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Brief paper

Barrier certificates for nonlinear model validation☆

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Abstract

Methods for model validation of continuous-time nonlinear systems with uncertain parameters are presented in this paper. The methods employ functions of state-parameter-time, termed barrier certificates, whose existence proves that a model and a feasible parameter set are inconsistent with some time-domain experimental data. A very large class of models can be treated within this framework; this includes differential-algebraic models, models with memoryless/dynamic uncertainties, and hybrid models. Construction of barrier certificates can be performed by convex optimization, utilizing recent results on the sum of squares decomposition of multivariate polynomials.

Keywords: Model validation; Nonlinear systems; Barrier certificates; Semidefinite programming relaxations

1. Introduction

Modelling is an important precursor to system analysis and controller design. For successful analysis and design, it is crucial to obtain a model that captures essential behaviors of the system under consideration. Model validation provides a way to evaluate the ability of a proposed model to represent observed system behaviors. However, as often mentioned in the literature (Dullerud & Smith, 2002; Poolla, Khargonekar, Tikku, Krause, & Nagpal, 1994; Smith & Doyle, 1992), "model validation" is actually a misnomer. It is impossible to validate a model, because to do so requires an infinite number of experiments and data. The role of model validation techniques is to *invalidate* a model by proving that some experimental data are inconsistent with the model, thus indicating that a refinement is required.

Model validation was first treated in Smith and Doyle (1992) in the context of invalidation using frequency-domain data. Other references include (Chen & Wang, 1996; Poolla et al., 1994), in which model validation using time-domain data was addressed, and (Rangan & Poolla, 1996; Smith & Dullerud, 1996), which considered sampled-data models. Model validation using mixed frequency-domain and time-domain data was investigated in Xu, Ren, Gu, and Chen (1999). Quite recently, nonlinear model validation was addressed in Dullerud and Smith (2002), Smith and Dullerud (1999), and model validation of linear parameter varying models was considered in Sznaier and Mazzaro (2003). Most of these work addressed deterministic model validation in the robust control domain—typically by representing the model as a linear fractional transformation (LFT) between a linear time invariant system and an uncertainty/nonlinearity block, and their results are obtained using operator theoretic approaches. In the statistical settings, model validation was addressed e.g. in Gevers, Bombois, Codrons, Scorletti, and Anderson (2003), Lee and Poolla (1996), Ljung and Guo (1997). Besides modelling, model validation is related to and has applications in the areas of system identification, fault detection, prediction, and verification. See e.g. Frenklach, Packard, and Seiler (2002) for results on prediction using model and data.

In this paper, we present a methodology for invalidation of continuous-time nonlinear models with uncertain parameters. The methodology is based on functions of state-parameter-time which we term *barrier certificates*, that are reminiscent of Lyapunov functions or storage functions (Willems, 1972). Some level sets of a barrier certificate act as "barriers" between possible model trajectories and time-domain experimental data, and such a function proves/certifies in an exact manner that the

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model and its associated parameter set are inconsistent with the data. Different from the methods presented in e.g. Dullerud and Smith (2002), Smith and Dullerud (1999), Sznaier and Mazzaro (2003), our approach draws inspiration from Lyapunov-based analysis in nonlinear systems theory, and can be directly applied to a state-space model without converting it to an LFT form first.

With this methodology, we are able to treat in a unified way model validation of a very large class of continuous-time nonlinear models—some of which have never been addressed before. This class of models, which is a much larger class than the one that can be handled by Dullerud and Smith (2002), Smith and Dullerud (1999), includes differential-algebraic models (Campbell, 1980), models with uncertain inputs (Megretski & Rantzer, 1997), models with memoryless and dynamic uncertainties (Khalil, 1996; Megretski & Rantzer, 1997), hybrid models (van der Schaft & Schumacher, 2000), and their combinations. Moreover, the methods are computationally tractable, as barrier certificates can be constructed using the sum of squares (SOS) decomposition (Parrilo, 2000) and semidefinite programming (Vandenberghe & Boyd, 1996), for which software tools (Prajna, Papachristodoulou, Seiler, & Parrilo, 2005) are available. These we consider as some of the most important features of our approach.

In Section 2, several invalidation settings are considered and basic results on invalidation using barrier certificates are presented. The key ideas will be illustrated using some simple, easy to visualize examples. Section 3 is devoted to computational issues. In particular, it will be shown how the search for a barrier certificate can be formulated as a convex optimization problem, based on the SOS decomposition. Sections 4 and 5, respectively, address the invalidation methods for models with constraints and hybrid models. An application example will be given in Section 6.

2. Invalidation using barrier certificates

2.1. The two-measurement case

Consider the following ordinary differential equation (ODE) model in the state-space form:

$$\dot{x}(t) = f(x(t), p, t), \tag{1}$$

where $x(t) \in \mathbb{R}^{n_x}$ is the vector of state variables, t is the time, and $p \in \mathbb{R}^{n_p}$ is the parameter vector, assumed to take its value in a set $P \subset \mathbb{R}^{n_p}$. Let an experiment be performed with the real system, and two sets of measurements be taken at time $t = 0$ and T. Suppose that these measurements indicate that $x(0) \in X_0 \subset \mathbb{R}^{n_x}$ and $x(T) \in X_T \subset \mathbb{R}^{n_x}$. In addition, assume that $x(t) \in X \subseteq \mathbb{R}^{n_x}$ for all $t \in [0, T]$. The invalidation problem can now be stated as follows:

Problem 1. Given the model (1), parameter set P, and trajectory information $\{X_0, X_T, X\}$, prove that for all possible parameter $p \in P$, model (1) cannot produce a trajectory $x(t)$ such that $x(0) \in X_0$, $x(T) \in X_T$, and $x(t) \in X$ $\forall t \in [0, T]$.

Before proceeding further, we would like to remark that necessarily $X_0 \subseteq X$ and $X_T \subseteq X$, and in most cases X will be *much larger* than X_0 or X_T. In fact, X can be the whole state space. The information about X may come from the experiment and/or a priori knowledge about the system,[1] and such information will strengthen the model validation test. Note also that output measurement using the output $y(t) = g(x(t))$ can be accommodated. For example, if measurements of the scalar output components $y_i(t) = g_i(x(t))$, $i = 1, \ldots, n_y$ indicate that $\underline{y}_i \leqslant y_i(t) \leqslant \overline{y}_i$ at time $t = 0$, then X_0 should be defined as $X_0 = \{x \in X : \underline{y}_i \leqslant g_i(x) \leqslant \overline{y}_i, \text{ for } i = 1, \ldots, n_y\}$.

If such a proof in Problem 1 can be found, then we say that the model (1) and parameter set P are invalidated by $\{X_0, X_T, X\}$. Traditional approaches for solving this problem include exhaustive simulation of (1) using parameters p and initial conditions $x(0)$ sampled randomly from P and X_0. If no trajectory $x(t)$ satisfying the initial hypothesis is found after many such simulations, then inconsistency is concluded. Indeed simulation (possibly after parameter fitting) is a way for proving that a model can reproduce *some* behaviors of the system it represents. However, for proving inconsistency, the required number of simulation runs will soon become prohibitive. Moreover, a proof by simulation alone is *never exact*, simply because it is impossible to test all p and $x(0)$.

On the other hand, our method relies on the existence of a function of state-parameter-time, which we term barrier certificate. A barrier certificate gives an *exact* proof of inconsistency by providing a barrier between possible trajectories of the model starting at X_0 and the final measurement X_T. This is accomplished without performing any simulation nor computing the flow of the model. The method is summarized in Theorem 2 below. Although for most physical models the solution to the ODE (1) starting from a given initial condition will be unique, such an assumption is not needed, and we only ask that the vector field $f(x, p, t)$ be continuous in x and t, enough to guarantee the local existence and also the continuous differentiability of solutions to the ODE.

Theorem 2. *Let the model* (1) *and the sets* P, X_0, X_T, X *be given, with* $f(x, p, t)$ *being continuous in x and t. Suppose that there exists a real-valued function* $B(x, p, t)$ *that is differentiable with respect to x and t, such that*

$$B(x_T, p, T) - B(x_0, p, 0) > 0 \quad \forall (x_T, x_0, p) \in X_T \times X_0 \times P, \tag{2}$$

$$\frac{\partial B}{\partial x}(x, p, t) f(x, p, t) + \frac{\partial B}{\partial t}(x, p, t) \leqslant 0 \quad \forall (x, p, t) \in X \times P \times [0, T]. \tag{3}$$

Then the model (1) *and its associated parameter set P are invalidated by* $\{X_0, X_T, T\}$. (*In the sequel, we will call the function* $B(x, p, t)$ *a barrier certificate*.)

[1] For example, in biological systems typical state variables are the concentration of some chemical substrates, which can be neither negative nor very large.

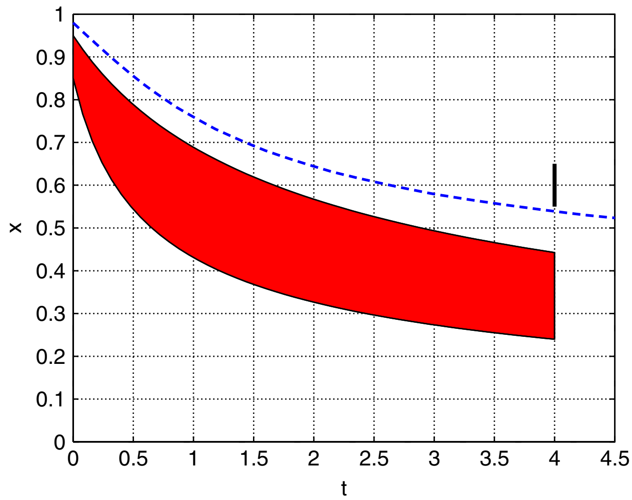

Fig. 1. A level set of the barrier certificate $B(x,t)$ in Example 4 is shown as the dashed curve. Bold line at $t=4$ is X_T, whereas the solid patch depicts all possible trajectories of the model starting at $x(0)\in X_0$, with $p\in P$. Since X_T is not reachable by these trajectories, the model is invalidated.

Proof. Our proof is by contradiction. Suppose that there exists a $B(x,p,t)$ satisfying conditions (2)–(3), while at the same time there are parameters $p\in P$ and initial conditions $x_0\in X_0$ such that a trajectory $x(t)$ of the model $\dot{x}=f(x,p,t)$ starting at $x(0)=x_0$ satisfies $x(t)\in X$ for all $t\in[0,T]$ and $x(T)\in X_T$. Condition (3) states that the total derivative of $B(x(t),p,t)$ with respect to time is non-positive on the time interval $[0,T]$, implying that $B(x(T),p,T)\leqslant B(x(0),p,0)$, which is contradictory to (2). Thus, the model (1) and parameter set P are invalidated by $\{X_0,X_T,X\}$. □

For illustration, consider the following simple examples.

Example 3. Consider a model $\dot{x}_1=x_1+2x_2$, $\dot{x}_2=x_1x_2-0.5x_2^2$ on $X=\mathbb{R}^2$. Let the measurement data be $X_0=[-1,1]^2$ and $X_T=[-1,1]\times[3,5]$ at $T=1$. We show that the measurements are inconsistent with the model by constructing a barrier certificate, $B(x)=-0.25x_1^2+x_2-2$. The zero level set of $B(x)$ provides a "barrier", in the sense that any flow starting at X_0 can never cross this set to reach X_T, as can be proven using the facts that $(\partial B/\partial x_1)\dot{x}_1+(\partial B/\partial x_2)\dot{x}_2=-0.5x_1^2-0.5x_2^2\leqslant 0$, $B(x)<0$ $\forall x\in X_0$, and $B(x)>0$ $\forall x\in X_T$.

Example 4. Consider the model $\dot{x}=-px^3$, with $X=\mathbb{R}$ and $P=[0.5,2]$. The measurement data used for invalidation are $X_0=[0.85,0.95]$ and $X_T=[0.55,0.65]$ at $T=4$. We construct a barrier certificate that is time dependent of the form $B(x,t)=B_1(x)+tB_2(x)$, where $B_1(x)$ and $B_2(x)$ are polynomials in x. Using the computational method that will be described in Section 3 and the software (Prajna et al., 2005), we obtain $B(x,t)=8.35x+10.4x^2-21.5x^3+9.86x^4-1.78t+6.58tx-4.12tx^2-1.19tx^3+1.54tx^4$ as a barrier certificate. It is shown in Fig. 1 how a level set of $B(x,t)$ serves as a barrier in the state-time space.

2.2. Piecewise constant inputs

An important class of model validation problems corresponds to the case where experiments are performed by applying inputs to the system, e.g. piecewise constant inputs (Rangan & Poolla, 1996; Smith & Dullerud, 1996). Suppose that the model is given by

$$\dot{x}(t)=f(x(t),p,u(t),t), \tag{4}$$

where $u(t)\in\mathbb{R}^{n_u}$ is the input. Let a sequence of inputs $u_0,u_1,\ldots,u_{N-1}$ be applied to the system by defining $u(t)=u_i$ for $t\in[T_i,T_{i+1})$, with $0\triangleq T_0<T_1<\cdots<T_{N-1}<T_N\triangleq T$, and $u(T)=u_{N-1}$. The exact values of u_i for $i=0,\ldots,N-1$ are not known, although it is known that they take values in some sets $U_0,U_1,\ldots,U_{N-1}\subseteq\mathbb{R}^{n_u}$. We assume that the measurements are performed at $t=0$ and T, with the results denoted using the same notations as in Section 2.1. For brevity, let us also define $I=\{0,1,\ldots,N-1\}$.

A straightforward approach to invalidation in this case is to use the test in Theorem 2, with (3) replaced by $(\partial B/\partial x)(x,p,t)f(x,p,u_i,t)+(\partial B/\partial t)(x,p,t)\leqslant 0$ for all $i\in I$ and $(x,p,u_i,t)\in X\times P\times U_i\times[T_i,T_{i+1})$. Unfortunately, this test is often too restrictive, as we require B (which is continuous in time) to satisfy the above condition for all $i\in I$. A more relaxed condition is obtained by using different B_i's for different i and concatenating them to form a barrier certificate on the whole interval. This is a special case of *discontinuous* barrier certificates, which we will also use for invalidation of hybrid models in Section 5. The conditions for invalidation are as follows.

Theorem 5. *Consider the model* (4) *with $f(x,p,u,t)$ being continuous in x and t, and let the sets P, X_0, X_T, X, $U_0,\ldots,U_{N-1}$ be given. Suppose there exist real-valued functions $B_i(x,p,u,t)$ for all $i\in I$, that are differentiable with respect to x and t, and satisfy*:

$$B_{N-1}(x_T,p,u_{N-1},T)-B_0(x_0,p,u_0,0)>0$$
$$\forall x_T\in X_T,\quad x_0\in X_0,\quad p\in P,\quad u_{N-1}\in U_{N-1},\quad u_0\in U_0, \tag{5}$$

$$\frac{\partial B_i}{\partial x}f(x,p,u_i,t)+\frac{\partial B_i}{\partial t}(x,p,u_i,t)\leqslant 0$$
$$\forall i\in I,\quad x\in X,\quad p\in P,\quad u_i\in U_i,\quad t\in[T_i,T_{i+1}), \tag{6}$$

$$B_{i+1}(x,p,u_{i+1},T_{i+1})-B_i(x,p,u_i,T_{i+1})\leqslant 0$$
$$\forall i\in I\backslash\{N-1\},\quad x\in X,\quad p\in P,\quad u_{i+1}\in U_{i+1},\quad u_i\in U_i. \tag{7}$$

Then the model (4) *and parameter set P are invalidated by* $\{X_0,X_T,X,U_0,\ldots,U_{N-1}\}$.

Proof. Suppose that some functions B_i satisfying (5)–(7) can be found, yet there exists a trajectory $x(t)$ of (4) for some $p\in P$ and input sequence $u_0,u_1,\ldots,u_{N-1}$ such that $x(0)\in X_0$, $x(T)\in X_T$, $x(t)\in X$ for all $t\in[0,T]$, and $u_i\in U_i$. Now consider the function $B(t)$ defined by $B(t)=B_i(x(t),p,u_i,t)$ for $t\in[T_i,T_{i+1})$, and $B(T_N)=B_{N-1}(x(T_N),p,u_{N-1},T_N)$.

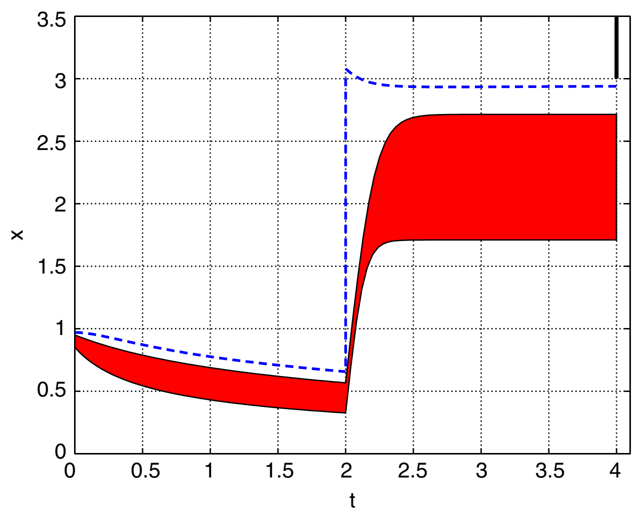

Fig. 2. A level set of the discontinuous barrier certificate in Example 6 is depicted by the dashed curve. Bold line at the upper right corner is X_T, whereas the solid patch is all possible trajectories of the model.

Condition (6) states that $B(t)$ is non-increasing on each of the time interval $[T_i, T_{i+1})$, while (7) states that it is also non-increasing at each T_{i+1}. Thus, the statement of the theorem follows via a contradiction with (5). □

Example 6. Consider the model $\dot{x} = -px^3 + u$, with $X = \mathbb{R}$ and $P = [0.5, 2]$. Assume that an input $u_0 \in [-0.05, 0.05]$ is applied on the time interval $[0, 2]$, followed by $u_1 \in [9.95, 10.05]$ on the interval $[2, 4]$. The measurement data used for invalidation are $X_0 = [0.85, 0.95]$ and $X_T = [3.00, 3.50]$ at $T = 4$. For this example, a continuous barrier certificate might be hard to find, due to the extreme discontinuity of the vector field at $t = 2$. However, invalidation can be performed using a discontinuous barrier certificate as suggested in Theorem 5. A level set of such barrier certificate is shown in Fig. 2.[2]

For invalidation of models with other kinds of inputs, such as uncertain inputs, see Section 4.

2.3. Three measurements and beyond

We will now discuss the case of three or more measurements. Assume that measurements performed at $t = T_0, T_1, \ldots, T_N$ indicate that $x(T_i) \in X_{T_i}$. These data will be used for invalidating the model (1).

A direct, computationally less expensive way to achieve this is to consider the measurements pairwise (for example at $t = T_i$ and T_j, where $i < j$), and use Theorem 2 to invalidate the model. Unfortunately, this approach may be conservative. The reason is that for all possible i and j the parameter sets $\tilde{P}_{ij} \subseteq P$ defined by

$$\tilde{P}_{ij} = \{p \in P : \exists x(t) \text{ s.t. } \dot{x} = f(x, p, t), x(T_i) \in X_i,\ x(T_j) \in X_j, \text{ and } x(t) \in X\ \forall t \in [T_i, T_j]\}$$

may not be empty, even if the set

$$\tilde{P} = \{p \in P : \exists x(t) \text{ s.t. } \dot{x} = f(x, p, t), x(T_i) \in X_i \text{ for } i = 0, \ldots, N, \text{ and } x(t) \in X\ \forall t \in [T_0, T_N]\}$$

is empty. Since the $\tilde{P}_{ij}$'s are not empty, each pair $\{X_{T_i}, X_{T_j}\}$ is consistent with the model, and therefore we will not be able to find a barrier certificate associated to it. On the contrary, the model is actually inconsistent with the data $X_0, \ldots, X_T$, because $\tilde{P}$ is empty.

To overcome this conservatism, all the measurement data need to be considered at once and the couplings between two segments of state trajectory (namely that $\lim_{t \to T_i^-} x(t) = \lim_{t \to T_i^+} x(t) = x(T_i)$) need to be taken into account. This is accomplished using an extended model that captures the evolution of all trajectory segments in parallel, as described in the next theorem.

Theorem 7. *Consider the model* (1) *with $f(x, p, t)$ being continuous in x and t, the parameter set P, and the trajectory data $\{X_{T_0}, \ldots, X_{T_N}, X\}$. Let $\Delta T_i = T_i - T_{i-1}$ for $i = 1, 2, \ldots, N$, and define the extended vector field $\tilde{f}(\tilde{x}, p, t)$ as follows*:

$$\tilde{f}(\tilde{x}, p, t) = \begin{bmatrix} \Delta T_1 f(\tilde{x}_1, p, t\Delta T_1 + T_0) \\ \Delta T_2 f(\tilde{x}_2, p, t\Delta T_2 + T_1) \\ \vdots \\ \Delta T_N f(\tilde{x}_N, p, t\Delta T_N + T_{N-1}) \end{bmatrix}, \tag{8}$$

where $\tilde{x} = (\tilde{x}_1, \tilde{x}_2, \ldots, \tilde{x}_N) \in \mathbb{R}^{Nn_x}$, $\tilde{x}_i \in \mathbb{R}^{n_x}$ for each i. Suppose that there exists a real-valued function $\tilde{B}(\tilde{x}, p, t)$, that is differentiable with respect to $\tilde{x}$ and t, such that

$$\tilde{B}(\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_N, p, 1) - \tilde{B}(\hat{x}_0, \hat{x}_1, \ldots, \hat{x}_{N-1}, p, 0) > 0 \quad \forall \hat{x}_i \in X_{T_i},\ i = 0, 1, \ldots, N, \text{ and } \forall p \in P, \tag{9}$$

$$\frac{\partial \tilde{B}}{\partial \tilde{x}}(\tilde{x}, p, t)\tilde{f}(\tilde{x}, p, t) + \frac{\partial \tilde{B}}{\partial t}(\tilde{x}, p, t) \leqslant 0 \quad \forall \tilde{x} \in X^N,\ p \in P,\ t \in [0, 1]. \tag{10}$$

Then the model (1) *and parameter set P are inconsistent with the data $\{X_{T_0}, \ldots, X_{T_N}, X\}$. Moreover, this test is more powerful than the test performed by considering the measurements pairwise, in the sense that if the pairwise measurement test can invalidate the model, then so can the test in this theorem, but not vice versa.*

Proof. Suppose that a $\tilde{B}(\tilde{x}, p, t)$ satisfying (9)–(10) can be found, but there exists also a trajectory $x(t)$ of (1) for some $p \in P$ satisfying $x(T_i) \in X_{T_i}$ for $i = 0, 1, \ldots, N$, and $x(t) \in X$ for all $t \in [T_0, T_N]$. Now consider the flow of the extended model $\dot{\tilde{x}} = \tilde{f}(\tilde{x}, p, t)$, starting with initial conditions

[2] For this plot, we deliberately fix u_0 and u_1 equal to 0 and 10. Otherwise a four-dimensional plot will be required to depict correctly both the trajectories and the level set of the barrier certificate, which is also a function of u_0 and u_1.

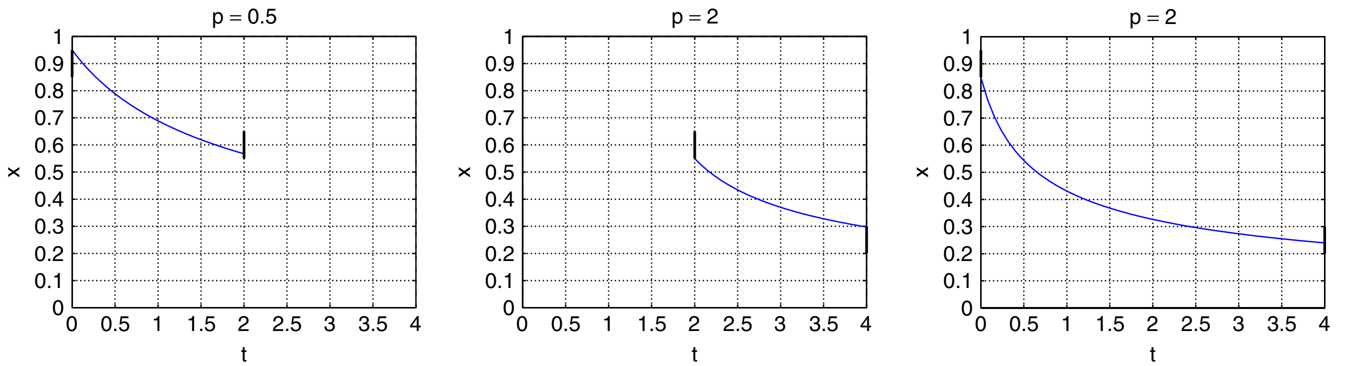

Fig. 3. When considered pairwise, the measurements in Example 8 do not invalidate the model. From left to right, the figures show trajectories connecting X_{T_0} to X_{T_1}, X_{T_1} to X_{T_2}, and X_{T_0} to X_{T_2}, for parameters $p=0.5, 2,$ and 2, respectively.

$\tilde{x}_1(0)=x(T_0)$, $\tilde{x}_2(0)=x(T_1),\ldots,\tilde{x}_N(0)=x(T_{N-1})$. At this point, notice that the vector field $\Delta T_i f(\tilde{x}_i, p, t\Delta T_i+T_{i-1})$ is obtained by time rescaling of the vector field $f(x,p,t)$, such that the time interval $[T_{i-1},T_i]$ for the original vector field corresponds to the interval [0, 1] for the new vector field. Because of this, for the initial conditions given above we have $\tilde{x}_1(1)=x(T_1)$, $\tilde{x}_2(1)=x(T_2),\ldots,\tilde{x}_N(1)=x(T_N)$. By considering the evolution of $\tilde{B}(\tilde{x}(t),p,t)$ on the time interval [0, 1], the inconsistency between the model and data can be proven in the same manner as in Theorem 2.

Finally, to prove that this test is more powerful than the pairwise measurement test, suppose that for some pair of measurements X_{T_i} and X_{T_j} (with $i<j$) a barrier certificate $B(x,p,t)$ satisfying the conditions stated in Theorem 2 can be found. From $B(x,p,t)$, a barrier certificate $\tilde{B}(\tilde{x},p,t)$ for the extended vector field can be constructed by defining $\tilde{B}(\tilde{x},p,t)=B(\tilde{x}_i,p,t\Delta T_{i+1}+T_i)+B(\tilde{x}_{i+1},p,t\Delta T_{i+2}+T_{i+1})+\cdots+B(\tilde{x}_{j-1},p,t\Delta T_j+T_{j-1})$. It can be verified that $\tilde{B}(\tilde{x},p,t)$ satisfies all the conditions in Theorem 7, showing that if the pairwise measurement test can invalidate the model, then so can the test in Theorem 7. The converse is not true, as can be seen from the arguments given at beginning of this subsection and also Example 8. □

Two things should be noted in relation to Theorem 7. First, the fact that the parameter of the system does not change along the whole trajectory $x(t)$ is taken into account by using the same parameter p for all the components $\Delta T_i f(\tilde{x}_i,p,t\Delta T_i+T_{i-1})$ of the extended vector field (8). Second, the continuation condition between the trajectory segments is actually imposed in (9). This is achieved by requiring the final value of $\tilde{x}_i(t)$, which enters as an argument of the first term in this inequality (cf. also condition (2)) and is denoted by $\hat{x}_i$, to be the same as the initial condition of $\tilde{x}_{i+1}(t)$, which enters as an argument of the second term.

Example 8. Consider the same model $\dot{x}=-px^3$ as in Example 4, with $X=\mathbb{R}$ and $P=[0.5,2]$. Let the measurement data be $X_{T_0}=[0.85,0.95]$, $X_{T_1}=[0.55,0.65]$, $X_{T_2}=[0.20,0.30]$, where $T_0=0$, $T_1=2$, and $T_2=4$. In this case, the pairwise measurement test will not be able to invalidate the model. In fact, each of the pairs $\{X_{T_0},X_{T_1}\}$, $\{X_{T_1},X_{T_2}\}$,and $\{X_{T_0},X_{T_2}\}$ is consistent with the model, because

- for $x(0)=0.95$ and $p=0.5$, we have $x(2)\in[0.55,0.65]$,
- for $x(2)=0.55$ and $p=2$, we have $x(4)\in[0.20,0.30]$,
- for $x(0)=0.85$ and $p=2$, we have $x(4)\in[0.20,0.30]$.

See Fig. 3. However, as the reader may expect already, these measurement data are actually inconsistent with the model. The barrier certificate $B(\tilde{x},t)=6.81\tilde{x}_1-57.9\tilde{x}_2+13.4\tilde{x}_1^2-50.3\tilde{x}_1\tilde{x}_2+94.4\tilde{x}_2^2-3.66t+2.53t\tilde{x}_1+9.05t\tilde{x}_2+.758t\tilde{x}_1^2+7.25t\tilde{x}_1\tilde{x}_2-25.9t\tilde{x}_2^2$ satisfies all the conditions in Theorem 7, thus proving the inconsistency.

Several variations of Theorem 7 can be derived for various other invalidation settings. Three of such instances are (i) invalidation of a model using several experiments that correspond to different initial conditions, (ii) invalidation of a model using several experiments, where some parameters may differ from one experiment to another, and (iii) invalidation of a model using piecewise constant inputs as in Section 2.2, but with measurements also performed at time $t=T_1,T_2,\ldots,T_{N-1}$. We leave it to the reader to derive suitable conditions for barrier certificates in the respective settings.

3. Construction of barrier certificates

Similar to the case of Lyapunov functions, construction of barrier certificates is in general not easy. In fact, even verifying that the conditions (2)–(3) are satisfied by a given barrier certificate is hard. However, for models with polynomial vector fields and sets P, X_{T_i}, X, U_i described by polynomial equalities and inequalities, a tractable computational relaxation for constructing barrier certificates exists. The relaxation is provided by the *sum of squares decomposition* (Parrilo, 2000).

A multivariate polynomial $p(x)$ is a SOS if there exist polynomials $p_1(x),\ldots,p_m(x)$ such that $p(x)=\sum_{i=1}^m p_i^2(x)$. This is equivalent to the existence of a positive semidefinite matrix Q and a properly chosen vector of monomials $Z(x)$ such that

$p(x)=Z^{\mathrm{T}}(x)QZ(x)$. An SOS decomposition for $p(x)$ can be computed using semidefinite programming (Vandenberghe & Boyd, 1996). Coupled with the property that $p(x)$ being an SOS implies[3] $p(x)\geqslant 0$, the SOS decomposition provides a computational relaxation for proving polynomial positivity, which belongs to the class of NP-hard problems.

The SOS decomposition has been exploited for algorithmically constructing Lyapunov functions for nonlinear systems (Papachristodoulou & Prajna, 2002; Parrilo, 2000). Similar idea can be used in the computation of barrier certificates. In this case, real coefficients $c_1, \ldots, c_m$ are used to parameterize a set of candidate barrier certificates in the following way:

$$\mathscr{B}=\left\{B(x,p,t): B(x,p,t)=\sum_{j=1}^{m} c_j b_j(x,p,t)\right\}, \qquad (11)$$

where the $b_j(x,p,t)$'s are some polynomials in x, p, t; for example they could be monomials of degree less than or equal to some pre-chosen bound. Then the search for a barrier certificate $B(x,p,t)\in\mathscr{B}$, or equivalently coefficients c_j's, such that the conditions in Theorems 2, 5, or 7 are satisfied can still be formulated as an SOS problem and solved using semidefinite programming.

More concretely, consider the two-measurement case with the model $\dot{x}=f(x,p,t)$, where f is polynomial. Assume that the parameter set is defined as follows:

$$P=\{p\in\mathbb{R}^{n_p} : g_{P,i}(p)\geqslant 0 \ \forall i\in I_P\}, \qquad (12)$$

where the $g_{P,i}(p)$'s are polynomials in p, and I_P is an index set. For example, when the components of p take values on the intervals $\underline{p_i}\leqslant p_i\leqslant \overline{p_i}$, we may define $g_{P,i}(p)=(p_i-\underline{p_i})(\overline{p_i}-p_i)$, for $i\in I_P=\{1,\ldots,n_p\}$. Similarly, let the trajectory data be defined by

$$X_0=\{x_0\in\mathbb{R}^{n_x} : g_{0,i}(x_0)\geqslant 0 \ \forall i\in I_0\}, \qquad (13)$$
$$X_T=\{x_T\in\mathbb{R}^{n_x} : g_{T,i}(x_T)\geqslant 0 \ \forall i\in I_T\}, \qquad (14)$$
$$X=\{x\in\mathbb{R}^{n_x} : g_{X,i}(x)\geqslant 0 \ \forall i\in I_X\}. \qquad (15)$$

Then a barrier certificate can be computed by solving the convex optimization problem given in Algorithm 9.

Algorithm 9.

(1) *Fix a degree bound for the barrier certificate, and parameterize $B(x,p,t)$ in terms of some unknown coefficients c_j's as in* (11), *by having all monomials whose degrees are less than the degree bound as the $b_j(x,p,t)$'s.*
(2) *In a similar way, fix some degree bounds and use some other unknown coefficients c_j's to parameterize polynomials $M_{P,i}(x_0,x_T,p)$ for all $i\in I_P$, $M_{0,i}(x_0,x_T,p)$ for all $i\in I_0$, $M_{T,i}(x_0,x_T,p)$ for all $i\in I_T$, $N_{P,i}(x,p,t)$ for all $i\in I_P$, $N_{X,i}(x,p,t)$ for all $i\in I_X$, and $N_t(x,p,t)$.*
(3) *Choose a small positive number ε.*
(4) *Find the values of c_j's which make the expressions* (16)–(17) *and the polynomials $M_{P,i}$'s, $M_{0,i}$'s, $M_{T,i}$'s, $N_{P,i}$'s, $N_{X,i}$'s, and N_t sums of squares.*

$$\begin{aligned}&B(x_T,p,T)-B(x_0,p,0)-\varepsilon\\&\quad-\sum_{i\in I_P} M_{P,i}(x_0,x_T,p)g_{P,i}(p)\\&\quad-\sum_{i\in I_0} M_{0,i}(x_0,x_T,p)g_{0,i}(x_0)\\&\quad-\sum_{i\in I_T} M_{T,i}(x_0,x_T,p)g_{T,i}(x_T),\end{aligned} \qquad (16)$$

$$\begin{aligned}&-\frac{\partial B}{\partial x}(x,p,t)f(x,p,t)-\frac{\partial B}{\partial t}(x,p,t)\\&\quad-\sum_{i\in I_P} N_{P,i}(x,p,t)g_{P,i}(p)\\&\quad-\sum_{i\in I_X} N_{X,i}(x,p,t)g_{X,i}(x)-N_t(x,p,t)(Tt-t^2).\end{aligned} \qquad (17)$$

The above problem is an SOS optimization problem, which is a convex programming problem and can be solved efficiently for the unknown coefficients c_j's using semidefinite programming, e.g., with the software (Prajna et al., 2005).

Proposition 10. *Let the model $\dot{x}=f(x,p,t)$ and the sets P, X_0, X_T, X in* (12)–(15) *be given. If the SOS optimization problem given in Algorithm* 9 *is feasible, then the polynomial $B(x,p,t)$ obtained by substituting the corresponding values of c_j's to its polynomial parameterization satisfies the conditions* (2)–(3) *of Theorem* 2, *and therefore $B(x,p,t)$ is a barrier certificate.*

Proof. First notice that the expressions (16)–(17) are nonnegative, since they are sums of squares. Now take any $x_0\in X_0$, $x_T\in X_T$, and $p\in P$. For any such triplets the last three terms in (16) are non-positive, and therefore it follows that $B(x_T,p,T)-B(x_0,p,0)-\varepsilon\geqslant 0$. Since ε is positive, condition (2) is immediately satisfied. Next, take any $t\in[0,T]$, $x\in X$, $p\in P$ and consider (17). Using the same argument as the above, it is straightforward to show that condition (3) is satisfied. □

Although the approach in this section assumes that the description of the model and sets are polynomial, non-polynomial descriptions can be handled (although possibly with conservatism) in at least two different ways. First, a non-polynomial vector field can be approximated by a polynomial vector field, and the approximation error can be "covered" by including some uncertainty description, which we will treat in Section 4. In a similar way we can cover sets with non-polynomial descriptions with those described using polynomials. Second, for some non-polynomial systems, algebraic recasting of variables can be used to transform the system to a polynomial system, possibly plus some algebraic constraints. The details of this can be found in Papachristodoulou and Prajna (2005).

[3] Note that the converse implication is true only in special cases. One such instance is when the polynomial is quadratic.

Generally speaking, there are other possible sources of conservatism with the methods presented in this paper. Theorem 2 and its variants are presented in sufficiency form, and it is currently not known whether a barrier certificate that satisfies the conditions in these theorems is guaranteed to exist when the model and parameter set are inconsistent with the data. Another source of conservatism comes from the computational method in this section, in which the barrier certificates are assumed to be *finite degree* polynomials. In relation to this, our experience seems to indicate that conservatism can be reduced by increasing the degree of the barrier certificates, or by dividing the time interval $[0, T]$ or state-parameter space to finer segments/partitions and then using a discontinuous barrier certificate similar to what was proposed in Section 2.2.

4. Invalidation of models with constraints

As mentioned in the Introduction, the methods we proposed in Section 2 can be extended to accommodate larger class of models. Consider the following model:

$$\dot{x}(t) = f(x(t), v(t), p, t), \tag{18}$$

$$0 = g(x(t), v(t), p, t), \tag{19}$$

$$0 \leqslant h(x(t), v(t), p, t), \tag{20}$$

$$0 \leqslant \int_0^T \sigma(x(t), v(t), p, t)\,\mathrm{d}t \quad \forall T \geqslant 0, \tag{21}$$

where $x(t)$ and p are the same as before, and $v(t) \in V \subseteq \mathbb{R}^{n_v}$ is a vector of auxiliary variables. We assume that f, g, h, and σ are continuous in x, v, and t. In general, g, h, and σ are vector-valued, for which (19)–(21) are interpreted entry-wise. This formulation includes a very large class of models, for example:

- Models described by differential-algebraic equations (DAEs) can be accommodated by including the equality constraints (19).
- Memoryless uncertainties (Khalil, 1996) relating some signals in the model can be taken into account by (20).
- Uncertain time-varying inputs can be characterized using (20) for inputs with bounded magnitude, or (21) for inputs with bounded energy (Megretski & Rantzer, 1997).
- Some classes of dynamic uncertainties can be described using *hard integral quadratic constraints* (IQCs) (Megretski & Rantzer, 1997), which is a special case of (21).

More importantly, their combinations clearly can still be described by (18)–(21).

Before proceeding further, we need to specify what is considered as a valid trajectory of the model. A trajectory $x : [0, T] \to X$ is a valid trajectory of (18)–(21) on the time interval $[0, T]$ if there exists a piecewise continuous and bounded $v : [0, T] \to V$ such that $x(t)$ is a solution of (18), and the constraints (20)–(21) are satisfied by $x(t)$ and $v(t)$ for all $t \in [0, T]$.

For handling this class of models, we will add the products of g, h, and σ given in (19)–(21) with some function multipliers satisfying certain positivity criteria to the conditions of Theorem 2. This can be regarded as a generalization of the so-called *S-procedure* (Yakubovich, 1977) (in which the multipliers are constants), and has been proposed for the construction of Lyapunov functions (Papachristodoulou & Prajna, 2002) for systems described by (18)–(21).

The extension of Theorem 2 is stated in Theorem 11. Similar extensions can be applied to the other results of Section 2, and thus are not included here. If the descriptions of the model and sets are polynomial, then a polynomial barrier certificate and polynomial multipliers can be searched using the method described in Section 3.

Theorem 11. *Let the model* (18)–(21) *and the sets* P, X_0, X_T, X, V *be given, with* f, g, h, σ *being continuous in* x, v, *and* t. *Suppose there exists a real-valued* $B(x, p, t)$ *that is continuously differentiable with respect to* x *and* t, *and multipliers* $\lambda_1(x, v, p, t)$, $\lambda_2(x, v, p, t)$, $\lambda_3(p)$, *where* λ_1 *and* λ_2 *are continuous with respect to* x, v, *and* t, *such that*

$$B(x_T, p, T) - B(x_0, p, 0) > 0 \quad \forall x_T \in X_T,\ x_0 \in X_0,\ p \in P, \tag{22}$$

$$\begin{aligned}&\frac{\partial B}{\partial x}(x, p, t) f(x, v, p, t) + \frac{\partial B}{\partial t}(x, p, t)\\ &\quad + \lambda_1(x, v, p, t) g(x, v, p, t)\\ &\quad + \lambda_2(x, v, p, t) h(x, v, p, t)\\ &\quad + \lambda_3(p)\sigma(x, v, p, t) \leqslant 0\\ &\quad \forall x \in X,\ v \in V,\ p \in P,\ t \in [0, T],\end{aligned} \tag{23}$$

$$\lambda_2(x, v, p, t) \geqslant 0 \quad \forall x \in X,\ v \in V,\ p \in P,\ t \in [0, T], \tag{24}$$

$$\lambda_3(p) \geqslant 0 \quad \forall p \in P. \tag{25}$$

Then the model (18)–(21) *and its associated parameter set* P *are invalidated by* $\{X_0, X_T, X\}$.

Proof. The proof is similar to the proof of Theorem 2, except that here the conditions (23)–(25) will be used to show that $B(x, p, t)$ is non-increasing along the trajectory of the model. That can be shown directly by integrating (23) with respect to time and using the fact that $\int_0^\tau [(\lambda_1 g + \lambda_2 h + \lambda_3 \sigma)(x(t), v(t), p, t)]\,\mathrm{d}t$ is non-negative for $\tau \in [0, T]$, which follows from (19)–(21) and (24)–(25). □

Remark 12. Notice that λ_3 is a function of p only. If g, h, and σ are vectors of functions, then the respective λ's will also be vectors of multipliers. In this case, their multiplications in (23) are interpreted as sums-of-products, and the inequalities in (24)–(25) are entry-wise.

5. Invalidation of hybrid models

Hybrid systems (van der Schaft & Schumacher, 2000) are systems whose dynamics involve both continuous and discrete processes. One class of models for these systems takes the form

$$\dot{x} = f_{i(t)}(x(t), p, t), \quad i(t) \in I = \{1, \ldots, N\}, \tag{26}$$

where $x(t) \in \mathbb{R}^{n_x}$ is the continuous state, $i(t)$ is the discrete state, $f_i(x, p, t)$ is the vector field describing the dynamics of the ith mode, and I is the index set. We assume that each f_i is continuous with respect to x and t. The evolution of the discrete state is governed by

$$i(t) = \phi(x(t), i(t^-)), \quad i(0) \in I_0, \tag{27}$$

with $\phi : \mathbb{R}^{n_x} \times I \to I$ and $I_0 \subseteq I$. Corresponding to the transition law ϕ, there exists an invariant, i.e., a region of the state space where a particular mode can be active. For the ith mode, the invariant is denoted by A_i, and for example can be described by $A_i = \{x \in \mathbb{R}^{n_x} : g_{ik}(x) \geqslant 0 \ \forall k \in K_{A_i}\}$ for some $g_{ik} : \mathbb{R}^{n_x} \to \mathbb{R}$, with K_{A_i} being a set of indices. In general, some x may belong to several invariants. The transition set from the jth mode to the ith mode is defined as $S_{ji} = \{x \in \mathbb{R}^{n_x} : i = \phi(x, j)\}$. It is assumed in this paper that the discrete state $i(t)$ is piecewise continuous in time. Systems with infinitely fast switching, such as those that have sliding modes, are excluded from our discussion.

Clearly, the model (26) is invalidated by some trajectory data X_0, X_T, X, if a barrier certificate $B(x, p, t)$ that satisfies conditions (2)–(3) for each $f_i(x, p, t)$ can be found. In fact, the existence of such a barrier certificate will prove that the model is inconsistent with the trajectory data for *any* discrete state sequence. However, this test is unnecessarily too restrictive if the discrete transition law (27) is specified, since in that case the discrete state sequence cannot be arbitrary.

In the latter case, ideas similar to those used in analysis of hybrid systems using piecewise Lyapunov functions (see Prajna & Papachristodoulou, 2003, and references therein) can be utilized to obtain a less conservative test. The key concept here is to invalidate the model using a *piecewise barrier certificate*, i.e., a barrier certificate patched from several functions $B_i(x, p, t)$. Each $B_i(x, p, t)$ corresponds to a discrete state i and needs to satisfy condition (3) *only inside* the invariant A_i of the mode. In addition, on the transition set S_{ji} it is only required that the value of $B_i(x, p, t)$ in the destination mode is less than or equal to the value of $B_j(x, p, t)$, as opposed to being exactly the same. The complete conditions are stated in Theorem 13. Again, for polynomial systems, the computation can be performed using the method described in Section 3.

Theorem 13. *Let the model* (26) *and the sets* A_i, S_{ji}, P, X_0, X_T, X *be given, with* f_i *being continuous in* x *and* t. *Define the sets* $\hat{I}_0$ *and* $\hat{I}_T$ *as follows*: $\hat{I}_0 = \{i \in I_0 : X_0 \cap A_i \neq \emptyset\}$, $\hat{I}_T = \{i \in I : X_T \cap A_i \neq \emptyset\}$. *If there exist real-valued functions* $B_i(x, p, t)$ *for all* $i \in I$, *each of which is differentiable with respect to* x *and* t, *such that*

$$B_i(x_T, p, T) - B_j(x_0, p, 0) > 0 \quad \forall i \in \hat{I}_T,\ j \in \hat{I}_0, \quad x_T \in X_T \cap A_i,\ \ x_0 \in X_0 \cap A_j,\ \ p \in P, \tag{28}$$

$$\frac{\partial B_i}{\partial x}(x, p, t) f_i(x, p, t) - \frac{\partial B_i}{\partial t}(x, p, t) \leqslant 0 \quad \forall i \in I,\ \ x \in A_i \cap X,\ \ p \in P,\ \ t \in [0, T], \tag{29}$$

$$B_i(x, p, t) - B_j(x, p, t) \leqslant 0 \quad \forall i, j \in I,\ \ x \in S_{ji} \cap X, \quad p \in P,\ \ t \in [0, T], \tag{30}$$

then the hybrid model (26) *with discrete transition law* (27) *and parameter set* P *is invalidated by* $\{X_0, X_T, X\}$.

Proof. Suppose that functions $B_i(x, p, t)$ satisfying (28)–(30) can be found, but at the same time there exists a trajectory $x(t)$ of the model for some parameter $p \in P$ with $x(0) \in X_0$, $x(T) \in X_T$, $x(t) \in X\ \forall t \in [0, T]$. The existence of such trajectory implies that there exists a corresponding sequence of discrete state $i_1, i_2, \ldots, i_N$ and time $0 \triangleq T_0 < T_1 < T_2 < \cdots < T_{N-1} < T_N \triangleq T$ such that $i(t) = i_k$ for $t \in [T_{k-1}, T_k)$, $k = 1, 2, \ldots, N$ and $i(T) = i_N$. Now define the function $B(t)$ on the time interval $[0, T]$ as $B(t) = B_{i_k}(x(t), p, t)$ for $t \in [T_{k-1}, T_k)$, and $B(T) = B_{i_N}(x(T), p, T)$. It follows by definition that $\hat{I}_0$ is the set of possible initial discrete states, $\hat{I}_T$ is the set of possible final discrete states, and thus condition(28) asserts that $B(T) > B(0)$. On the other hand, conditions (29)–(30) together imply that $B(T) \leqslant B(0)$ and therefore we obtain a contradiction. This shows that such a trajectory $x(t)$ cannot exist and we conclude that the model and its parameter set are invalidated by $\{X_0, X_T, X\}$. □

6. Application example: enzymatic reactions

In this section, we present a physically motivated example to illustrate the use of the results in this paper. The system we consider is a system of enzymatic reactions:

$$\left.\begin{aligned} &S_1 + E_1 \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C_1, \\ &C_1 \xrightarrow{k_2} S_2 + E_1, \\ &\quad \vdots \\ &C_N \xrightarrow{k_{2N}} S_{N+1} + E_N. \end{aligned}\right\} \tag{31}$$

Systems of this type are found in the metabolic pathway of living organisms. See Murray (2002) for more background and modelling details. In this system, a substrate S_1 reacts with an enzyme E_1 in a reversible reaction to form a complex C_1, which is then converted into a product S_2 and the enzyme E_1. The product S_2 is converted through a series of reactions to result in the final product S_{N+1}. The dotted part in (31) is assumed unknown, but will be represented by an uncertain operator in our model.

A model of this system and the list of variables in it are given in Table 1. All the p_i's are time-invariant parameters, with $p_2 > p_1$. The rationale in the derivation of this model will be explained now.

The equations describing evolution of the concentration of S_1, E_1, and C_1 (denoted by square brackets) can be obtained using the *law of mass action* (Murray, 2002) as follows: $\mathrm{d}[S_1]/\mathrm{d}t = -k_1[E_1][S_1] + k_{-1}[C_1]$, $\mathrm{d}[E_1]/\mathrm{d}t = -k_1[E_1][S_1] + (k_{-1} + k_2)[C_1]$, $\mathrm{d}[C_1]/\mathrm{d}t = k_1[E_1][S_1] - (k_{-1} + k_2)[C_1]$. These differential equations can be simplified because of two facts. First, $[E_1] + [C_1]$ is constant and therefore the state equation for $[E_1]$ can be eliminated. Second, the formation of the

Table 1
An enzymatic reactions model and the list of variables

$\dot{x}_1(t) = -x_1(t) + (x_1(t) + p_1)v_1(t),$ (32)	$0 = x_1(t) - (x_1(t) + p_2)v_1(t),$ (35)
$\dot{x}_2(t) = p_3 v_1(t) - v_2(t)x_2(t),$ (33)	$0 \leqslant (v_2(t) - \underline{v_2})(\overline{v_2} - v_2(t)),$ (36)
$\dot{x}_3(t) = v_3(t),$ (34)	$0 \leqslant \int_0^T [x_2^2(t) - v_3^2(t)]\,\mathrm{d}t \quad \forall T \geqslant 0.$ (37)
$x_1(t)$:dimensionless concentration of S_1	$v_1(t)$: dimensionless concentration of C_1
$x_2(t)$: dimensionless concentration of S_2	$v_2(t)$: time-varying uncertain feedback gain for S_2
$x_3(t)$: dimensionless concentration of S_{N+1}	$v_3(t)$: dimensionless concentration of C_2

complexes is very fast and most of the time it is in equilibrium, implying $\mathrm{d}[C_1]/\mathrm{d}t \approx 0$. After a suitable non-dimensionalization, this results in the DAEs (32) and (35).

The evolution of S_2 can be modelled in a similar manner. The substrate S_2 is produced from C_1 and consumed by the forward reactions in the chain. However, since these reactions are not known, we will assume that the consumption of S_2 is represented by an uncertain negative feedback with time-varying feedback gain $v_2(t)$. Thus, we obtain (33), where $v_2(t)$ is assumed to satisfy (36). Finally, the unknown reactions from S_2 to C_N are modelled by an uncertain operator with L_2-gain equal to one, which is represented by the IQC (37), and the dynamics of the final product S_{N+1} is described by (34).

Since x_1, x_2, x_3, v_1, and v_3 represent physical substrate concentrations, they can be neither negative nor very large. Thus, we assume that they take their values on the interval $[0, 10]$. This defines the sets X and V in Theorem 11. We let v_2 be "free", although it will be constrained by (36), for which it is assumed that $\underline{v_2} = 0.5$ and $\overline{v_2} = 2$. The parameters are assumed to be in the following intervals: $p_1 \in [0.5, 1.5]$, $p_2 \in [2, 3]$, $p_3 \in [0.5, 2.5]$. These define the set P.

Suppose now that measurements of the initial and final substrates $x_1(t)$, $x_3(t)$ are performed with the real system at time $t = 0$ and $t = 1 \triangleq T$. For our purpose here, an "experiment with the real system" is just a simulation of the full model of (31) where the dotted part is given by $S_2 + E_2 \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} C_2$, $C_2 \xrightarrow{k_4} S_3 + E_2$, $S_3 + E_N \underset{k_{-5}}{\overset{k_5}{\rightleftharpoons}} C_N$, and the initial conditions and parameters of the system are fixed at some values. The measurement results indicate that $x_1(0) \in [0.9, 1.1]$, $x_1(1) \in [0.4, 0.6]$, $x_3(0) \in [0.9, 1.1]$, $x_3(1) \in [3.9, 4.1]$. Other values of the states are hidden from the experimenter. We want to assess the ability of our model to account for the above observation. Neither $x_2(0)$ nor $x_2(1)$ is measured; however, it is known that the initial quantity of x_2 is not abundant and therefore we assume that $x_2(0) \in [0, 2]$. No further restriction is put on $x_2(1)$. All these information define the sets X_0 and X_T.

In this example, the model and its parameter set turn out to be inconsistent with the measurement data. A barrier certificate and multipliers that satisfy the conditions in Theorem 11 exist and can be computed using the method described in Section 3. In particular, we have computed a barrier certificate $B(x, t)$ that is of the form $B(x, t) = B_0(x) + tB_1(x) + t^2 B_2(x)$, with B_0, B_1, and B_2 being quadratic. The semidefinite program corresponding to this computation can be solved in less than 2 min on a Pentium III 600 MHz machine.

Having the model invalidated, the modeller should then try to refine the structure of the model and/or the parameter ranges in order to have one that is a closer description of the real system. At present, the question on how one should modify the model or parameter ranges after they have been invalidated is still an open problem. Ideally, feedback from the invalidation process should be used when refining the model. For example, sensitivity analysis using the multipliers appearing in Algorithm 9 may be useful in identifying which parameter constraints or measurements data are the most important. We hope to address this issue in a future publication.

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