Computers and Chemical Engineering 52 (2013) 10–25

Contents lists available at SciVerse ScienceDirect

Computers and Chemical Engineering

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

Computing fuzzy trajectories for nonlinear dynamic systems

D. Andrei Măceş, Mark A. Stadtherr*

Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN 46556, USA

ARTICLE INFO

Article history:
Received 16 May 2012
Received in revised form
21 November 2012
Accepted 29 November 2012
Available online 22 December 2012

Keywords:
Uncertainty
Fuzzy sets
Fuzzy numbers
Nonlinear dynamic systems
Interval analysis
Dynamic simulation

ABSTRACT

One approach for representing uncertainty is the use of fuzzy sets or fuzzy numbers. A new approach is described for the solution of nonlinear dynamic systems with parameters and/or initial states that are uncertain and represented by fuzzy sets or fuzzy numbers. Unlike current methods, which address this problem through the use of sampling techniques and do not account rigorously for the effect of the uncertain quantities, the new approach is not based on sampling and provides mathematically and computationally rigorous results. This is achieved through the use of explicit analytic representations (Taylor models) of state variable bounds in terms of the uncertain quantities. Examples are given that demonstrate the use of this new approach and its computational performance.

1. Introduction

In the context of engineering and science, nonlinear dynamic models typically involve uncertain quantities. For example, in an initial value problem (IVP) described by a system of ordinary differential equations (ODEs), the initial conditions may be uncertain, and there may be uncertain parameters in the ODE model. Determining the effect of such uncertainties on the model outputs is clearly an important issue. To address this problem requires first that an appropriate representation of the uncertain quantities be chosen, and then that these be propagated through the nonlinear ODE model to determine the corresponding uncertainties in the model outputs.

There are a number of approaches that can be used to represent uncertainty. A common approach is to treat an uncertain quantity as a random variable described by some probability distribution. However, the true probability distribution may itself be uncertain. This gives rise to the concept of a probability distribution variable, as described by Li and Hyman (2004), which is typically characterized by a probability box (p-box) (Ferson, Ginzburg, & Akçakaya, 1996; Williamson & Downs, 1990) that provides bounds on the probability distribution function. However, many types of uncertainty arise from lack of knowledge, not from randomness, and so may not be appropriately represented through the use of probabilities. In this case, one simple approach is to treat an uncertain quantity as an interval. This requires only knowledge of an upper and lower bound on the uncertainty, and implies nothing about the distribution of the uncertainty. If there is more insight into the nature of the uncertainty, then it might be represented using a fuzzy set (Zadeh, 1965) or a fuzzy number (a particular type of fuzzy set) (Dubois & Prade, 1980; Hanss, 2005; Kaufmann & Gupta, 1985; Nahmias, 1977). Fuzzy sets can be viewed as representing *possibilities*, not probabilities, and form the basis for a theory of possibility (Zadeh, 1978) that is a counterpart to the traditional theory of probability. The relationships between possibilities and probabilities have been well explored (e.g., Dubois, Foulloy, Mauris, & Prade, 2004; Dubois & Prade, 1982; Gupta, 1993; Klir & Parviz, 1992), with a basis in Zadeh's (1978) possibility/probability consistency principle. This states that something must be possible before it can be probable. Thus, one simple interpretation of possibility is as an upper bound on probability. A fuzzy number can be interpreted as a nested set of intervals, with each successively smaller interval representing a range that is "more possible" than the larger one before it.

Hanss (2005) provides several examples of the use of fuzzy numbers to represent uncertainties in engineering problems involving linear and nonlinear ODE and PDE models. The formulation and solution of such "fuzzy-parameterized" models is a subdomain of fuzzy set theory that has received relatively little attention, with much more work having been focused on the use of fuzzy logic and reasoning methods. For example, just within the field of chemical engineering, there have been many applications of fuzzy logic and reasoning, in process control (e.g., Andujar & Bravo, 2005; Chen

* Corresponding author.
E-mail addresses: dmaces@nd.edu (D.A. Măceş), markst@nd.edu (M.A. Stadtherr).

0098-1354/$ – see front matter
http://dx.doi.org/10.1016/j.compchemeng.2012.11.008

& Chang, 2006; Chen, Chang, & Shieh, 2001; Gromov, Kafarov, & Matveikin, 1995; Kaucsár, Axente, Cosma, & Baldea, 2007; Sanjuan, Kandel, & Smith, 2006; Zhang, Ye, Chu, Zhuang, & Guo, 2006), safety and reliability analysis (e.g., Guimarães & Lapa, 2004; Hassana et al., 2009; Meel & Seider, 2006; Takeda, Shibata, Tsuge, & Matsuyama, 1994; Yong, Zheng, Zheng, Youxian, & Zheng, 2007; Yu & Lee, 1991), knowledge processing (e.g., Arva & Csukas, 1987; Claudel, Fonteix, Leclerc, & Lintz, 2003; Dohnal, Exall, Carsky, Morris, & Dohnalova, 1994; Gromov, Kafarov, & Matveikin, 1996; Hanratty & Joseph, 1992; Hanratty, Joseph, & Dudukovic, 1992; Johansen & Foss, 1997; Schmitz & Aldrich, 1998; Stephane & Marc, 2008; Tsekouras, Sarimveis, Raptis, & Bafas, 2002; Vrba, 1991), and other areas.

In this paper, we will focus on the use of fuzzy sets and fuzzy numbers to represent uncertainties in nonlinear dynamic models, and consider how to compute the resulting fuzzy trajectories in a verified way. For propagation of fuzzy uncertainties in dynamic models, a typical approach is to solve the underlying ODE problem multiple times using prescribed and/or arbitrary samples of the uncertainty quantities. For example, this is the basis of the "transformation method" of Hanss (2002, 2005). In general, however, this approach is not rigorous and may underestimate the true effect of an uncertain quantity on the model outputs, as discussed in more detail below. We will describe here a much different strategy for the propagation of fuzzy uncertainties in dynamic models. This approach is not based on sampling, and provides mathematically and computationally rigorous results in all cases. Our method is based on the use of techniques (Lin & Stadtherr, 2007) developed for the verified solution of parametric ODE systems. These techniques provide explicit analytic representations (Taylor models) of the state variables, from which rigorous interval bounds on the state variables can be obtained. We explore here how to extend these techniques to provide rigorous fuzzy set bounds on the state variables in fuzzy-parameterized, nonlinear dynamic models.

The remainder of this paper is structured as follows: In the next section we will provide a concise formulation of the problem to be solved. In Section 3, we will provide background on some of the concepts and methods that we will utilize. This includes background on interval analysis, fuzzy sets and numbers, fuzzy arithmetic, and Taylor models. Then, in Section 4 we will describe our new approach for the rigorous solution of fuzzy-parameterized, nonlinear dynamic models, with examples and results given in Section 5. Finally in Section 6 we will provide concluding remarks about this work.

2. Problem statement

We will consider nonlinear dynamic systems described by IVPs of the form

$$\frac{\mathrm{d}\boldsymbol{y}}{\mathrm{d}t} = \boldsymbol{f}(\boldsymbol{y}, \boldsymbol{\theta}), \qquad \boldsymbol{y}(t_0) = \boldsymbol{y}_0, \quad t \in [t_0, t_m]. \tag{1}$$

Here the n state variables are represented by the state vector $\boldsymbol{y}$ and have initial values $\boldsymbol{y}_0$. There are p time-invariant parameters represented by the parameter vector $\boldsymbol{\theta}$. The parameters and initial values are uncertain and bounded by the intervals $\boldsymbol{\Theta}$ and $\boldsymbol{Y}_0$, respectively. That is,

$$\boldsymbol{\theta} \in \boldsymbol{\Theta}, \qquad \boldsymbol{y}_0 \in \boldsymbol{Y}_0. \tag{2}$$

Additional information about the uncertainties is available in the form of fuzzy numbers or, more generally, in the form of fuzzy sets. That is, for a parameter $\theta_i \in \Theta_i$, the interval Θ_i supports a fuzzy set denoted by $\tilde{\Theta}_i$, $i = 1, \ldots, p$, and we define the fuzzy parameter vector $\tilde{\boldsymbol{\Theta}} = (\tilde{\Theta}_1, \ldots, \tilde{\Theta}_p)^{\mathrm{T}}$. Similarly, for an initial value $y_{0,i} \in Y_{0,i}$, the interval $Y_{0,i}$ supports a fuzzy set $\tilde{Y}_{0,i}$, $i = 1, \ldots, n$, and we define the fuzzy initial state vector $\tilde{\boldsymbol{Y}}_0 = (\tilde{Y}_{0,1}, \ldots, \tilde{Y}_{0,n})^{\mathrm{T}}$. In these terms, the uncertainties can now be described by

$$\boldsymbol{\theta} \in \tilde{\boldsymbol{\Theta}}, \qquad \boldsymbol{y}_0 \in \tilde{\boldsymbol{Y}}_0. \tag{3}$$

Fuzzy sets and numbers will be described in more detail in Section 3.2. Our goal is to rigorously propagate these uncertainties, thus computing fuzzy sets $\tilde{Y}_i(t)$, $i = 1, \ldots, n$, that characterize the uncertainty in the state trajectories $y_i(t)$, $i = 1, \ldots, n$. That is, we seek to determine the fuzzy state vector $\tilde{\boldsymbol{Y}}(t) = (\tilde{Y}_1(t), \ldots, \tilde{Y}_n(t))^{\mathrm{T}}$.

We assume that $\boldsymbol{f}$ is representable by a finite number of standard functions, and that it is sufficiently differentiable for the verified ODE solver used (see Section 4.1). We also note that if the ODE model is nonautonomous, or involves parameters with time dependence of a known form, then such a model can easily be converted into the form of Eq. (1).

3. Background

3.1. Interval analysis

A real (closed) interval $X = [\underline{X}, \overline{X}]$ can be defined as the set $X = \{x \in \mathbb{R} \mid \underline{X} \le x \le \overline{X}\}$. Here an underline is used to indicate the lower bound of an interval and an overline is used to indicate the upper bound. The width of an interval is $w(X) = \overline{X} - \underline{X}$. A real interval vector $\boldsymbol{X} = (X_1, \ldots, X_n)^{\mathrm{T}}$ has n real interval components and can be interpreted geometrically as an n-dimensional rectangle. Basic arithmetic operations with intervals X and Y are defined by $X \circ Y = \{x \circ y \mid x \in X, y \in Y\}$, $\circ \in \{+, -, \times, \div\}$, with division in the case of $0 \in Y$ allowed only in extensions of interval arithmetic (Hansen & Walster, 2004). Interval versions of the elementary functions are similarly defined. The endpoints of an interval are computed with a directed (outward) rounding; that is, the lower bound is rounded down and the upper bound is rounded up. Thus, interval operations are guaranteed to produce bounds that are rigorous both mathematically and computationally. A number of good introductions to interval analysis and computing with intervals are available (Hansen & Walster, 2004; Jaulin, Kieffer, Didrit, & Walter, 2001; Kearfott, 1996; Moore, Kearfott, & Cloud, 2009; Neumaier, 1990).

For a real function $f(\boldsymbol{x})$ with interval-valued variables $\boldsymbol{x} \in \boldsymbol{X}$, the interval extension $F(\boldsymbol{X})$ can be defined as a real interval that bounds the range of $f(\boldsymbol{x})$ for $\boldsymbol{x} \in \boldsymbol{X}$. One way to compute $F(\boldsymbol{X})$ is to substitute $\boldsymbol{X}$ into the expression for $f(\boldsymbol{x})$ and then to evaluate with interval arithmetic. However, the tightness of these bounds depends on the form of the expression used to evaluate $f(\boldsymbol{x})$. If this is a single-use expression, in which no variable appears more than once, then the exact function range will be obtained (within roundout). However, if any variable appears multiple times, then overestimation of the range may occur. This overestimation is due to the "dependency" problem of interval arithmetic. A variable may take on any value within its interval, but it must take on the *same* value each time it occurs in an expression. Unfortunately, this dependency is not detected when the interval extension is computed using standard interval arithmetic. For example, consider the case $f(x) = (1 - x)/(2 - x)$, with $x \in [0, 1]$. Using interval arithmetic gives $F([0, 1]) = (1 - [0, 1])/(2 - [0, 1]) = [0, 1]/[1, 2] = [0, 1]$. This correctly bounds, but significantly overestimates, the true function range of $[0, 1/2]$. Using a different expression for this function, $f(x) = 1/(x - 2) + 1$, which is now a single-use expression, and evaluating with interval arithmetic gives $F([0, 1]) = 1/([0, 1] - 2) + 1 = 1/[-2, -1] + 1 = [-1, -1/2] + 1 = [0, 1/2]$, the true function range. We could also obtain the true range by noting that, for $x \neq 2$, $f(x)$ is a monotonically decreasing function. Thus, $F([0, 1]) = [f(1), f(0)] = [0, 1/2]$. For more general cases,