Computers and Chemical Engineering 71 (2014) 94–103

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

An algorithm for the identification and estimation of relevant parameters for optimization under uncertainty

David Müller[*,1], Erik Esche[1], Diana C. López C., Günter Wozny

Technische Universität Berlin, School of Process Sciences, Department of Process Dynamics and Operation, Sekr. KWT-9, Straße des 17. Juni 135, D-10623 Berlin, Germany[2]

ARTICLE INFO

Article history:
Received 23 January 2014
Received in revised form 8 July 2014
Accepted 14 July 2014
Available online 21 July 2014

Keywords:
Optimization under uncertainty
Parameter estimation
Identifiable parameter subset selection
Monte Carlo simulation

ABSTRACT

Models are prone to errors, often due to uncertain parameters. For optimization under uncertainty, the larger the amount of uncertain parameters, the higher the computational effort and the possibility of obtaining unrealistic results. In this contribution it is assumed that not all uncertain parameters need to be regarded and focus should be laid on a subset. As a first step in the algorithm, a parameter estimation is carried out to determine expected values, followed by a linear-dependency analysis and a ranking of the uncertain parameters. Parameters with a high linear-dependency are fixed, while others are left uncertain. This is followed by a subset selection regarding the sensitivity of the parameters toward the model and toward a user-defined objective function. Thus, only parameters with the largest sensitivities are selected as uncertain parameters and considered for optimization under uncertainty. A case study is presented in which the algorithm is applied.

© 2014 Elsevier Ltd. All rights reserved.

1. Introduction

In many disciplines, such as economics, biology, or chemical engineering, uncertainty plays a crucial role in the decision making process (Arellano-Garcia, 2006). On an industrial scale, uncertainty is often compensated with conservative measures such as worst case assumptions, over-estimation of operating parameters, over-design of equipment, or implementation of risk-values to minimize possible losses of profit. Often enough, mathematical models of systems are created to simulate or even optimize the system regarding an objective function. Currently, several approaches exist to incorporate the uncertainty of parameters into optimization studies, e.g. Arellano-Garcia (2006), Binder (2012), and Quaglia et al. (2013). In general, all of these approaches are computationally expensive, with the computation time drastically increasing with the number of uncertain parameters (Dyer and Stougie, 2006). For strategies such as chance constrained optimization under uncertainty, this is a critical issue (Wendt et al., 2002). The basis of all uncertainty estimation is measurements and thereon based parameter estimation. Depending on the system the parameter estimation will distribute the measurement uncertainty on all estimated parameters of the system. Usually, identifiability or relevance of parameters for the application of the model is not considered. This can lead to the effect that poorly estimated parameters, in terms of large uncertainty, can add unrealistic behavior to the system. Therefore, it is obviously not sensible to implement the uncertainty for all uncertain parameters into the entire user-defined optimization problem. The goal of this contribution is to present an approach with which the relevant uncertain parameters can be ranked according to their uncertainty and identifiability. Hereby, a consideration of the sensitivity toward the objective function in optimization under uncertainty as well as the incorporation of the variance of the uncertain parameters is necessary as well as taking linear independence of the uncertainty of the parameters into account.

2. Status quo

Dealing with uncertainty in optimization has been a very prominent issue in the last years. Some approaches are scenario based optimization: Examples can be found in Mars and Hundt (2009), Dembo (1992), or Laird and Biegler (2008). More recently, Quaglia et al. (2013) have applied these approaches to enterpise-wide optimization problems. In these approaches different scenarios are optimized for different sets of parameter values. Other approaches are concerned with chance constrained optimization under uncertainty, also found in Arellano-Garcia (2006) or Li et al. (2008). Herein, probabilities are attached to certain inequality constraints,

* Corresponding author. Tel.: +49 03031421634.
E-mail addresses: david.mueller@tu-berlin.de (D. Müller), erik.esche@tu-berlin.de (E. Esche).
[1] David Müller and Erik Esche have contributed equally to this article and are both considered primary authors.
[2] www.dbta.tu-berlin.de.

http://dx.doi.org/10.1016/j.compchemeng.2014.07.007
0098-1354/© 2014 Elsevier Ltd. All rights reserved.

which do not need to be adhered to at all times. The expected value of the objective function is minimized. As a result, the stochastic optimization problem is turned into a deterministic one. For all these approaches, the different sources of uncertainty need to be identified. A classification of uncertainty can be found in Ierapetritou et al. (1996):

- model-inherent uncertainty such as kinetic constants or physical properties;
- process-inherent uncertainty such as plant data of flow rates, pressures, or temperatures;
- external uncertainty, mainly determined by external factors such as the demand-market for a product or feed availability and pricing; and
- discrete uncertainty such as equipment availability or other random discrete events.

In general, all these sources should be considered when working in the field of optimization under uncertainty. The fact remains though that the computational load increases exponentially with the number of uncertain parameters. At the same time, badly estimated uncertainties can lead to a wrong prediction of the behavior of the actual system at hand by causing fluctuations into areas where the true system cannot go. Therefore, the sources that are truly worth regarding should somehow be selected and an information condensation into a desirably small number of uncertain parameters is required. Several strategies exist to improve the quality of a parameter estimation result. In Binder (2012), different strategies for robust parameter estimation are discussed. These strategies can include gross-error in the basic measurement data sets, which least squares parameter estimation cannot handle. However, given the fact that the optimization problem using robust estimators is not twice continuously differentiable and non-standard solution algorithms have to be applied, these methods will be neglected here. In the contribution by Burth et al. (1999), subset selection for improved non-linear least squares parameter estimation is examined. Herein it is shown that a partitioning of the to be estimated parameters into well-conditioned and ill-conditions subsets followed by a fixation of the ill-conditioned parameters greatly enhances the quality of the estimated parameters and reduces unreliability of the results. Several other authors, such as Fink et al. (2007) or López C et al. (2013), have successfully implemented this approach for very different applications. Due to these successful implementations of subset selection methods in non-linear parameter estimation and the achieved initial reduction of uncertain parameters, this contribution extends subset selection as a means to identify relevant uncertain parameters for optimization.

3. Algorithm for the relevant uncertain parameter selection

In order to design an algorithm for the selection of the relevant uncertain parameters for optimization purposes, issues such as linear independence of parameters, identifiability, and sensitivity of the parameters regarding the outputs or a user-defined objective function regarding a specific process should be considered. Firstly, identifiability theory states that some models may not be completely identifiable. Hence, it is necessary to find a subset of parameters, on which it is at least partially identifiable. Using the whole set of parameters would lead to unnecessary noise in the parameter estimation. Badly estimated parameters may then add unrealistic behavior to the system. This again would distort the optimization result. In case the model is theoretically able to fully depict the real behavior of a process, this subset of identifiable parameters considering their variances should be able cover the entire area of the measurement data. In most cases, however, the subset will still contain additional information that is solely important for intermediate values in the model. With respect to optimization under uncertainty, only the behavior of certain outputs of the model with respect to a specific user-defined objective function is of importance. Hence, it should be possible to further reduce the subset of identifiable parameters to an even smaller set containing the most vital uncertain parameters, whose expected values and variances are then to be implemented into optimization under uncertainty, while all other parameters are fixed to their expected values. This of course demands the formulation of the user-defined objective function before tackling the parameter estimation and subset selection.

The general idea is to perform a pre-screening of the parameters regarding their identifiability. Methods from design of experiments, also described in Montgomery (2013) or Anderson and Whitcomb (2000), are known. Here, parameter fitting strategies, such as fixation and relaxation of parameters have been widely investigated. A simple example of a pair of non-identifiable parameters is the heat capacity C_p, which is usually the product of the specific heat, density, and volume:

$$C_p = c_p \cdot \rho \cdot V \tag{1}$$

Here, a separate identification of c_p and ρ will not be directly possible, as long as they do not appear separately in the model equations and sufficient measurement data is available to identify either of them. Strategies for the determination and ranking of linearly independent parameters can be found in López C et al. (2013), Velez-Reyes and Verghese (1995), Grah (2004), and Quaiser and Monnigmann (2009) and a focus on the sensitivities of identifiable parameters is made in Brun et al. (2002), Chu and Hahn (2009), Yao et al. (2003), Chandrakant and Bisaria (1998), and Weijers and Vanrolleghem (1997). The strategies implemented as part of this contribution will be discussed in the next section.

As a next step, the parameters are ranked according to their sensitivity regarding the state variables (including immeasurable ones) and according to their sensitivity regarding a user-defined objective function. The subsets of the two rankings are combined. These then are the relevant uncertain parameters. With respect do the desired reduction of the number of parameters, the worst case would be an outcome, in which the final subset selection contains all initially provided parameters. The general schematic of the algorithm is displayed in Fig. 1.

Before starting with the description of the algorithm, the following assumptions are made:

- A model of the system is available or has been discriminated.
- The model is either fully discretized or consists of a first order differential algebraic equation system.
- Measurement data have been produced and is available for various operation points or conditions.
- Variances for all measurement devices are available.

3.1. Subset selection I – identifiability and linear independence

The measurement data accumulation and model discrimination are the first step of the algorithm. From the model structure it is not obvious which parameter values can or should be fixed initially. The first step is followed by a definition of expected values, lower bounds, and upper bounds for all uncertain parameters. This step is based on heuristics. If the results of parameter estimation are not satisfactory, a relaxation of the bounds should be done.

Download English Version:

https://daneshyari.com/en/article/6595509

Download Persian Version:

https://daneshyari.com/article/6595509

Daneshyari.com