Abstract

Mathematical models are versatile tools to gain valuable insights into dynamic complex processes of real-world phenomena. Dynamic systems are generally modelled as a set of algebraic and differential equations involving a set of input parameters or variables that are not precisely known, but may vary within some ranges. This stochastic nature of the parameters leads to variability in the model outcome as well. Thus, in order to obtain realistic predictions from the formulated model, such parameters must be selected precisely. This may pose computational challenges in case of high dimensional complex mathematical models involving a large number of uncertain parameters. This thesis addresses an important and challenging task of parameter estimation using a combined framework of uncertainty quantification (UQ) and sensitivity analysis (SA). UQ refers to the process of estimating uncertainty riddled in the model outcome. The SA aims to provide the ranking of the input parameters in the order of their influence on the model response. The main findings of this thesis are summarized in the following paragraphs.

In **Chapter 1**, we give motivation of the thesis explaining the problem of parameter estimation in mathematical models. A detailed literature review on UQ methods is given along with some existing techniques to carry out sensitivity analysis.

In **Chapter 2**, we present a systematic methodology based on UQ and SA for precise estimation of uncertain parameters in a dynamic mathematical model. This strategy involves nonintrusive polynomial chaos expansion (PCE) method and the Sobol' sensitivity indices to quantify uncertainties in the model outcomes due to parameter uncertainties. In addition, the Monte Carlo (MC) method is used to investigate the accuracy of the PCE method for uncertainty quantification. Three case studies using the crystallization population balance models for L-asparagine monohydrate and pyrazinamide are used to demonstrate the effectiveness of the proposed methodology.

In **Chapter 3**, we investigate the sigma point method for uncertainty quantification and proposes a three-step process for computation of Sobol' sensitivity indices using the sigma point method. The proposed sensitivity analysis approach is implemented on several case studies, including a PBM for a sonocrystallization process. The sigma point-based sensitivity results are compared with that of the PCE method. Additionally, the MC simulations are employed to compare the accuracy levels of the two methods in estimating mean and standard deviations of the stochastic function.

In **Chapter 4**, we present a modified perturbance moments (PM) method that achieves a significantly higher degree of accuracy in estimating the statistical moments of a stochastic function as compared to the existing PM method, while maintaining the same computational expense. An investigation is conducted based on computing the error produced by both methods in approximating the mean of the response function. Our findings reveal that the existing PM method may lead to errors, even when dealing with linear stochastic problems. In contrast, our proposed PM method constitutes at least a third-order approximation technique that gives accurate estimation of the exact response mean for polynomials up to degree three. A numerical comparison between the two methods clearly demonstrates the superiority of the proposed PM method over the existing one.

In **Chapter 5**, we present a comparative error analysis of several point estimation methods (PEMs) in estimating the statistical moments of a stochastic function. The error produced by these methods in estimating the first moment (mean) of the response function are computed and then the order of approximation of these methods are obtained. Different cases of correlated and independent random variables having symmetric or skewed distributions are studied. Further, a detailed numerical comparison is carried out in estimating the first four moments of a stochastic function using several case studies used in engineering applications. The accuracy of the methods is investigated for different nonlinearity of the stochastic system with varying magnitude of input uncertainties. This comparison provides a clear understanding of the methods for the selection of the most appropriate method that gives least error and requires minimum computational effort in handling correlated/random variables having symmetric/skewed distributions.

In **Chapter 6**, we give some concluding remarks and future scope for improvements in the existing UQ methods and also some ideas for the establishment of new UQ methods.

Keywords: Computational efficiency, Error in mean approximation, Modified perturbance moments method, Monte Carlo simulations, Parameter estimation, Polynomial chaos expansion, Sensitivity analysis, Uncertainty quantification.

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