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Systematic Parameter Selection for Optimization under Uncertainty

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Abstract

Considering uncertainty is crucial for the decision making process in chemical engineering. However, when working in optimization under uncertainty a systematic selection of relevant uncertain parameters is required. In this contribution, an algorithm is presented in which uncertain parameters are selected based on their linear-independence to one another, their sensitivity towards state variables, and their sensitivity towards a user-defined process objective function. This workflow is applied in a case study. To analyze the information loss due to the reduction of uncertain parameters, Monte Carlo simulations are performed.

Keywords: Uncertainty, Parameter Estimation, Optimization, Monte Carlo Simulation

1. Introduction

Consideration of uncertainties is generally vital for making decisions in various disciplines. This is especially the case in optimization of chemical processes. A negligence of uncertainties or a faulty introduction of uncertainties into an optimization problem may lead to unrealistic and possibly devastating results when implemented into an actual chemical plant (Binder, 2012). Furthermore, independent of how uncertainties are introduced into the optimization problem, it is known that with a higher number of uncertain parameters, the computational complexity for solving the optimization problem increases (Dyer et al., 2006). This is especially the case for strategies such as chance constrained optimization under uncertainty (Wendt et al., 2002). Adding to this, badly estimated uncertainty can add behavior to the system, which is unrealistic. Therefore, the question arises if it is possible to assist engineers in selecting the most relevant uncertain parameters for optimization under uncertainty.

In optimization under uncertainty it is often assumed that the required uncertainties of various parameters are available. This, however, is not always the case. Furthermore, a selection of the relevant uncertain parameters is often performed with the best knowledge of the process engineer. Whilst this is an acceptable method for small systems with a limited number of uncertain parameters, for larger systems on the other hand, this becomes questionable.

In this contribution a method is presented, in which strategies from parameter estimation are combined with ideas from optimization under uncertainty in order to tackle the problem discussed above. The presented method herein aims towards quantifying uncertain parameters in terms of expected values and

variances followed by a ranking of their relevance regarding the process model equations and the user-defined process objective function.

2. Workflow for Uncertain Parameter Selection

In Fig. 1 the entire workflow for the selection of uncertain parameters is presented. Of course, all possible sources of uncertainties should be considered, but the focus herein is lain on identifying the most relevant uncertain parameters.

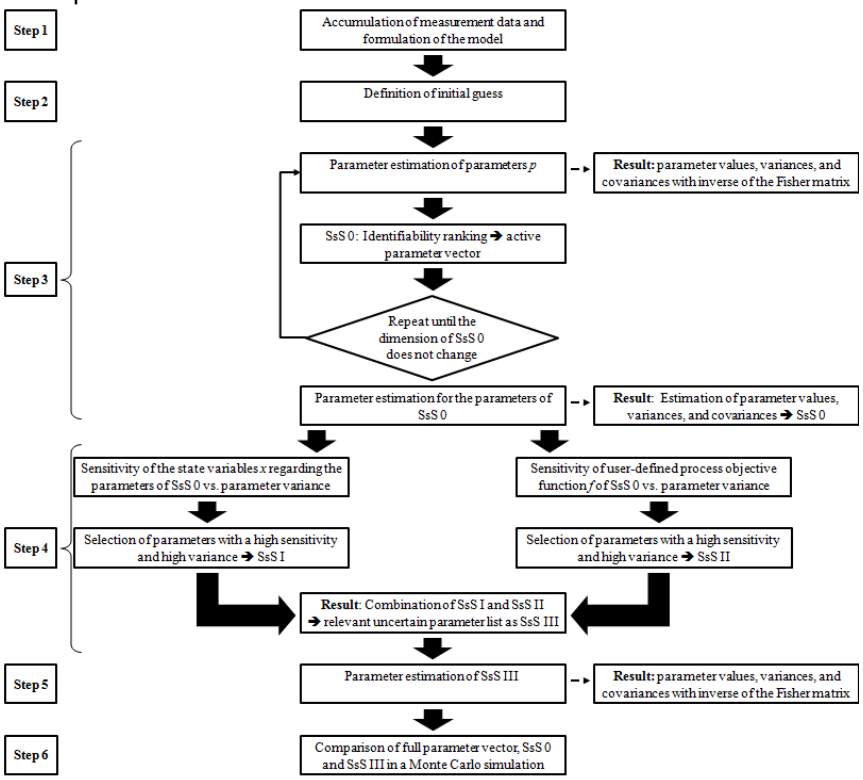

Figure 1. Parameter selection workflow for optimization under uncertainty.

Several approaches for parameter estimation exist, some of which are described in e.g. (Bard, 1974) and (Binder, 2012). The ideas to incorporate the linear independence and identifiability of parameters into the estimation process (Burth et al. 1999, Lopez et al. 2013) are exploitable for the purpose of this contribution and are shown in Fig. 1. Under the assumption of the availability of measurement data and a model with unknown or uncertain parameters, the algorithm can be started (Step 1). The initial guess for the uncertain parameters p has to be specified (Step 2). This is followed by a loop of parameter determinations based on the selection of identifiable parameters (Step 3) as described in Lopez et al. (2013). After the first parameter estimation (minimization of the sum of least squares method), the sensitivity matrix S ($S= \partial y/\partial p$) is calculated for the measureable output variables y with respect to the estimated parameter values. The sensitivity matrix is analyzed according to the linear independence of its columns. Then, a subset of identifiable parameters

(active parameters) is selected. Thus, a reduced set of parameters is determined. The reduced parameter estimation performed only with the active parameters is then guaranteed to be well-conditioned. Parameter estimation and subset selection are repeated on the obtained subset, until the number of active parameter no longer changes. Estimated values and variances for the remaining, identifiable parameters are stored. The non-identifiable parameters are fixed at their estimated values. The aim of the algorithm (Fig. 1) is to select a sensible set of parameters for optimization under uncertainty. Therefore, the effect of each active parameter from step 3 on a user-defined process objective function *f* (Eq. 1) and the model state variables *x* should be analyzed in greater detail (Step 4). The process model is represented by *g* in Eq. 1. Therein, *u* is the set of control variables and *p* the set of both fixed and uncertain parameters. The standard deviation σ is derived from the results of the parameter estimation. For the non-active or fixed parameters σ is set to 0.

$$\min_{u} f(\dot{x}, x, u, p) \quad with\ p \sim N(\mu, \sigma)$$
$$\text{s.t. } g(\dot{x}, x, u, p) = 0 \tag{1}$$

The model equations *g* are differentiated with respect to *p* to derive expressions for the time derivative of *dx/dp*. These sensitivity equations are hence integrated simultaneously to the model equations. Thus, *dx/dp* is available for any point in time. The sensitivity of *f* with respect to *p* is also calculated as *df/dp*. This way, the gradient of the user-defined objective function with respect to the parameters can also be calculated. Those parameters, that have a large influence on the objective function, should be selected for optimization under uncertainty (subset SsS I). Furthermore, those parameters that greatly influence the state variables *x* of the system, should also be selected for optimization under uncertainty (subset SsS II). Here, all states *x* are considered, which is an extension to the first part of the algorithm, where only measurable state variables *y* were analyzed. These two subsets are combined (SsSI U SsS III) to form subset SsS III. A further parameter estimation with the remaining subset is carried out (Step 5). The results of the different subsets are compared in a Monte-Carlo simulation (Step 6), to see, if the information loss due to fixation of the parameters is high.

3. Case Study

To test the algorithm, a case study is investigated. A heated continuously stirred tank reactor (CSTR) with three reactions is presented in Fig. 2.

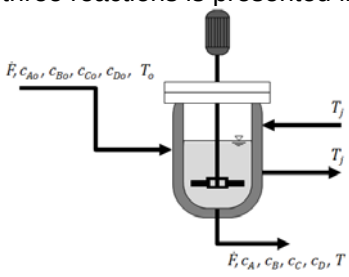

Figure 2. General scheme of the CSTR including all inputs and outputs.

In the first reaction, educt A reacts to product C: A ➔ C. In the second reaction B turns into A: B ➔ A. In the third reaction, C's isomer D is formed from A: A ➔ D. All reactions adhere to Arrhenius equation. The aim of this CSTR is to produce the product C. In general, the differential equations shown in Eq. 3 to 7 apply.

$$\frac{\partial c_A}{\partial t} = \frac{\dot{F}}{V} \cdot (c_{Ao} - c_A) - k_{1o} \cdot c_A \cdot e^{-\frac{E_1}{R \cdot T}} + k_{2o} \cdot c_B \cdot e^{-\frac{E_2}{R \cdot T}} - k_{3o} \cdot c_A \cdot e^{-\frac{E_3}{R \cdot T}} \tag{3}$$

$$\frac{\partial c_B}{\partial t} = \frac{\dot{F}}{V} \cdot (c_{Bo} - c_B) - k_{2o} \cdot c_B \cdot e^{-\frac{E_2}{R \cdot T}} \tag{4}$$

$$\frac{\partial c_C}{\partial t} = \frac{\dot{F}}{V} \cdot (c_{Co} - c_C) + k_{1o} \cdot c_C \cdot e^{-\frac{E_1}{R \cdot T}} \tag{5}$$

$$\frac{\partial c_D}{\partial t} = \frac{\dot{F}}{V} \cdot (c_{Do} - c_D) + k_{3o} \cdot c_C \cdot e^{-\frac{E_3}{R \cdot T}} \tag{6}$$

$$\begin{aligned} \frac{\partial T}{\partial t} = \frac{\dot{F}}{V} \cdot (T_o - T) + \frac{U \cdot A}{\rho \cdot c_p \cdot V} + \frac{-\Delta h_1}{\rho \cdot c_p} \cdot k_{1o} \cdot c_A \cdot e^{-\frac{E_1}{R \cdot T}} \\ + \frac{-\Delta h_2}{\rho \cdot c_p} \cdot k_{2o} \cdot c_B \cdot e^{-\frac{E_2}{R \cdot T}} + \frac{-\Delta h_3}{\rho \cdot c_p} \cdot k_{3o} \cdot c_A \cdot e^{-\frac{E_3}{R \cdot T}} \end{aligned} \tag{7}$$

In this system, nine unknown parameters exist. The algorithm is used to select the most relevant of these: the activation energies of the three reactions, E_1, E_2, E_3, the pre-exponential factors of the three reactions, k_{1o}, k_{2o}, k_{3o}, the heat transfer coefficient $U \cdot A$, the specific heat c_p, and the average density ρ. In order to model the system, it is assumed that the volume of the reactor (V = 1m³), the mass flow into the reactor ($\dot{F}$ = 6.5·10^{-4} m³/s), and the heat of each reaction (Δh_1 = 45·10^{-4} J/mol, Δh_2 = -55·10^{-4} J/mol, Δh_3 = 45·10^{-4} J/mol) is constant. Furthermore, the reaction is performed for one hour (3600s), whereby a sample is taken every 20 minutes. In this case study, it is only possible to measure the concentrations of components A and B as well as the temperature T.

3.1. Parameter Identification and Subset Selection

Step 1 of the algorithm is modeling the system and gathering data. The model of the system is shown above, therefore measurements are still required. In order to obtain these, experiments are simulated. The controls u are the input values c_{Ao}, c_{Bo}, T_0, and the jacket temperature T_j. Since four input variables are used, 16 + 1 experiments are performed. For this purpose, the following ranges of the inputs are applied: c_{Ao} 5 to 10 mol/m³, c_{Bo} 10 to 14 mol/m³, and T_0 and T_j 273 to 373 K, thus creating an experiment "hypercube" (full factorial design with mean-value experiment). For the parameters, the real parameter values shown in Tab. 1 are implemented. The measureable variables c_A, c_B, and T are subject to random normal noise with a standard deviation $\sigma_{A/B}$ of 0.5 for the two concentrations and σ_T of 1 for the temperature. Thus, measurement errors are simulated. The process is very sensitive to temperature and concentration changes.

Table 1. True and initial kinetic parameter values.

	E_1 [J/(molK)]	E_2 [J/(molK)]	E_3 [J/(molK)]	k_{1o} [1/s]	k_{2o} [1/s]	k_{3o} [1/s]
True	$69 \cdot 10^3$	$72 \cdot 10^3$	$69 \cdot 10^3$	$5.0 \cdot 10^6$	$1.0 \cdot 10^7$	$5.0 \cdot 10^5$
Initial	$42 \cdot 10^3$	$115 \cdot 10^3$	$42 \cdot 10^3$	$3.0 \cdot 10^6$	$2.0 \cdot 10^7$	$3.0 \cdot 10^5$

Table 2. True and initial values for other uncertain parameters.

	ρ [kg/m³]	c_p [J/(kg K)]	$U \cdot A$ [kW/K]
True	800	3.5	1.4
Initial	500	5.0	0.8

The aim now is to select the relevant uncertain parameters and quantify their uncertainty. In Step 2 initial values for the uncertain parameters are defined (Tab. 1 and Tab 2.). All initial guesses have an offset of more than 40% to their true values.

In Step 3, parameter estimation and subset selection strategies are used, to systematically reduce the number of parameters based on their identifiability (linear independence). The subset selection reduces the parameters from nine to four (SsS 0 = {E_1, E_2, E_3, k_{3o}}). In Fig. 3 measurement values of a randomly chosen experiment are compared to the initial guess and to the subset SsS 0 after the parameter estimation. It is apparent that the initial guess is strongly off target and the trajectory after the parameter estimation fits the experimental values quite nicely. For c_B the noise is larger than the actual change in the variable. Nevertheless, for optimization under uncertainty, a further reduction of the amount of parameters is required.

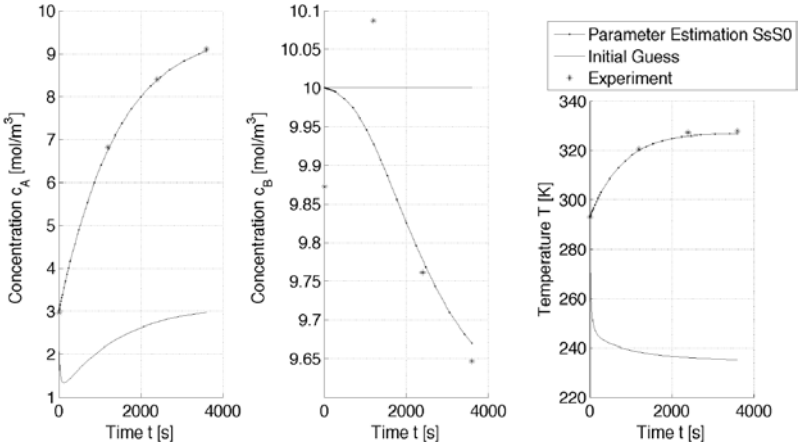

Figure 3. Comparison of measurements, initial guess, and SsS0 for experiment 11.

First of all in Step 4, the sensitivity of the user-defined objective function to the parameters is analyzed. A threshold of 10% of the sensitivity of the most sensitive parameter was used for the selection. In this example, three

parameters are seen as vital (SsS III = {E_1, E_2, E_3}). From an engineering point of view, the results are reasonable. The activation energies of reaction 1 (product producing reaction) and reaction 3 (byproduct producing reaction) have an exponential influence on the production of c_A. Analyzing the sensitivity of the state variables regarding the parameters also shows a reduction of the subset. Again, only the activation energies are selected. The combination of the two subsets leads to subset SsS III, which contains only E_1, E_2, and E_3.

3.2. Monte Carlo Simulation

A Monte Carlo simulation with 200 simulations is applied to analyze the information loss due to the reduced number of parameters. In Fig. 4 the concentration for c_B is exemplarily analyzed in greater detail for one of the 17 experiments. It becomes apparent, that the first parameter estimation leads to unrealistic results of the state variables x, which are widely off-target regarding the experiments. At this point the parameter estimation is still ill-conditioned. Using the variances thereof in optimization under uncertainty would therefore also lead to unrealistic optimization results and could be devastating if implemented into an actual chemical plant. SsS 0 after Step 4 of the algorithm leads to better results. These lie closer to the actual experimental values. The further reduction of the subset slightly reduces the uncertainty, but still contains a large degree of information that is applicable for optimization under uncertainty. In Fig. 4 (c) the last measurement point is not in the Monte Carlo set. A reason for this could be that the measurement is a stochastic outlier or the applied threshold for the final subset selection is too high. Improvements on the later are currently under research.

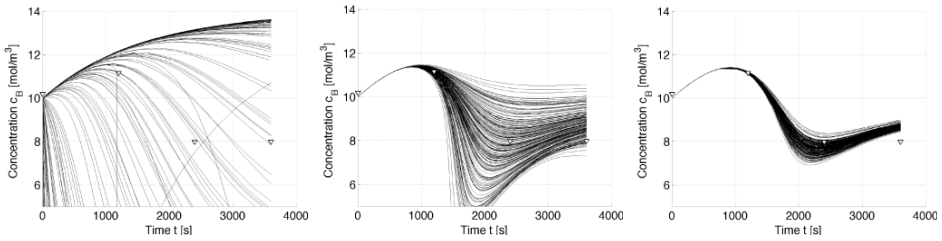

Figure 4. Monte Carlo simulation for the first parameter estimation with all parameters (a), with SsS 0 (b), and with SsS III (c) (from left to right) for experiment 7.

4. Conclusions

In this contribution an algorithm is shown, in which parameters based on their identifiability and their relevance regarding the model state variables and a user-defined process objective function are selected for optimization under uncertainty. The algorithm was successfully applied to a case study. In future investigations, systems will be analyzed, in which the model structurally differs from the experimental data. Adding to this, the influence of the thresholds will be investigated. Furthermore, this algorithm will be tested on larger models of whole chemical plants. Using the determined uncertain parameters, optimization under uncertainty of the models of these the chemical plants will be carried out.

Acknowledgments

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