

Computing Guaranteed Bounds for Uncertain Cooperative and Monotone Nonlinear Systems

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Abstract: Models of biological or technical applications are represented by nonlinear systems, which are defined by ordinary differential equations. These systems generally contain multiple uncertain or unknown parameters. These uncertainties result from measurement errors or from modeling, e.g. numerical modeling. For several applications, the guaranteed enclosure of all possible solutions of an initial value problem (IVP) of a given uncertain system is demanded. In general the calculation of guaranteed bounds of the given uncertain nonlinear system cannot be done directly, because the solution set of an IVP can be solved algebraically only in certain cases. Furthermore, most numerical methods which compute the solution of IVPs cannot handle systems with uncertain parameters. But for the class of cooperative systems tight guaranteed bounds for all solutions of the IVP can be computed. This class satisfies certain monotony conditions. Moreover the computation of guaranteed lower and upper bounds can be applied to a larger class of ordinary differential equations, which does not satisfy all conditions for uncertain cooperative systems. For this class of monotone systems the guaranteed enclosure can show some overestimation. Some examples illustrate the methods described in this contribution.

Keywords: Application of nonlinear analysis and design; Uncertainty descriptions; Parameter-varying systems.

1. INTRODUCTION

A wide range of biological and technical systems is represented by ordinary differential equations. The representation of such systems is given by

$$\dot{\mathbf{x}}(t) = \tilde{\mathbf{f}}(\mathbf{x}, t) \text{ with } \mathbf{x}(0) = \mathbf{x}_0, \quad (1)$$

where the number of states is given by n . The right hand side is given by the function $\tilde{\mathbf{f}}$ which does not depend on any uncertain parameters. But these systems often contain uncertain parameters, due to model uncertainties or measurement errors. Also numerical system modeling methods, e.g. Finite Element Methods, can result in uncertain parameters. The uncertainties are represented by intervals, which means that the value of each parameter p lies between the infimum p^L and the supremum p^R . This representation also denotes the left and right end of the corresponding interval p^I . Thus, a system with uncertain parameters is given by

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}, t; \mathbf{p}) \text{ with } \mathbf{x}(0) = \mathbf{x}_0 \text{ and } \mathbf{p} \in \mathbf{p}^I \quad (2)$$

where \mathbf{p}^I represents the interval parameter vector. The number of uncertain parameters is given by P .

The set of all possible solutions of the given IVP of the system (2) with respect to the uncertain parameters is often needed. In general the solution is hard to find for nonlinear systems and guaranteed bounds for uncertain nonlinear systems cannot be computed directly. The Monte-Carlo method is a common method to determine a solution subset of the given IVP (2). With this method the IVP is solved several times with randomly chosen values from the interval vector \mathbf{p}^I . Thus, in general the Monte-Carlo method does not deliver a guaranteed enclosure for all possible solutions; it returns only a subset of the designated domain enclosed by the guaranteed bounds.

The main target is to determine guaranteed bounds for uncertain systems as an exact enclosure. This can be done for so called cooperative systems. Moreover, for monotone systems guaranteed bounds can also easily be computed, although these bounds may suffer from overestimation. This means that the given set of all possible solutions of the IVP of a monotone system is only a conservative enclosure. Nevertheless the computed solution does give a guaranteed enclosure of all IVP solutions with respect to the uncertain parameters and in general compute a tighter enclosure than other guaranteed bounds for uncertain systems providing methods, c.f. Tibken and Gennat (2005, 2006); Gennat and Tibken (2007); Aschemann et al. (2005).

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2. COOPERATIVE SYSTEMS

Nonlinear uncertain systems that fulfill certain monotony conditions, are called cooperative systems, c.f. Angeli and Sontag (2003); Smith (1986, 1998). For systems which fulfill the conditions for cooperative systems the simulation has to be done two times, one for the lower bound and one for the upper bound. The region between the bounds define the set of all possible solutions given by the uncertainties. In this contribution a simulation of a nonlinear system means the numerical solution of an IVP given by an ordinary differential equation (2). This can be done e.g. by using the Matlab ODE-solver, c.f. Shampine and Reichelt (1997). A validated solution of the IVP can be computed by using Lohner's AWA-algorithm, see Lohner (1988); Ludyk (1990).

A given system (1) is called a cooperative system, if all states of the system are monotone and leave the nonnegative orthant invariant. A system is monotone if it preserves the ordering of the initial data. This means the system (1) is monotone, if two states \mathbf{x}, \mathbf{y} for the ordering

$$\mathbf{x} \geq \mathbf{y} \text{ and } x_i = y_i \quad (3)$$

the condition

$$\tilde{f}_i(\mathbf{x}, t) \geq \tilde{f}_i(\mathbf{y}, t) \quad \forall t \geq 0 \quad (4)$$

is fulfilled for all $i = 1, \dots, n$. An additional condition for cooperative systems is given by the property that all states of the system do not leave the nonnegative orthant or in other words that $\mathbf{x}(t) \geq 0 \forall t \geq 0$. The nonnegative orthant is given by

$$\mathbb{R}_{\geq 0} = \{\mathbf{x} \mid x_i \geq 0 \forall i = 1, \dots, n, \mathbf{x} \in \mathbb{R}^n\}. \quad (5)$$

The examination of the condition (4) and the nonnegativity condition can be done with necessary and sufficient conditions for the continuously differentiable functions on the right hand side of the system (1).

The continuously differentiable system (1) is a cooperative system, if and only if

$$\mathbf{x} \in \mathbb{R}_{\geq 0} \quad (6)$$

and

$$\frac{\partial \tilde{f}_i}{\partial x_j}(\mathbf{x}, t) \geq 0 \quad \forall i \neq j \text{ with } i, j = 1, \dots, n. \quad (7)$$

hold. All elements of the Jacobian of $\tilde{\mathbf{f}}$ except those on the main diagonal have to be positive or zero.

2.1 Uncertain Cooperative Systems

The expansion of these conditions to uncertain systems (2), which also depend on the parameters \mathbf{p} , is accomplished by expanding the system of differential equations. The resulting new system is given by

$$\begin{pmatrix} \dot{\mathbf{x}}(t) \\ \dot{\mathbf{p}} \end{pmatrix} = \begin{pmatrix} \mathbf{f}(\mathbf{x}, t; \mathbf{p}) \\ 0 \end{pmatrix}, \quad \mathbf{x}(0) = \mathbf{x}_0, \mathbf{p} \in \mathbf{p}^I \quad (8)$$

or $\dot{\mathbf{z}}(t) = \mathbf{g}(\mathbf{z}, t; \mathbf{p})$

with $\mathbf{z} = (\mathbf{x} \ \mathbf{p})^T$. This system has to fulfill conditions (6) and (7). Thus, the conditions for cooperativity of uncertain systems are reformulated as follows. The continuously

differentiable system (8) is a cooperative system, if and only if

$$\mathbf{x} \in \mathbb{R}_{\geq 0} \quad (9)$$

and

$$\frac{\partial g_i}{\partial z_j}(\mathbf{z}(t), t; \mathbf{p}) \geq 0 \quad \forall i \neq j, \text{ with } i, j = 1, \dots, n + P. \quad (10)$$

hold. In this case, the uncertain system (8) is cooperative for all $\mathbf{p} \in \mathbf{p}^I$. To prove the nonnegativity of the states for all times, the states dependency on the parameters has also to be examined. The nonnegativity can be proven by showing

$$\frac{d}{dt} x_i|_{x_i=0} = f_i(\mathbf{x}; \mathbf{p})|_{x_i=0} \geq 0 \quad \forall i = 1, \dots, n \text{ and} \quad (11)$$

$$\frac{d}{dt} \left(\frac{\partial x_i}{\partial p_j} \right) \Big|_{\frac{\partial x_i}{\partial p_j}=0} \geq 0 \quad \forall i = 1, \dots, n, j = 1, \dots, P \quad (12)$$

$$(13)$$

$$\text{with } x_k \geq 0, \left(\frac{\partial x_k}{\partial p_l} \right) \geq 0, k = 1, \dots, n, l = 1, \dots, P.$$

Then, the time derivatives of all states (11) and all states' partial derivatives with respect to all parameters (12) are nonnegative. Uncertain systems which fulfill the conditions (10), (11) and (12) are named uncertain cooperative systems in this contribution.

Lower and upper bounds to include all possible solutions of the IVP (2) can be computed by solving the two IVPs of the systems

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}, t; \mathbf{p}^L) \text{ with } \mathbf{x}(0) = \mathbf{x}_0 \quad (14)$$

and

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}, t; \mathbf{p}^R) \text{ with } \mathbf{x}(0) = \mathbf{x}_0. \quad (15)$$

Thus, the system (8) is cooperative with respect to the uncertain parameters and the solutions of IVPs (14) and (15) determine the lower and upper bound of the set of all possible solutions of (2).

2.2 First Example

To illustrate the idea of cooperative systems and their guaranteed enclosure, a simple arbitrary two-dimensional example is given. Consider a system represented by the differential equations

$$\begin{aligned} \dot{x}_1 &= p_1 x_2 + p_2 x_1^2 \\ \dot{x}_2 &= x_1 - x_2^2 + x_1 x_2 \end{aligned} \quad (16)$$

with initial values $\mathbf{x}(0) = (5 \ 0)^T$. The uncertain parameters are given by $p_1^I = [1, 1.1]$ and $p_2^I = [-1, -0.9]$. To examine the conditions (9) and (10) the Jacobian has to be computed. It results in

$$\frac{\partial \mathbf{g}}{\partial \mathbf{z}}(\mathbf{z}, t; \mathbf{p}) = \begin{pmatrix} 2 p_2 x_1 & p_1 & x_2 & x_1^2 \\ 1 + x_2 & -2 x_2 + x_1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Assuming all states are nonnegative, all elements of the Jacobian except those on the main diagonal are also nonnegative. Thus, (10) is fulfilled. The nonnegativity

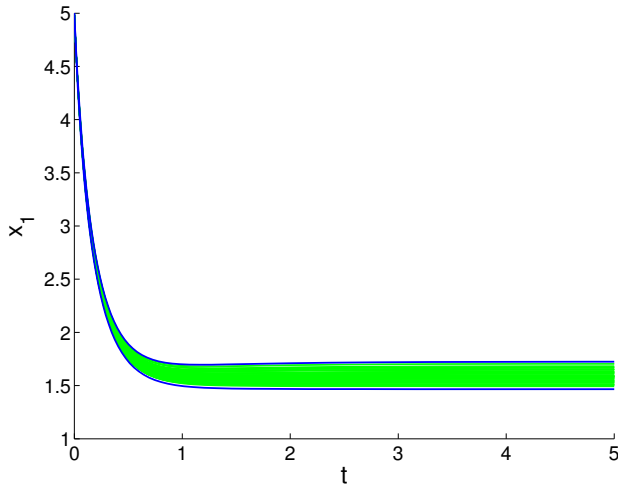


Fig. 1. first example: simulation of x_1 with guaranteed bounds and Monte-Carlo simulations

conditions (11) and (12) are examined in the following. The inequalities

$$f_1(0, x_2) \geq 0 \text{ with } x_2 \geq 0 \text{ and} \quad (17)$$

$$f_2(x_1, 0) \geq 0 \text{ with } x_1 \geq 0 \quad (18)$$

prove the nonnegativity of the system with respect to the states. The nonnegativity with respect to the parameters is shown by examination of

$$\frac{d}{dt} \left(\frac{\partial \mathbf{x}}{\partial \mathbf{p}} \right) = \frac{\partial \mathbf{f}}{\partial \mathbf{x}}(\mathbf{x}; \mathbf{p}) \cdot \frac{\partial \mathbf{x}}{\partial \mathbf{p}} + \frac{\partial \mathbf{f}}{\partial \mathbf{p}} \quad (19)$$

$$\frac{d}{dt} \left(\frac{\partial \mathbf{x}}{\partial \mathbf{p}} \right) = \begin{pmatrix} 2 p_2 x_1 & p_1 \\ 1 + x_2 & -2 x_2 + x_1 \end{pmatrix} \begin{pmatrix} \frac{\partial x_1}{\partial p_1} & \frac{\partial x_1}{\partial p_2} \\ \frac{\partial x_2}{\partial p_1} & \frac{\partial x_2}{\partial p_2} \end{pmatrix} + \begin{pmatrix} x_2 & x_1^2 \\ 0 & 0 \end{pmatrix}.$$

From (17) and (18) follows

$$\begin{aligned} f_1(0, x_2) &= p_1 x_2 \geq 0, \\ f_2(x_1, 0) &= x_1 \geq 0 \end{aligned}$$

and from (19) the inequalities

$$\begin{aligned} \frac{d}{dt} \left(\frac{\partial x_1}{\partial p_1} \right) \Big|_{\frac{\partial x_1}{\partial p_1}=0} &= p_1 \left(\frac{\partial x_2}{\partial p_1} \right) + x_2 \geq 0 \\ \frac{d}{dt} \left(\frac{\partial x_2}{\partial p_1} \right) \Big|_{\frac{\partial x_2}{\partial p_1}=0} &= (1 + x_2) \left(\frac{\partial x_1}{\partial p_1} \right) \geq 0 \\ \frac{d}{dt} \left(\frac{\partial x_1}{\partial p_2} \right) \Big|_{\frac{\partial x_1}{\partial p_2}=0} &= p_1 \left(\frac{\partial x_2}{\partial p_2} \right) + x_1^2 \geq 0 \\ \frac{d}{dt} \left(\frac{\partial x_2}{\partial p_2} \right) \Big|_{\frac{\partial x_2}{\partial p_2}=0} &= (1 + x_2) \left(\frac{\partial x_1}{\partial p_2} \right) \geq 0 \end{aligned}$$

are derived. With (17), (18) and (19) it is shown that all solutions of the IVP given by the system (16) stay in the nonnegative orthant for all times.

To determine the guaranteed lower and upper bound, the two IVPs (14) and (15) has to be solved. The resulting graphs of the solutions are shown in Fig. 1 and Fig. 2, where the green graphs represent 64 Monte-Carlo simulations for comparison only.

3. UNCERTAIN MONOTONE SYSTEMS

It is possible to get tight guaranteed lower and upper bounds for a nonlinear system, which does not fulfill the

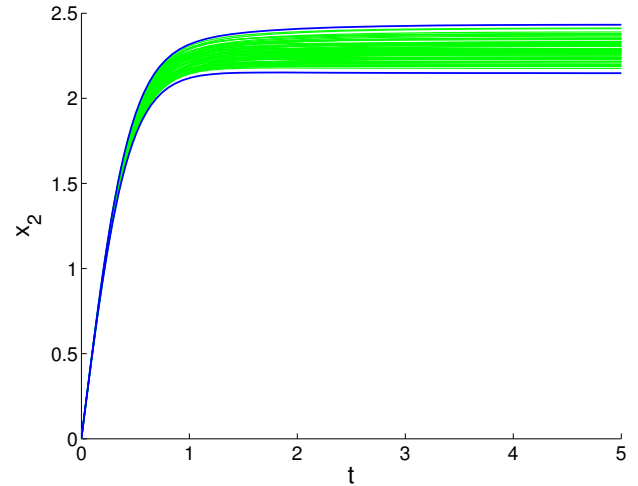


Fig. 2. first example: simulation of x_2 with guaranteed bounds and Monte-Carlo simulations

conditions for uncertain cooperative systems. If the system represents a cooperative system without considering the uncertain parameters, an expansion of the parameter vector \mathbf{p} can turn the uncertain system into an uncertain monotone system. Thus, guaranteed bounds can be computed easily with a modification of the equations in (14) and (15). This type of system is called uncertain monotone system. It is not an uncertain cooperative system, because the condition (10) for the parameters is not fulfilled. The expansion of the parameter vector and the computation of the lower and upper bounds for the uncertain system are described in the following.

To fulfill the condition (10) for all uncertain parameters, the parameter vector \mathbf{p} will be augmented to $\tilde{\mathbf{p}}$, thus every component of the parameter vector \mathbf{p} in the system (2) will occur exactly one time in the system

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}, t; \tilde{\mathbf{p}}) \text{ with } \mathbf{x}(0) = \mathbf{x}_0 \text{ and } \tilde{\mathbf{p}} \in \tilde{\mathbf{p}}^I \quad (20)$$

with the new interval parameter vector $\tilde{\mathbf{p}}^I$. If a parameter p_i occurs two or more times in the system (2), the new vector $\tilde{\mathbf{p}}$ is augmented by one or more components, depending on the number of occurrences of p_i . The new uncertain parameter \tilde{p}_{P+1}^I is set to p_i^I on the second occurrence of p_i , the new uncertain parameter \tilde{p}_{P+2}^I is set to p_i^I on the third and so on. The number of the components in $\tilde{\mathbf{p}}^I$ after the expansion described above is denoted by \tilde{P} . This expansion has to be done for all parameters p_i in the original system (2).

To fulfill the condition (10), all new and unique parameters \tilde{p}_i are multiplied by -1 , which causes negative signs in the Jacobian. For that, a leading signs vector $\boldsymbol{\alpha}$ is introduced. All components of $\boldsymbol{\alpha}$ are set to -1 , whose corresponding parameters \tilde{p}_i are causing the negative Jacobian entries. In addition a new vector is given by $\hat{\mathbf{p}} = \boldsymbol{\alpha} \tilde{\mathbf{p}}$. If the new vector $\hat{\mathbf{p}}$ with its uncertain parameters and leading signs vector leads to a system

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}, t; (\boldsymbol{\alpha} \hat{\mathbf{p}})), \hat{\mathbf{p}} \in (\boldsymbol{\alpha} \tilde{\mathbf{p}})^I \text{ with } \mathbf{x}(0) = \mathbf{x}_0, \quad (21)$$

for which condition (10) holds, guaranteed bounds can be computed for all solutions of the IVP of the uncertain monotone system (21).

For this computing guaranteed enclosure, the leading signs vector α needs not be determined. It is sufficient to compute the solutions of $2^{\bar{P}}$ IVPs of the system with all possible infima and suprema combinations of the uncertain parameters. Thus, the solutions of the following IVPs

$$\begin{aligned} \dot{\mathbf{x}}(t) &= \mathbf{f}(\mathbf{x}(t), t; [\tilde{p}_1^L, \tilde{p}_2^L, \dots, \tilde{p}_{\bar{P}}^L]) \\ \dot{\mathbf{x}}(t) &= \mathbf{f}(\mathbf{x}(t), t; [\tilde{p}_1^R, \tilde{p}_2^R, \dots, \tilde{p}_{\bar{P}}^R]) \\ \dot{\mathbf{x}}(t) &= \mathbf{f}(\mathbf{x}(t), t; [\tilde{p}_1^L, \tilde{p}_2^R, \dots, \tilde{p}_{\bar{P}}^L]) \\ \dot{\mathbf{x}}(t) &= \mathbf{f}(\mathbf{x}(t), t; [\tilde{p}_1^R, \tilde{p}_2^L, \dots, \tilde{p}_{\bar{P}}^R]) \\ &\vdots \\ \dot{\mathbf{x}}(t) &= \mathbf{f}(\mathbf{x}(t), t; [\tilde{p}_1^R, \tilde{p}_2^R, \dots, \tilde{p}_{\bar{P}}^R]) \end{aligned} \quad (22)$$

with initial condition $\mathbf{x}(0) = \mathbf{x}_0$ have to be computed.

Due to the expansion of the parameter vector, all uncertain parameters are unique in (21). Moreover, two solutions of all $2^{\bar{P}}$ IVPs (22) represent the guaranteed lower and upper bounds for all possible solutions of the IVP of the original system (2). Thus, not all solutions of the $2^{\bar{P}}$ IVPs has to be computed, if the leading signs vector α is determined. With the acknowledgment of α , the lower and upper bounds for the enclosure of the system (21) are computed according to (14) and (15) with

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}, t; (\alpha \hat{\mathbf{p}})^L) \text{ with } \mathbf{x}(0) = \mathbf{x}_0 \quad (23)$$

and

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}, t; (\alpha \hat{\mathbf{p}})^R) \text{ with } \mathbf{x}(0) = \mathbf{x}_0. \quad (24)$$

Nevertheless, the expansion of the parameter vector can lead to overestimation, which means that the guaranteed lower and upper bounds are conservative and not tight. In the case of overestimation these bounds are not part of solution set which represents the precise enclosure set of all possible solutions. The term overestimation comes from interval arithmetic and denotes an overly conservative enclosure of a solution set, c.f. Moore (1966); Alefeld and Herzberger (1974); Hansen (1992); Didrit et al. (2001).

3.1 Second Example

Taking the uncertain system of the first example, the second differential equation is has also made dependent on the uncertainties. Thus, the new system is given by

$$\begin{aligned} \dot{x}_1 &= p_1 x_2 + p_2 x_1^2 \\ \dot{x}_2 &= -p_2 x_1 - p_3 x_2^2 + p_3 x_1 x_2 \end{aligned} \quad (25)$$

and the initial values are once again, set to $\mathbf{x}(0) = (5 \ 0)^T$. The uncertain parameters are given by $p_1^I = [1, 1.1]$, $p_2^I = [-1, -0.9]$ and $p_3^I = [0.9, 1.1]$. These slight changes make the system noncooperative in the sense of section 1. This can be easily verified by computing the Jacobian and examining condition (10). The Jacobian results in

$$\frac{\partial \mathbf{g}}{\partial \mathbf{z}} = \begin{pmatrix} 2 p_2 x_1 & p_1 & x_2 & x_1^2 & 0 \\ -p_2 + p_3 x_2 & -2 p_3 x_2 + p_3 x_1 & 0 & -x_1 & x_1 x_2 - x_2^2 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

As one can see, several elements of the Jacobian except those on the main diagonal are negative. Thus, the described above expansion of the parameter vector will be

used. The parameter vector expansion leads to a new system

$$\begin{aligned} \dot{x}_1 &= \tilde{p}_1 x_2 + \tilde{p}_2 x_1^2 \\ \dot{x}_2 &= -\tilde{p}_4 x_1 - \tilde{p}_3 x_2^2 + \tilde{p}_5 x_1 x_2. \end{aligned} \quad (26)$$

To meet conditions (10), the leading signs vector α is defined as

$$\alpha = (1 \ 1 \ -1 \ -1 \ 1)^T,$$

thus the new parameter vector $\hat{\mathbf{p}} = \alpha \tilde{\mathbf{p}}$ transforms the system (26) to

$$\begin{aligned} \dot{x}_1 &= \hat{p}_1 x_2 + \hat{p}_2 x_1^2 \\ \dot{x}_2 &= \hat{p}_4 x_1 + \hat{p}_3 x_2^2 + \hat{p}_5 x_1 x_2. \end{aligned} \quad (27)$$

The Jacobian of the system (27) with $\mathbf{z} = (\mathbf{x} \ \hat{\mathbf{p}})^T$ equates to

$$\frac{\partial \mathbf{g}}{\partial \mathbf{z}} = \begin{pmatrix} 2\hat{p}_2 x_1 & \hat{p}_1 & x_2 & x_1^2 & 0 & 0 & 0 \\ \hat{p}_4 + \hat{p}_5 x_2 & 2\hat{p}_3 x_2 + \hat{p}_5 x_1 & 0 & 0 & x_2^2 & x_1 & x_1 x_2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \vdots & & & & & & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

with the newly defined uncertain parameter vector $\hat{\mathbf{p}}$ consisting of $\hat{p}_1^I = [1, 1.1]$, $\hat{p}_2^I = [-1, -0.9]$, $\hat{p}_3^I = [-1.1, -0.9]$, $\hat{p}_4^I = [0.9, 1]$ and $\hat{p}_5^I = [0.9, 1.1]$. To prove the cooperativity of the transformed system (27), the nonnegativity conditions (11) and (12) have to be examined. The inequalities

$$f_1(0, x_2) = \hat{p}_1 x_2 \geq 0 \text{ and } f_2(x_1, 0) = \hat{p}_4 x_1 \geq 0$$

fulfill the nonnegativity condition (11) with respect to the states for all $x_1, x_2 > 0$ and all $\hat{p}_1 \in \hat{p}_1^I$ as well as $\hat{p}_4 \in \hat{p}_4^I$. Moreover, condition (12) with respect to the parameters is examined with

$$\begin{aligned} \frac{d}{dt} \left(\frac{\partial \mathbf{x}}{\partial \hat{\mathbf{p}}} \right) &= \begin{pmatrix} 2 \hat{p}_2 x_1 & \hat{p}_1 \\ \hat{p}_4 + \hat{p}_3 x_2 & 2 \hat{p}_3 x_2 + \hat{p}_2 x_1 \end{pmatrix} \begin{pmatrix} \frac{\partial x_1}{\partial \hat{\mathbf{p}}} \\ \frac{\partial x_2}{\partial \hat{\mathbf{p}}} \end{pmatrix} \\ &\quad + \begin{pmatrix} x_2 & x_1^2 & 0 & 0 & 0 \\ 0 & 0 & x_2^2 & x_1 & x_1 x_2 \end{pmatrix}, \end{aligned}$$

which leads to the set of inequalities

$$\begin{aligned} \frac{d}{dt} \left(\frac{\partial x_1}{\partial \hat{p}_1} \right) \Big|_{\frac{\partial x_1}{\partial \hat{p}_1} = 0} &= \hat{p}_1 \left(\frac{\partial x_2}{\partial \hat{p}_1} \right) + x_2 &> 0 \\ \frac{d}{dt} \left(\frac{\partial x_2}{\partial \hat{p}_1} \right) \Big|_{\frac{\partial x_2}{\partial \hat{p}_1} = 0} &= (\hat{p}_4 + \hat{p}_5 x_2) \left(\frac{\partial x_1}{\partial \hat{p}_1} \right) &> 0 \\ \frac{d}{dt} \left(\frac{\partial x_1}{\partial \hat{p}_2} \right) \Big|_{\frac{\partial x_1}{\partial \hat{p}_2} = 0} &= \hat{p}_1 \left(\frac{\partial x_2}{\partial \hat{p}_2} \right) + x_1^2 &> 0 \\ \frac{d}{dt} \left(\frac{\partial x_2}{\partial \hat{p}_2} \right) \Big|_{\frac{\partial x_2}{\partial \hat{p}_2} = 0} &= (\hat{p}_4 + \hat{p}_5 x_2) \left(\frac{\partial x_1}{\partial \hat{p}_2} \right) &> 0 \\ \frac{d}{dt} \left(\frac{\partial x_1}{\partial \hat{p}_3} \right) \Big|_{\frac{\partial x_1}{\partial \hat{p}_3} = 0} &= \hat{p}_1 \left(\frac{\partial x_2}{\partial \hat{p}_3} \right) &> 0 \\ \frac{d}{dt} \left(\frac{\partial x_2}{\partial \hat{p}_3} \right) \Big|_{\frac{\partial x_2}{\partial \hat{p}_3} = 0} &= (\hat{p}_4 + \hat{p}_5 x_2) \left(\frac{\partial x_1}{\partial \hat{p}_3} \right) + x_2^2 &> 0 \\ \frac{d}{dt} \left(\frac{\partial x_1}{\partial \hat{p}_4} \right) \Big|_{\frac{\partial x_1}{\partial \hat{p}_4} = 0} &= \hat{p}_1 \left(\frac{\partial x_2}{\partial \hat{p}_4} \right) &> 0 \\ \frac{d}{dt} \left(\frac{\partial x_2}{\partial \hat{p}_4} \right) \Big|_{\frac{\partial x_2}{\partial \hat{p}_4} = 0} &= (\hat{p}_4 + \hat{p}_5 x_2) \left(\frac{\partial x_1}{\partial \hat{p}_4} \right) + x_1 &> 0 \\ \frac{d}{dt} \left(\frac{\partial x_1}{\partial \hat{p}_5} \right) \Big|_{\frac{\partial x_1}{\partial \hat{p}_5} = 0} &= \hat{p}_1 \left(\frac{\partial x_2}{\partial \hat{p}_5} \right) &> 0 \\ \frac{d}{dt} \left(\frac{\partial x_2}{\partial \hat{p}_5} \right) \Big|_{\frac{\partial x_2}{\partial \hat{p}_5} = 0} &= (\hat{p}_4 + \hat{p}_5 x_2) \left(\frac{\partial x_1}{\partial \hat{p}_5} \right) + x_1 x_2 &> 0, \end{aligned}$$

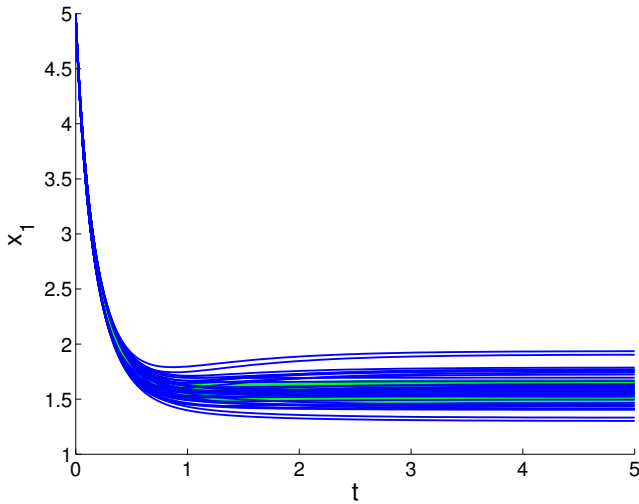


Fig. 3. second example: simulation of x_1 with guaranteed bounds and Monte-Carlo simulations

which is fulfilled for all nonnegative \mathbf{x} and all $\hat{\mathbf{p}} \in \hat{\mathbf{p}}^I$. In this example the computation of the guaranteed bounds is achieved by solving the 2^5 IVPs given by scheme (22), which is shown in Fig. 3 and Fig. 4. The most outward lying graphs determine the set of the guaranteed enclosure of all possible solutions of the IVP of the given system (25). These solution graphs can be computed by solving (23) and (24), but for this computation, the leading signs vector α has to be identified. It depends on the system and its uncertain parameters, whether the computation of $2^{\hat{P}}$ solutions of an IVP or the identification of α and then only 2 computations of solutions of an IVP leads to an easier and faster guaranteed enclosure.

The green graphs are achieved by computing 64 Monte-Carlo simulations. As one can see, the guaranteed enclosure of all possible solutions apparently leads to some overestimation.

4. REDUCING OVERESTIMATION FOR UNCERTAIN MONOTONE SYSTEMS

The overestimation can be reduced for some uncertain monotone systems. The reduction can be achieved by using another or not any parameter expansion method. A general method of parameter expansion cannot be given, it depends on the system's differential equations and their dependence on the parameters. But in general not all parameters have to be separated. Separation means the parameter expansion; the parameters p_i , which occur twice or more, are substituted by \tilde{p}_k with $k > P$.

To get a guaranteed enclosure of all possible solutions of the IVP with uncertain parameters, test with all α from

$$\begin{aligned}
 \alpha &= (1 \ 1 \ \dots \ 1)^T \\
 \alpha &= (-1 \ 1 \ \dots \ 1)^T \\
 \alpha &= (1 \ -1 \ \dots \ 1)^T \\
 \alpha &= (-1 \ -1 \ \dots \ 1)^T \\
 &\vdots \\
 \alpha &= (-1 \ -1 \ \dots \ -1)^T
 \end{aligned} \tag{28}$$

and the resulting parameter vectors $\hat{\mathbf{p}} = \alpha \tilde{\mathbf{p}}$ the conditions

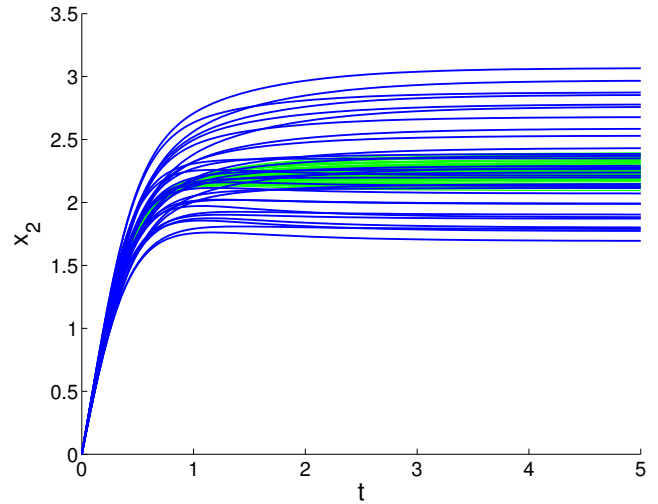


Fig. 4. second example: simulation of x_2 with guaranteed bounds and Monte-Carlo simulations

$$\frac{d}{dt} x_i |_{x_i=0} = f_i(\mathbf{x}; \hat{\mathbf{p}}) |_{x_i=0} \geq 0 \quad \forall i = 1, \dots, n \text{ and} \tag{29}$$

$$\frac{d}{dt} \left(\frac{\partial x_i}{\partial \hat{p}_j} \right) \Big|_{\frac{\partial x_i}{\partial \hat{p}_j}=0} \geq 0 \quad \forall i = 1, \dots, n, j = 1, \dots, P \tag{30}$$

$$\text{with } x_k \geq 0, \left(\frac{\partial x_k}{\partial \hat{p}_l} \right) \geq 0, k = 1, \dots, n, l = 1, \dots, P \text{ and}$$

$$\frac{\partial g_i}{\partial z_j}(\mathbf{z}(t), t; \hat{\mathbf{p}}) \geq 0 \quad \forall i \neq j, \text{ with } i, j = 1, \dots, n + P. \tag{31}$$

If (29), (30) and (31) hold with different α and their resulting parameter vectors $\hat{\mathbf{p}}$ for all times, then a guaranteed enclosure of all possible solutions of the IVP of the system (20) can be computed. This guaranteed enclosure is achieved by the union of all guaranteed enclosure sets, which are computed by solving the IVPs of (22). To illustrate the results of reducing the overestimation, the second example is investigated once again.

4.1 Second Example with Reduced Overestimation

To compute the guaranteed enclosure of the uncertain system of the second example, the parameters do not need to be expanded. Choosing $\alpha = (1 \ -1 \ 1)^T$, the Jacobian of the condition (31) results in

$$\frac{\partial \mathbf{g}}{\partial \mathbf{z}} = \begin{pmatrix} -2 \hat{p}_2 x_1 & \hat{p}_1 & x_2 x_1^2 & 0 \\ \hat{p}_2 + \hat{p}_3 x_2 & -2 \hat{p}_3 x_2 + \hat{p}_3 x_1 & 0 & x_1 x_1 x_2 - x_2^2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

The conditions (29) are

$$f_1(0, x_2) = \hat{p}_1 x_2 \geq 0 \text{ and } f_2(x_1, 0) = -\hat{p}_2 x_1 \geq 0.$$

The conditions (30) result in

$$\begin{aligned}
 \frac{d}{dt} \left(\frac{\partial x_1}{\partial \hat{p}_1} \right) \Big|_{\frac{\partial x_1}{\partial \hat{p}_1}=0} &= \hat{p}_1 \left(\frac{\partial x_2}{\partial \hat{p}_1} \right) + x_2 \geq 0 \\
 \frac{d}{dt} \left(\frac{\partial x_2}{\partial \hat{p}_1} \right) \Big|_{\frac{\partial x_2}{\partial \hat{p}_1}=0} &= (\hat{p}_2 + \hat{p}_3 x_2) \left(\frac{\partial x_1}{\partial \hat{p}_1} \right) \geq 0
 \end{aligned}$$

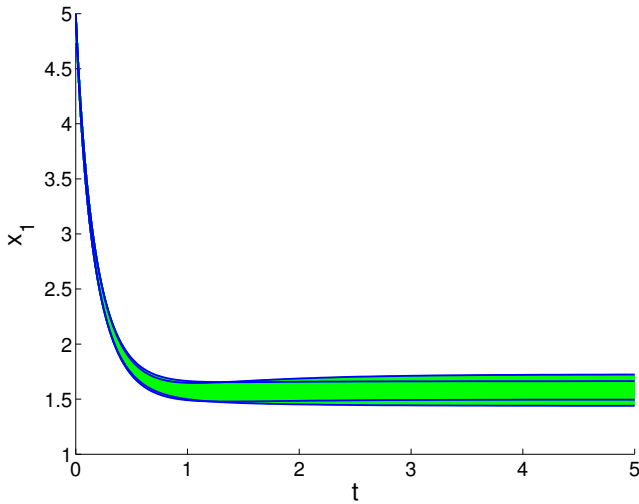


Fig. 5. second example with no overestimation: simulation of x_2 with guaranteed bounds and Monte-Carlo simulations

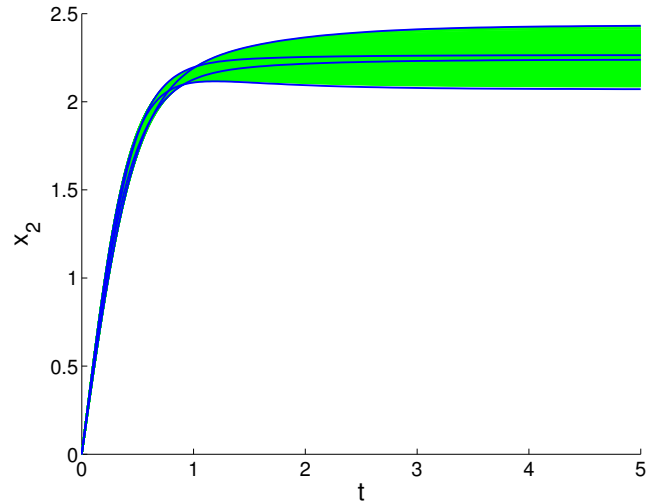


Fig. 6. third example with no overestimation: simulation of x_2 with guaranteed bounds and Monte-Carlo simulations

$$\begin{aligned} \frac{d}{dt} \left(\frac{\partial x_1}{\partial \hat{p}_2} \right) \Big|_{\frac{\partial x_1}{\partial \hat{p}_2}=0} &= \hat{p}_1 \left(\frac{\partial x_2}{\partial \hat{p}_2} \right) + x_1^2 \geq 0 \\ \frac{d}{dt} \left(\frac{\partial x_2}{\partial \hat{p}_2} \right) \Big|_{\frac{\partial x_2}{\partial \hat{p}_2}=0} &= (\hat{p}_2 + \hat{p}_3 x_2) \left(\frac{\partial x_1}{\partial \hat{p}_2} \right) + x_1 \geq 0 \\ \frac{d}{dt} \left(\frac{\partial x_1}{\partial \hat{p}_3} \right) \Big|_{\frac{\partial x_1}{\partial \hat{p}_3}=0} &= \hat{p}_1 \left(\frac{\partial x_2}{\partial \hat{p}_3} \right) \geq 0 \\ \frac{d}{dt} \left(\frac{\partial x_2}{\partial \hat{p}_3} \right) \Big|_{\frac{\partial x_2}{\partial \hat{p}_3}=0} &= (\hat{p}_2 + \hat{p}_3 x_2) \left(\frac{\partial x_1}{\partial \hat{p}_3} \right) + x_1 x_2 - x_2^2 \geq 0. \end{aligned}$$

The conditions (29), (30) and (31) are satisfied for $x_1 \geq x_2$ because in the (2, 5)-entry of the Jacobian as well as in $\frac{d}{dt} \left(\frac{\partial x_2}{\partial \hat{p}_3} \right)$ the term $x_1 x_2 - x_2^2$ does not fulfill the nonnegativity condition for all \mathbf{x} . Thus, a second parameter vector with $\boldsymbol{\alpha} = (1 \quad -1 \quad -1)^T$ is chosen. Now, the Jacobian results in

$$\frac{\partial \mathbf{g}}{\partial \mathbf{z}} = \begin{pmatrix} -2 \hat{p}_2 x_1 & \hat{p}_1 & x_2 & x_1^2 & 0 \\ \hat{p}_2 + \hat{p}_3 x_2 & 2 \hat{p}_3 x_2 - \hat{p}_3 x_1 & 0 & x_1 & -x_1 x_2 + x_2^2 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

The partial derivative of interest is given by

$$\frac{d}{dt} \left(\frac{\partial x_2}{\partial \hat{p}_3} \right) \Big|_{\frac{\partial x_2}{\partial \hat{p}_3}=0} = (\hat{p}_2 + \hat{p}_3 x_2) \left(\frac{\partial x_1}{\partial \hat{p}_3} \right) - x_1 x_2 + x_2^2 \geq 0$$

Thus, the conditions (29), (30) and (31) are satisfied for $x_1 \leq x_2$. The guaranteed enclosure of all possible solutions of the IVP given by the system (25) is computed by the union of both guaranteed enclosures using the parameter vectors $\hat{\mathbf{p}}$ above given. The simulation results are shown in Fig. 5 and 6. As one can see, the union set of the guaranteed enclosures is almost completely filled by the 512 green Monte-Carlo simulations. Strictly speaking the computed guaranteed bounds provided by the method of section 4 are the exact enclosure of all possible solutions of the IVP of the uncertain system (25).

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