE-session". This contribution provides a perspective on advanced sensitivity and uncertainty analysis and the important role they play in computer-aided process engineering from process understanding, to risk-based decision making for process synthesis and design and operation optimisation and control applications. Like other methods and tools in PSE toolbox, these methods aims to contribute to reliable and first-time right solution for novel and sustainable product-process development challenges.

Traditionally sensitivity analysis has relied on differential analysis of the model outputs with respect to inputs. For a model with a generic form of $y = f(\theta)$, the sensitivity of model outputs, y, to, model inputs, θ, is computed as:

$$s = \frac{\partial y}{\partial \theta} \text{ and } \delta^{msqr} = \frac{1}{n}\sqrt{\sum_{i}^{n}(s_i)^2}$$

As importance of input factors on the outputs, an absolute measure, e.g. mean squared value of sensitivity functions is typically used to rank the importance of the input on the output. This analysis is local and referred to as one-factor-at-a-time (OAT) approach, since the first order derivative is calculated at a given nominal value, making the results dependent on the selected nominal point.

Likewise uncertainty analysis of model outputs due to uncertainty in model inputs is traditionally also computed using a local method using linear error propagation. In this method, given the uncertainty in model inputs, characterised by a covariance matrix, *cov(*θ*)*, the resulting uncertainty of model outputs, *cov(y)*, is computed as follows:

$$\operatorname{cov}(y) \approx \left(\frac{\partial y}{\partial \theta}\right) \cdot \operatorname{cov}(\theta) \cdot \left(\frac{\partial y}{\partial \theta}\right)^T$$

Again the derivative needs to be evaluated at a given nominal point. The covariance matrix of model inputs can be estimated, if experimental data available, by using maximum likelihood theory (e.g. nonlinear least squares) method or Bayesian inference such as Markov Chain Monte Carlo sampling (MCMC) algorithms.

Advances in sensitivity and uncertainty analysis emphasize the importance of extending the analysis of model behaviour into a broader range of model input domain, as opposed to one point fixed in the input domain, as is the case in local methods. Hence the term global is commonly used to denote this class of methods. In these techniques, the sensitivity analysis is viewed as variance decomposition problem, while uncertainty analysis is viewed as the calculation of the variance of model outputs given an input uncertainty domain.

To carry out the global uncertainty and sensitivity analysis, first the uncertainty in model inputs needs to be characterised. In this representation, each element in the input is defined to follow a probability distribution function: $D_1, D_2, D_3, \ldots D_m$, where D_1 is associated with distribution of θ_1 and m is the total number of elements in the model inputs. Jointly these representations define an input probability domain, Ω, for the uncertainty analysis. Uncertainty analysis is then concerned with calculation of multidimensional integrals which provides inferential statistics such as mean and variance of the model outputs:

$$E(y) = \int_{\Omega} f(\theta)\, d\theta = \int f(\theta_1 \ldots \theta_m)\, d^m\theta \text{ and } \mathrm{var}(y) = \int_{\Omega} \left(E(y) - f(\theta)\right)^2 d\theta$$

To compute these multi-dimensional integrals, Monte Carlo technique is most commonly used, which employs sampling based techniques to evaluate the integrals.

Once the variance of the model outputs is computed in uncertainty analysis step, the sensitivity analysis is performed by decomposing the output variance with respect to the inputs. Global sensitivity analysis methods perform this variance decomposition by means of meta-models. The simplest form of a meta-model is a linear regression model, which describes the model outputs as a linear function of model inputs:

$$y_{meta} = b_0 + \sum_{j=1}^{M} b_j \theta_j + \varepsilon$$

Assuming this linear model describes sufficiently the model outputs (at least with a model determination coefficient,R^2, of 0.7), the linear coefficient of this model indicates the importance of input parameters. A sensitivity measure, β, is defined as the ratio of contribution of variance from each input to the total variance of the output:

$$\beta_j^2 = \frac{\mathrm{var}_{\theta j}}{\mathrm{var}(y)} \quad \textit{where}\ \mathrm{var}_{\theta j} = \left(b_j \sigma_{\theta j}\right)^2$$

This sensitivity measure is also called standardised regression coefficient and can take a value from [-1 1] and used to rank the importance of model inputs. Other global sensitivity analysis methods includes variance decomposition using higher dimensional metamodels (such as Sobol's index), Morris screening among others.

In this contribution a generic framework for advanced uncertainty and sensitivity analysis in computer-aided process engineering is presented. The framework provides a structured and systematic use of global as well as local uncertainty and sensitivity analysis methods for many product-process development problems. The framework includes the following tasks: (i) manage knowledge, data, models, associated methods, algorithms, tools integrated with work-flows/data-flows for specific product-process design problems, and (ii) manage uncertainties (of data, parameters, models, and their predictions) and their impact on decision-making related to specific product-process design problems.

The sensitivity and uncertainty analysis framework is highlighted on a various applications related to different product-process development challenges: (i) process understanding which enables factors prioritisation and focusing of experimental efforts, (ii) model development and discrimination, (iii) process design and (iv) synthesis/design processing network.

In summary one can conclude that advances in sensitivity and uncertainty analysis brought a wealth of methods that contribute to early stage of product and process development by providing better process understanding, focused experimental efforts, generation of many ideas and alternatives for improving process development under uncertainties among others. This complements and facilitates better engineering decisions under various uncertainties in data and models and the tools employed in the computer-aided process engineering paradigm.

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