

# Propagating Uncertainties in Modeling Nonlinear Dynamic Systems

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**Abstract.** Engineering analysis and design problems, either static or dynamic, frequently involve uncertain parameters and inputs. Propagating these uncertainties through a complex model to determine their effect on system states and outputs can be a challenging problem, especially for dynamic models. In this work, we demonstrate the use of Taylor model methods for propagating uncertainties through nonlinear ODE models. We concentrate on uncertainties whose distribution is not known precisely, but can be represented by a probability box (p-box), and show how to use p-boxes in the context of Taylor models. This allows us to obtain p-box representations of the uncertainties in the state variables and outputs of a nonlinear ODE model. Examples are used to demonstrate the potential of this approach for studying the effect of uncertainties with imprecise probability distributions.

**Keywords:** Ordinary differential equations, Interval analysis, Probability bounds analysis

## 1. Introduction

Ordinary differential equations (ODEs) are the basis for many mathematical models in the sciences and engineering. Often a system of ODEs is formulated as an initial value problem (IVP), in which the model is integrated through time beginning with specified initial values of the state variables. Especially in cases where no analytical solution exists, the numerical integration of these systems is necessary to obtain the trajectories of ODE systems.

Of particular interest here is the verified, or mathematically guaranteed, solution of systems of ODEs, especially such systems that involve uncertainty in initial conditions or model parameters. Traditional numerical methods, such as Euler's method or the Runge-Kutta schemes, only approx-

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imate the trajectory of an ODE system since truncation errors from both function approximation and machine arithmetic are present. Furthermore, if any particular parameter or initial state is uncertain, normal use of these methods will not fully guarantee that all possible trajectories are found.

In response to the need for guaranteed results, both with and without uncertainty, interval methods have been proposed. Computations with intervals, as opposed to real numbers, can provide mathematical and computational guarantees, and further, intervals are a logical way to deal with uncertainty in any parameters or initial conditions. An excellent review of interval methods for IVPs has been given by Nedialkov et al. (1999), and more recent work has been reviewed by Neher et al. (2007). Much work has been done for the case in which the initial values are given by intervals, and there are several available software packages that deal with this case, including AWA (Lohner, 1992), VNODE (Nedialkov et al., 2001), and COSY VI (Berz and Makino, 1998). These methods can also deal with interval-valued parameters, by treating them as additional state variables with derivative of zero. In the work described here, we will use a new validated IVP solver for parametric ODEs (Lin and Stadtherr, 2007b) called VSPODE (Validating Solver for Parametric ODEs), which is used to produce guaranteed bounds on the solutions of nonlinear dynamic systems with interval-valued initial states and parameters. VSPODE treats interval-valued parameters directly without the need to increase the number of state variables. Both COSY VI and VSPODE use Taylor models (Makino and Berz, 1996; Makino and Berz, 1999; Makino and Berz, 2003), but in different ways, to deal with the uncertain quantities (parameters and initial values).

Other methods exist to solve ODE systems with uncertainty, but they do not provide a mathematical guarantee that all possible trajectories are enclosed. These methods are often a combination of a Monte Carlo process with a standard integration scheme, such as Runge-Kutta. While such methods cannot guarantee that all solutions are enclosed, they can propagate uncertainty in ways that standard interval methods cannot. Interval methods do not use knowledge about the distribution of uncertainty in a variable or parameter, while such knowledge can be put to use in Monte Carlo methods to discern the most probable trajectory of an ODE system.

When the concepts of intervals and probability distributions are combined, the result has been called a probability distribution variable (PDV), and theorems and computations with this data type have been presented by Li and Hyman (2004). Intervals and “probability boxes” (p-boxes) can be viewed as specific enclosures of the more broadly defined PDV. If there are only upper and lower bounds on the uncertainties but no known probability distribution, then this can be represented by an interval. If there is some knowledge of the probability distribution, but it is uncertain, then this can be represented by a probability box (p-box). For computations with p-boxes, we use here the risk analysis software RAMAS Risk Calc (Ferson, 2002).

In this paper, we demonstrate the use of Taylor model methods for propagating uncertainties through nonlinear ODE models. We concentrate here on uncertainties represented by p-boxes, and show how to use p-boxes in the context of Taylor models. This allows us to obtain p-box representations of the uncertainties in the state variables. Examples are used to demonstrate the potential of this approach for studying the effect of uncertainties with imprecise probability distributions.

This paper is divided as follows. The next section will provide a general statement of the problem to be addressed. Section 3 gives background on interval analysis, Taylor models, and p-boxes. In

Section 4 we outline the specific method that is used, and in Section 5 we show the results of applying this method to some specific examples.

## 2. Problem Statement

Here we introduce the notation used in the paper as we describe the problems to be solved. We will consider the verified solution of the parametric autonomous IVP

$$y'(t) = f(y, \theta), \quad y(t_0) = y_0 \in Y_0, \quad \theta \in \Theta, \quad (1)$$

where  $t \in [t_0, t_m]$  for some  $t_m > t_0$ . Here  $y$  is the  $n$ -dimensional vector of state variables with initial value  $y_0$ , and  $\theta$  is a  $p$ -dimensional vector of *time-invariant* parameters. The vectors  $Y_0$  and  $\Theta$  are intervals that enclose uncertainties in the initial states and parameters, respectively. Additional information about these uncertainties is available in the form of p-boxes, as described in the next section, for at least one component of  $Y_0$  or  $\Theta$ . We assume that  $f$  maps the variable and parameter space back to the variable space and that  $f$  is  $(k - 1)$  times continuously differentiable with respect to  $y$  and  $(q + 1)$  times continuously differentiable with respect to  $\theta$ . Here  $k$  is the order of the truncation error in the interval Taylor series (ITS) method used by VSPODE, and  $q$  is the order of the Taylor model in VSPODE used to represent dependence on parameters and initial values. We also assume that  $f$  can be represented by a finite number of standard functions. Our goal is to obtain a guaranteed enclosure of the state variables  $y$  at time  $t_m$  and a probability distribution, in the form of a p-box, for the values of  $y$  within the enclosure.

## 3. Background

### 3.1. INTERVAL ANALYSIS

A real interval  $X$  is the set of real numbers between and inclusive of its lower bound (denoted  $\underline{X}$ ) and upper bound (denoted  $\overline{X}$ ). The width of an interval, denoted  $w(X)$ , is equal to  $\overline{X} - \underline{X}$ , while the midpoint  $m(X)$  is  $(\overline{X} + \underline{X})/2$ . A real interval vector  $X = (X_1, X_2, \dots, X_n)^T$  has  $n$  real interval components and can be interpreted as an  $n$ -dimensional rectangle or box. Interval matrices are similarly defined.

Basic arithmetic operations are defined on intervals according to

$$X \text{ op } Y = \{x \text{ op } y \mid x \in X, y \in Y\}, \quad \text{op} \in \{+, -, \times, \div\}. \quad (2)$$

Division in the case of  $Y$  containing zero is only allowed in extensions of interval arithmetic (Hansen and Walster, 2004). Addition and multiplication are commutative and associative but only subdistributive. Interval versions of the elementary functions can also be defined.

For a real function  $f(x)$ , the interval extension  $F(X)$  encloses the range of  $f(x)$  for  $x \in X$ . When  $f(x)$  can be written as a series of arithmetic operations and elementary functions, the natural interval extension is obtained by substituting the given interval  $X$  into  $f(x)$  and evaluating using

interval arithmetic. Computing the interval extension in this way often results in overestimation of the function range due to the “dependency” problem. While a variable may take on any value within its interval, it must take on the *same* value each time it occurs in an expression. However, this type of dependency is not recognized when the natural interval extension is computed. In effect, when the natural interval extension is used, the range computed for the function is the range that would occur if each instance of a particular variable was allowed to take on a different value in its interval range.

Another source of overestimation that may arise in the use of interval methods is the “wrapping” effect. This occurs when an interval is used to enclose (wrap) a set of results that is not an interval. If this overestimation is propagated from step to step in an integration procedure for ODEs, it can quickly lead to the loss of a meaningful enclosure.

Several good introductions to interval analysis, as well as interval arithmetic and other aspects of computing with intervals, are available (Hansen and Walster, 2004; Jaulin et al., 2001; Kearfott, 1996; Neumaier, 1990). Implementations of interval arithmetic and elementary functions are also readily available, and recent compilers from Sun Microsystems directly support interval arithmetic and an interval data type.

### 3.2. TAYLOR MODELS

Makino and Berz (1996) have described a remainder differential algebra (RDA) approach for bounding function ranges and control of the dependency problem of interval arithmetic (Makino and Berz, 1999). In this method, a function is represented using a model consisting of a Taylor polynomial and an interval remainder bound. Such a model is called a Taylor model.

One way of forming a Taylor model of a function is by using the Taylor theorem. Consider a real function  $f(x)$  that is  $(q + 1)$  times partially differentiable on  $X$  and let  $x_0 \in X$ . The Taylor theorem states that for each  $x \in X$ , there exists a real  $\zeta$  with  $0 < \zeta < 1$  such that

$$f(x) = p_f(x - x_0) + r_f(x - x_0, \zeta), \quad (3)$$

where  $p_f$  is a  $q$ -th order polynomial (truncated Taylor series) in  $(x - x_0)$ , and  $r_f$  is a remainder, which can be quantitatively bounded over  $0 < \zeta < 1$  and  $x \in X$  using interval arithmetic or other methods to obtain an interval remainder bound  $R_f$ . A  $q$ -th order Taylor model  $T_f = p_f + R_f$  for  $f(x)$  over  $X$  then consists of the polynomial  $p_f$  and the interval remainder bound  $R_f$  and is denoted by  $T_f = (p_f, R_f)$ . Note that  $f \in T_f$  for  $x \in X$ , and thus  $T_f$  encloses the range of  $f$  over  $X$ .

In practice, it is more useful to compute Taylor models of functions by performing Taylor model operations. Arithmetic operations with Taylor models can be done using the RDA operations described by Makino and Berz (1996; 1999; 2003), which include addition, multiplication, reciprocal, and intrinsic functions. Using these, it is possible to start with simple functions such as the constant function  $f(x) = k$ , for which  $T_f = (k, [0, 0])$ , and the identity function  $f(x_i) = x_i$ , for which  $T_f = (x_{i0} + (x_i - x_{i0}), [0, 0])$ , and then to compute Taylor models for very complicated functions. Therefore, it is possible to compute a Taylor model for any function representable in a computer environment by simple operator overloading through RDA operations. It has been shown that, compared to other rigorous bounding methods, the Taylor model often yields sharper bounds for modest to

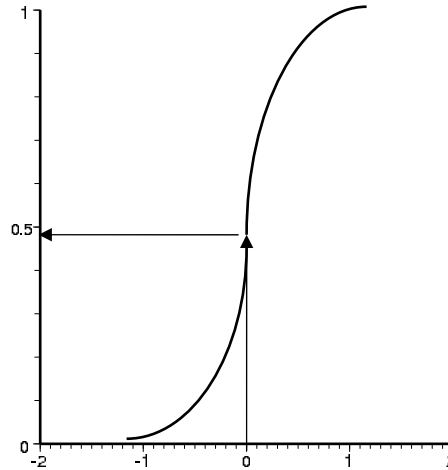


Figure 1. A cumulative probability density function is a one-to-one function where the value of a quantity  $x$  is on the abscissa and the corresponding cumulative probability is given by the ordinate. Here,  $P(x \leq 0) = 0.48$ .

complicated functional dependencies (Makino and Berz, 1996; Makino and Berz, 1999; Neumaier, 2003). A discussion of the uses and limitations of Taylor models has been given by Neumaier (2003).

### 3.3. P-BOXES

For some quantity (variable or parameter)  $x$ , the cumulative distribution function (CDF)  $F(z)$  gives the probability that  $x \leq z$ . A sample CDF is shown in Figure 1. Here, for example, the probability that  $x \leq 0$  is 0.48. Probability boxes, or p-boxes, are similar, but provide an interval of cumulative probability values represented by a pair of CDFs. A sample p-box is shown in Figure 2. This indicates, for example, that the probability of  $x \leq 0$  is  $[0.40, 0.59]$ . The slightly stepped appearance of the p-box curves, here and below, is due to the discretized representation of a p-box used by Risk Calc. This representation is used in the implementation of p-box arithmetic.

A probability box, then, is essentially a hybrid of an interval and a probability distribution. As an interval bounds a range of real numbers, a p-box bounds a range of probability distributions. Also, as a probability distribution gives a real-valued probability for the value of a real parameter, a p-box provides an interval-valued probability for the value of a real parameter (Ferson, 2002). Read in another way, for a real-valued probability, a p-box provides the interval of values corresponding to that probability. Formally, a p-box is a pair of functions  $(F, G)$  such that the true probability distribution  $H$  of a number satisfies  $F \geq H \geq G$ . The function  $F$  is called the left bound of the p-box, while the function  $G$  is the right bound, which should be apparent from the definition. For a given real-valued probability, the left bound provides the lower bound of the parameter, and the right bound corresponds to the upper bound. For a given value of a parameter, the left bound corresponds to the upper bound of its probability and the right bound to its lower bound.

When the probabilities of parameters are independent, computations with p-boxes are analogous to those with intervals. They are defined beginning with arithmetic and standard functions, again using Eq. (2). In this case, p-boxes encounter the same dependency issues that intervals do. However,

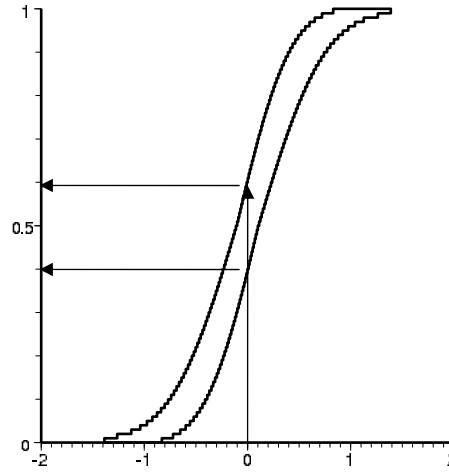


Figure 2. A p-box encloses the cumulative probability distribution function for a quantity  $x$ . Now the corresponding cumulative probability is an interval. Here,  $P(x \leq 0) = [0.4, 0.59]$ .

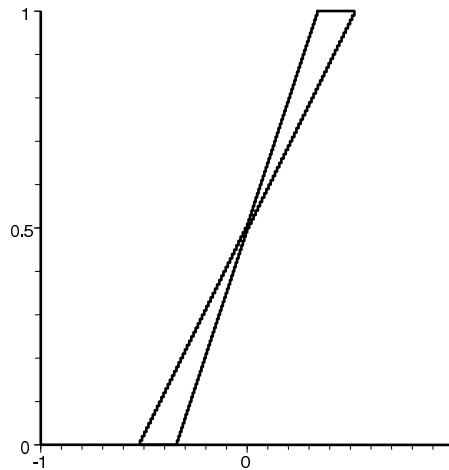


Figure 3. Sample p-box with bounds obtained from a uniform distribution with a mean of 0 and standard deviation in  $[0.2, 0.3]$ .

p-box arithmetic can vary depending on assumptions about the parameters; much more detail is provided by Ferson et. al. (2004).

There are three types of p-boxes employed in the examples used in Section 5. The first, as illustrated in Figure 3, is a p-box with bounds obtained from a uniform distribution with a fixed mean and an interval-valued standard deviation. Note that such a p-box encloses both uniform (straight line) and nonuniform CDFs. The second is a p-box with bounds obtained from a normal distribution, again with fixed mean and an interval-valued standard deviation, as shown in Figure 4. The third type of p-box used is shown in Figure 5 and corresponds to the case of an uncertain distribution with a specified minimum and maximum and fixed mean and standard deviation. This is referred to as the mmms distribution.

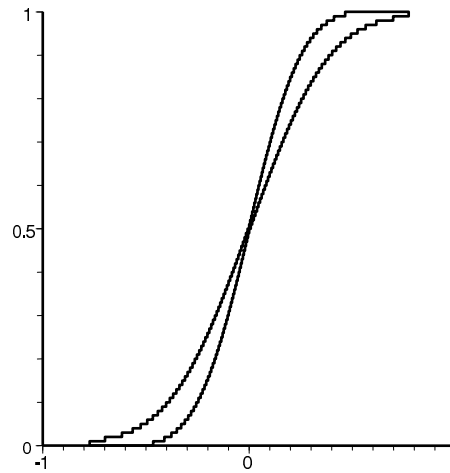


Figure 4. Sample p-box with bounds obtained from a normal distribution with a mean of 0 and standard deviation in  $[0.2, 0.3]$ .

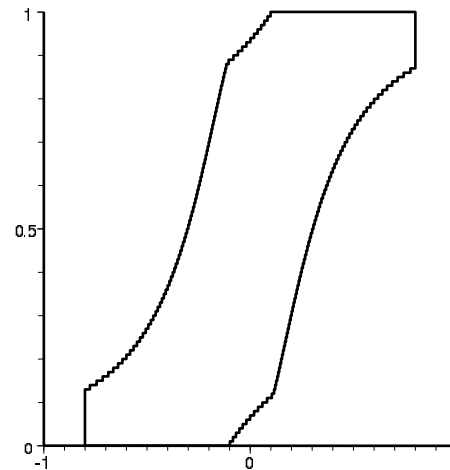


Figure 5. Sample p-box for mmms distribution. This p-box has a minimum of  $-0.8$ , maximum of  $0.8$ , mean of  $0$ , and standard deviation of  $0.3$ .

#### 4. Solution Procedure

In this section, we outline the method used for solving the problem described in Section 2. This involves using the VSPODE program for the verified integration of the IVP given by Eq. (1) and the RAMAS Risk Calc software for calculations with p-boxes. More detailed descriptions of the VSPODE program and RAMAS Risk Calc software can be found elsewhere (Lin and Stadtherr, 2007b; Ferson, 2002).

As a first step, VSPODE is used to integrate the IVP. This provides a guaranteed enclosure of the state variables at each time step in the integration and a Taylor model representation of the

final state  $y_m = y(t_m)$ . This Taylor model,  $T_{y_m} = T_{y_m}(y_0, \theta)$ , is a polynomial in  $y_0$  and  $\theta$  with an interval remainder bound, and is valid for all  $y_0 \in Y_0$  and  $\theta \in \Theta$ .

Then, in the second step, information about the distribution of  $y_0$  and  $\theta$  values is substituted into the Taylor model  $T_{y_m}$ , and the distribution of final state values is computed using Risk Calc. Each initial state and parameter is given by either an interval (no distribution known) or by a p-box, and Risk Calc can do the necessary arithmetic with either. To reduce the occurrence of overestimation in these calculations, Risk Calc can employ a subinterval reconstitution (SIR) procedure. These methods are described in more detail by Ferson and Hajagos (2004).

## 5. Examples

The following examples illustrate the solution procedure when applied to a model from population ecology and to three reactor modeling problems from chemical engineering. On all of the example problems, the order of the interval Taylor series used in VSPODE was  $k = 17$ , and the order of the Taylor models used was  $q = 5$ . Unless specified otherwise, a constant step size of 0.2 was used in VSPODE, though this step size may be automatically reduced during the integration procedure if needed.

### 5.1. LOTKA-VOLTERRA MODEL

One of the most basic population ecology models is the Lotka-Volterra model of a predator-prey system. The model equations, with parameter uncertainties, can be written as

$$\frac{dx_1}{dt} = \theta_1 x_1 (1 - x_2), \quad x_1(0) = 1.2, \quad \theta_1 \in [2.99, 3.01] \quad (4)$$

$$\frac{dx_2}{dt} = \theta_2 x_2 (x_1 - 1), \quad x_2(0) = 1.1, \quad \theta_2 \in [0.99, 1.01]. \quad (5)$$

This example has served as a test problem for comparing interval-based ODE solvers (Lin and Stadtherr, 2007b), in which uncertainty is represented as an interval. Figure 6 reproduces the interval trajectories computed by VSPODE for  $t = [0, 10]$ . The Taylor model describing the solution at  $t = 10$  can be combined with probability bound analysis when more specific information regarding the distribution of uncertainty is known. Figures 7 and 8 show the p-box solutions if both parameters are described by a p-box with bounds obtained from a uniform distribution with standard deviation of  $[0.0050, 0.0057]$  and mean at the interval midpoint. If the parameters were simply intervals (no distribution known), then only an interval enclosure of the states would be obtained, and these upper and lower bounds would match the upper and lower bounds of the p-boxes shown in Figures 7 and 8. If no probability bounds analysis was done, we could only say that the probability that  $x_1 \leq 1.14$  is in  $[0, 1]$ . However, using p-boxes it can be seen from Figure 7 that the probability that  $x_1 \leq 1.14$  is in the interval  $[0.05, 0.5]$ . We can run subinterval reconstitution to make the p-boxes tighter. Figures 9 and 10 show that the areas of the p-boxes can be drastically reduced with this technique. Now, the probability that  $x_1 \leq 1.14$  is shown to be about  $[0.13, 0.36]$ . The choice of a uniform



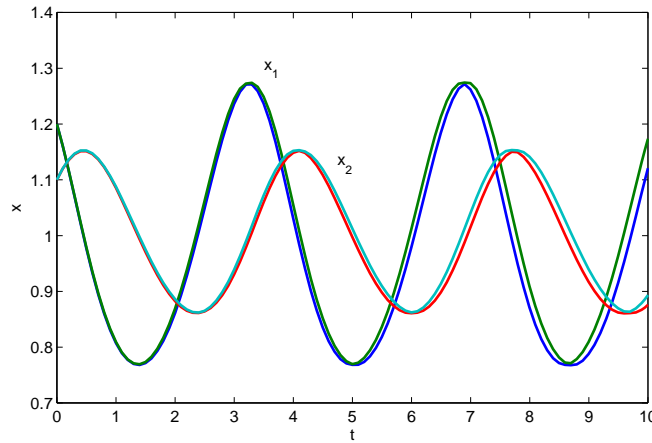


Figure 6. The interval bounds on the state trajectories of Lotka-Volterra model as computed by VSPODE.

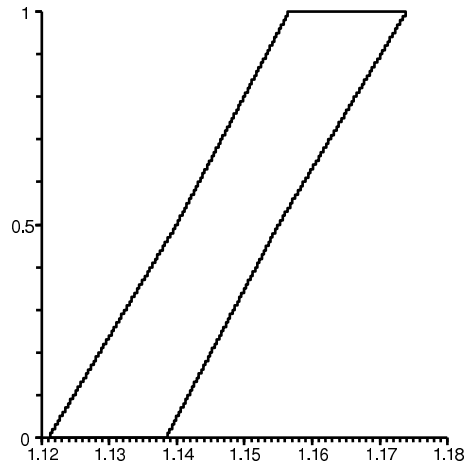


Figure 7. The p-box enclosure of  $x_1$  at time  $t = 10$  in the Lotka-Volterra model as computed by Risk Calc.

distribution for the p-box bounds in this problem was an arbitrary one. Other types of p-boxes could also be used.

### 5.2. MICROBIAL GROWTH MODEL WITH MONOD KINETICS

The system of equations for a simple bioreactor model (Lin and Stadtherr, 2007a) is

$$\frac{dX}{dt} = (\mu - \alpha D)X \tag{6}$$

$$\frac{dS}{dt} = D(S_f - S) - k\mu X, \tag{7}$$

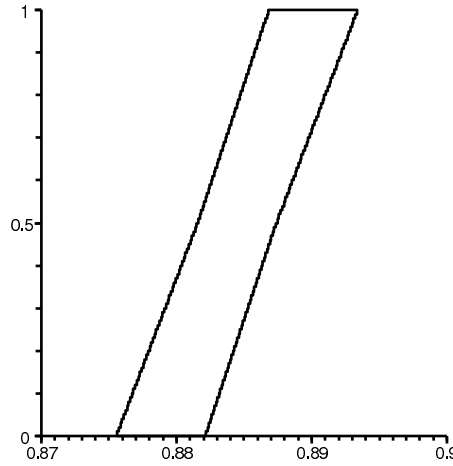


Figure 8. The p-box enclosure of  $x_2$  at time  $t = 10$  in the Lotka-Volterra model as computed by Risk Calc.

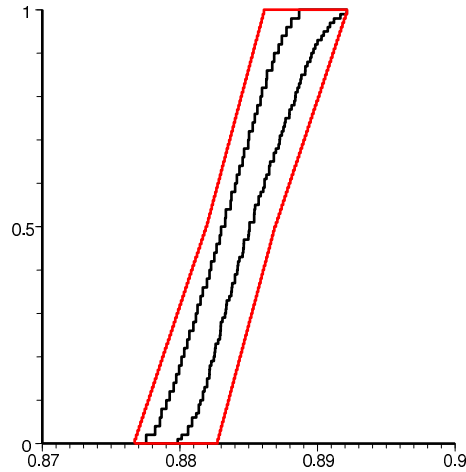


Figure 9. The inner curves show the p-box enclosure of  $x_1$  at time  $t = 10$  in the Lotka-Volterra model as computed by Risk Calc, now using the subinterval reconstitution technique. The outer box corresponds to the solution shown in Figure 7 for comparison.

where  $X$  represents the concentration of cells in the system, and  $S$  represents the concentration of substrate. The parameters  $\alpha$ ,  $D$ ,  $S_f$ , and  $k$  represent the heterogeneity parameter, the dilution rate of substrate, the feed concentration of substrate, and the yield coefficient, respectively. The growth rate of cells,  $\mu$ , is dependent on the concentration of substrate,  $S$ . This term may take a variety of forms. For a simple initial example, we consider Monod kinetics (Bastin and Douchain, 1990; Bequette, 2003), where

$$\mu = \frac{\mu_{max}S}{K_S + S}. \quad (8)$$

In the above expression,  $\mu_{max}$  is the maximum growth rate, and  $K_S$  is the saturation parameter.

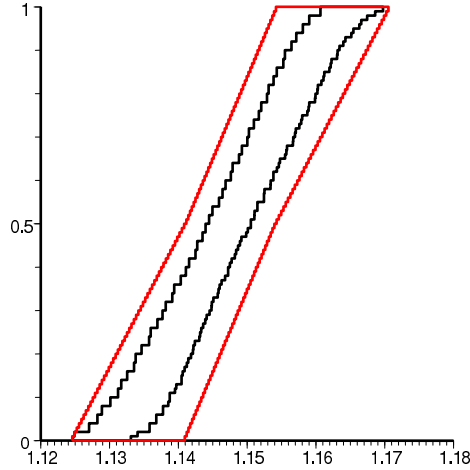


Figure 10. The inner curves show the p-box enclosure of  $x_2$  at time  $t = 10$  in the Lotka-Volterra model as computed by Risk Calc, now using the subinterval reconstitution technique. The outer box corresponds to the solution shown in Figure 8 for comparison.

We explore a subset of the uncertain conditions and parameters used by Lin and Stadtherr (2007a):  $X_0 \in [0.794, 0.864]$  g/L,  $\mu_{max} \in [1.15, 1.25]$  day<sup>-1</sup>, and  $K_S \in [6.8, 7.2]$  g/L. We assume an mmms distribution for these parameters, with the mean being the midpoint of the interval, and the standard deviation being one tenth of the width of the interval (these are arbitrary choices). Other initial conditions and parameters are expressed as real numbers:  $S_0 = 0.8$  g/L,  $\alpha = 0.5$ ,  $D = 0.36$  day<sup>-1</sup>,  $S_f = 5.7$  g/L, and  $k = 10.53$  g substrate/ g cells. We employ VSPODE to integrate the equation from  $t = 0$  to  $t = 10$  days. The biomass trajectory produced by VSPODE is shown in Figure 11. The resulting Taylor model that describes  $X$  and  $S$  at  $t = 10$  is used with Risk Calc, and the p-box calculations give bounds on the probability distributions for the state variables as shown in Figures 12 and 13. This shows, for example, that the probability that the biomass of cells is less than or equal to 0.85 g is in the interval  $[0.9, 1.0]$ .

### 5.3. MICROBIAL GROWTH MODEL WITH HALDANE KINETICS

The same bioreactor model described by Eqs. (6)-(7) can be solved using the slightly more complicated Haldane kinetics (Bastin and Douchain, 1990; Lin and Stadtherr, 2007a), also called substrate inhibition kinetics (Bequette, 2003). Here we replace the growth rate equation previously given as Eq. (8) with

$$\mu = \frac{\mu_{max} S}{K_S + S + K_I S^2}. \quad (9)$$

The new parameter,  $K_I$ , is called the inhibition parameter. Following Lin and Stadtherr (2007a), we will treat this new parameter as uncertain, with its value lying in the interval  $[0.0025, 0.01]$  and its uncertainty described again using the mmms p-box as discussed above.

Integrating this equation the same way as before, we obtain the transient biomass trajectory shown in Figure 14 and a Taylor model describing the variables at time  $t = 10$ . The p-box enclosures

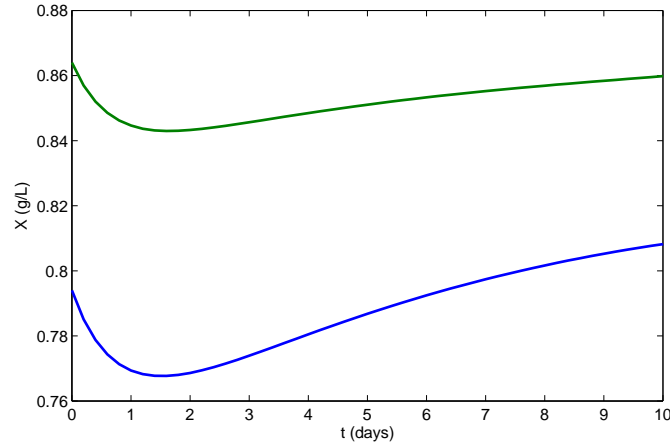


Figure 11. Interval bounds on trajectory of cell biomass  $X$  under Monod kinetics as computed by VSPODE.

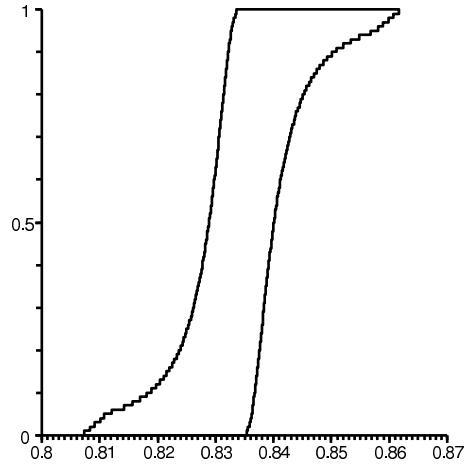


Figure 12. P-box enclosure of cell biomass  $X$  at  $t = 10$  for Monod kinetics as computed by Risk Calc.

computed by Risk Calc for the state variables are shown in Figures 15 and 16. These enclosures are larger than the enclosures determined in the previous example, which is expected because there is an additional uncertain parameter. Now the probability that the biomass of cells is less than or equal to 0.85 g is in the interval  $[0.86, 1.0]$ .

#### 5.4. THREE-STATE BIOREACTOR MODEL

A second bioreactor model explored by Lin and Stadtherr (2007a) is a three-state biochemical reactor. Here, we model the growth of cells  $x_1$  that consume substrate  $x_2$ , but which also form a product  $x_3$ . The model is

$$\frac{dx_1}{dt} = (\mu - D)x_1 \quad (10)$$

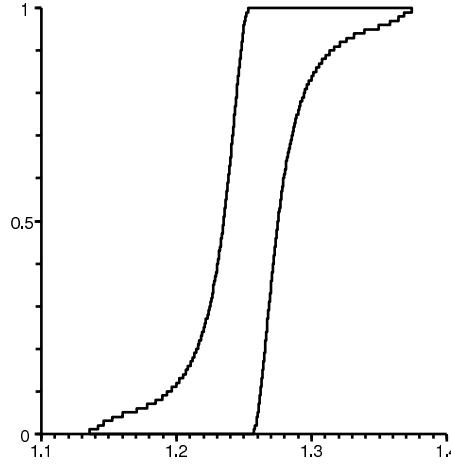


Figure 13. P-box enclosure of substrate  $S$  at  $t = 10$  for Monod kinetics as computed by Risk Calc.

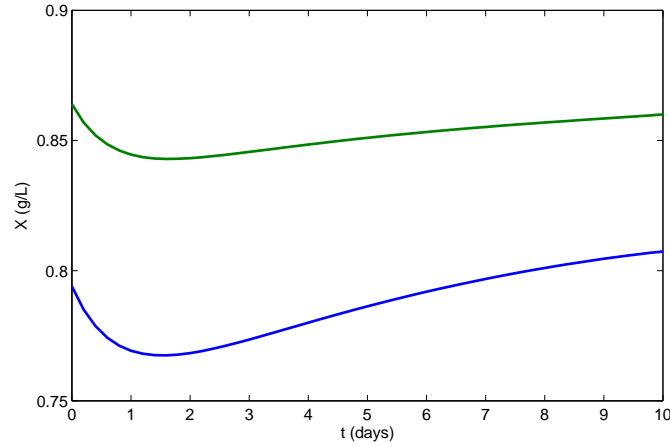


Figure 14. Interval bounds on trajectory of biomass  $X$  under Haldane kinetics as computed by VSPODE.

$$\frac{dx_2}{dt} = D(x_{2f} - x_2) - \frac{\mu x_1}{Y} \quad (11)$$

$$\frac{dx_3}{dt} = -Dx_3 + (\alpha\mu + \beta)x_1, \quad (12)$$

with the growth rate as a function of both substrate and product concentrations,

$$\mu = \frac{\mu_{max} [1 - (x_3/x_{3m})] x_2}{k_s + x_2}. \quad (13)$$

In the above equations, the initial concentration of cells is unknown but within  $[6.4549, 6.5676]$ , and is represented by a p-box with bounds obtained from a uniform distribution with standard deviation of  $[0.028170, 0.032533]$ . Two parameters are uncertain; the maximum growth rate  $\mu_{max} \in$

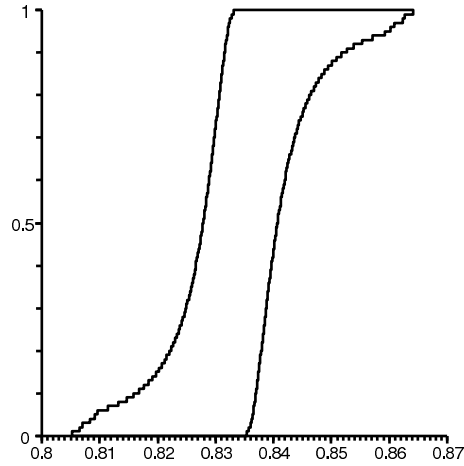


Figure 15. P-box enclosure of cell biomass  $X$  at  $t = 10$  for Haldane kinetics as computed by Risk Calc.

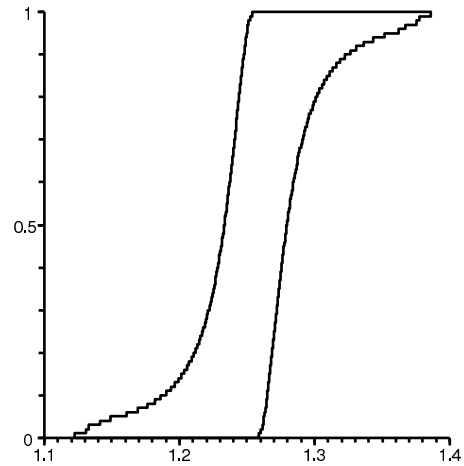


Figure 16. P-box enclosure of substrate  $S$  at  $t = 10$  for Haldane kinetics as computed by Risk Calc.

$[0.46, 0.47]$  is represented by a p-box with bounds obtained from a normal distribution with standard deviation of  $[0.0282, 0.0325]$ , and the saturation parameter  $k_s \in [1.03, 1.1]$  is represented by a p-box corresponding to the mmms distribution with standard deviation equal to 0.007. All p-box means are at the interval midpoint. All other initial conditions and parameters are known exactly:  $x_{20} = 5$  g/L,  $x_{30} = 15$  g/L,  $Y = 0.4$  g/g,  $\beta = 0.2$  hour $^{-1}$ ,  $D = 0.202$  hour $^{-1}$ ,  $\alpha = 2.2$  g/g,  $x_{3m} = 50$  g/L, and  $x_{2f} = 20$  g/L.

VSPODE provides the biomass trajectory shown in Figure 17 and the Taylor model used in Risk Calc to create Figures 18, 19, and 20, which give the probability distribution for the state variables as p-boxes at time  $t = 10$ . One purpose for this example is to show the ability to have uncertain conditions under a variety of probability distributions. Such an ability is essential in complicated biological models where a variety of distributions is likely.

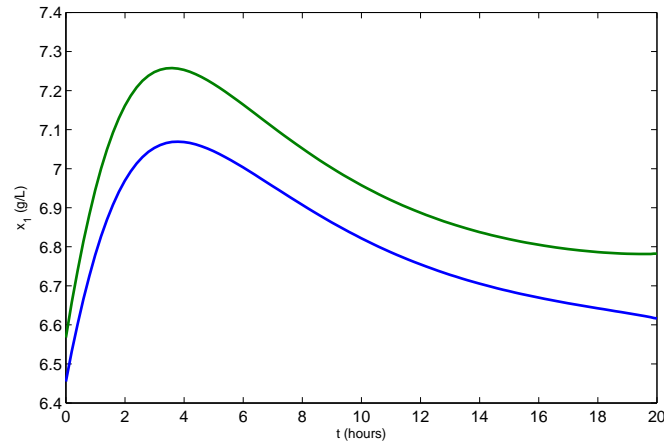


Figure 17. Interval bounds on trajectory of biomass  $x_1$  in three-state reactor as computed by VSPODE.

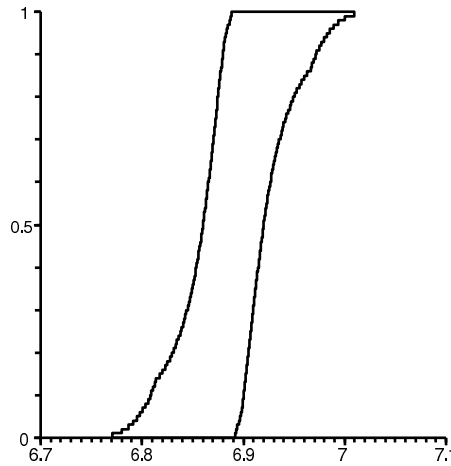


Figure 18. P-box enclosure of biomass  $x_1$  at  $t = 10$  in three-state reactor as computed by Risk Calc.

## 6. Concluding Remarks

The verified ODE solver VSPODE (Lin and Stadtherr, 2007b) provides a powerful tool for bounding the solutions of parametric nonlinear ODEs. Because it provides output in the form of Taylor models, VSPODE is also useful in situations in which uncertainties in parameters and initial states are represented by p-boxes. In this case, the Taylor models from VSPODE can be combined with the p-box uncertainties in initial states and parameters using RAMAS Risk Calc, resulting in a propagation of these uncertainties into the final values of the state variables. In this way, probability distributions (p-boxes) for the final state values can be obtained, as demonstrated in several example problems.

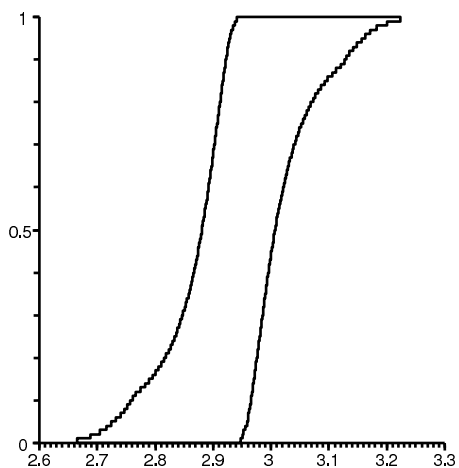


Figure 19. P-box enclosure of substrate mass  $x_2$  at  $t = 10$  in three-state reactor as computed by Risk Calc.

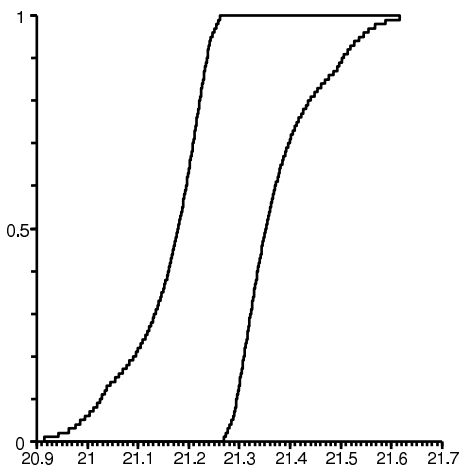


Figure 20. P-box enclosure of product mass  $x_3$  at  $t = 10$  in three-state reactor as computed by Risk Calc.

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