Barrier Certificates for Nonlinear Model Validation

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Outline

- Model validation: background and problem statement.
- Invalidation using barrier certificates.
- Computational methods.
- Extensions and examples.
- Conclusions.

Model Validation

- Model validation provides a way to assess the quality of a proposed model.
- Previous work e.g. in the robust control paradigm (Doyle, Dullerud, Poolla, Smith, and others).
- However, “model validation” is a *misnomer*: it is impossible to validate a model. Its proper role is to *invalidate* a model.
- Invalidating a model serves several purposes, e.g.:
  - Pointing out the inadequacy of a model in explaining an observed behavior
  - Showing that *a priori* information on the parameters is inconsistent with some experimental results
  - For finding a parameter range which may be consistent with the experimental results.

Basic Model Validation Setting

- Nonlinear model:

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

where $x(t) \in \mathbb{R}^n$ is the state and $p \in P \subseteq \mathbb{R}^m$ is the parameter.

- Some measurements are performed with the real system, indicating that

$$x(0) \in X_0, \quad x(T) \in X_T, \quad \text{and} \quad x(t) \in X \text{ for all } t \in [0, T]$$

- X_0, X_T and X are sets in $\mathbb{R}^n$, and necessarily $X_0, X_T \subseteq X$.
- We use sets as X_0 and X_T for handling *measurement uncertainty*.
- Information on X may come from the experiment, or from *a priori* knowledge about the system.

Problem Statement

- Given the model $\dot{x} = f(x, p, t)$, parameter set P, and trajectory information $\{X_0, X_T, X\}$, provide a proof that the model and its parameter set are inconsistent with the trajectory information.
- That is:

  Prove that for all possible parameter $p \in P$, the model cannot produce a trajectory $x(t)$ such that

$$x(0) \in X_0,$$

$$x(T) \in X_T,$$

$$x(t) \in X \quad \forall t \in [0, T].$$

- Traditional approaches for solving this problem include *exhaustive simulation* with many p and $x(0)$ sampled randomly from P and X_0.
- Indeed simulation (possibly after parameter fitting) is a good way for proving that a model can reproduce *some* behaviors of the system.
- However, for proving inconsistency, the required number of simulation runs soon becomes prohibitive.
- Moreover, a proof by simulation alone is *never exact*.
- With our method, we can prove inconsistency without running simulation, and the proof is exact.

Invalidation using Barrier Certificates

- **Theorem:** Suppose that there exists $B(x, p, t)$ — a barrier certificate — such that the following two conditions hold:

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

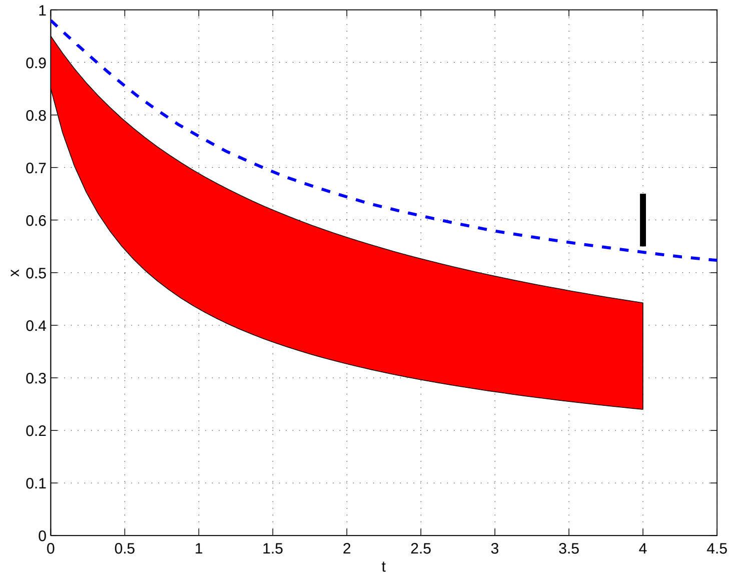
$$\frac{\partial B}{\partial x} f(x, p, t) + \frac{\partial B}{\partial t}(x, p, t) \leq 0 \quad \forall t \in [0, T], x \in X, p \in P.$$

Then, the model $\dot{x} = f(x, p, t)$ and parameter set P are inconsistent with $\{X_0, X_T, X\}$.

Example 1

- Consider the model $\dot{x} = -px^3$, with $X = \mathbb{R}$ and $p \in P = [0.5, 2]$.
- The measurement data are $X_0 = [0.85, 0.95]$ and $X_T = [0.55, 0.65]$ at $T = 4$.
- We found the following barrier certificate, which proves inconsistency.

$$
\begin{aligned}
B(x,t) = {} & 8.35x + 10.4x^2 - 21.5x^3 \\
& + 9.86x^4 - 1.78t + 6.58tx \\
& - 4.12tx^2 - 1.19tx^3 + 1.54tx^4.
\end{aligned}
$$



Computational Methods

- Similar to the case of Lyapunov functions, construction of barrier certificates is generally not easy.
- However, if the vector field is polynomial and the parameter and data sets are semialgebraic, *sum of squares* techniques can be directly used in this construction.
- More concretely, consider $\dot{x} = f(x, p, t)$ with f being a polynomial. Assume that P is defined as $P = \{p \in \mathbb{R}^m : g_P(p) \geq 0\}$, where $g_P(p)$ is a vector of polynomials. Define X_0, X_T, and X in a similar manner.

- **Proposition:** Let the model and the various set descriptions be given. Suppose there exist a polynomial $B(x,p,t)$, a positive number ϵ, and vectors of sums of squares M's and N's such that

$$B(x_T,p,T) - B(x_0,p,0) - \epsilon - M_P^T(\cdot)g_P(\cdot) - M_{X_0}^T(\cdot)g_{X_0}(\cdot) - M_{X_T}^T(\cdot)g_{X_T}(\cdot)$$

and

$$-\frac{\partial B}{\partial x}f(x,p,t) - \frac{\partial B}{\partial t}(x,p,t) - N_P^T(\cdot)g_P(\cdot) - N_X^T(\cdot)g_X(\cdot) - N_t(\cdot)(Tt - t^2)$$

are sums of squares. Then the solution $B(x,p,t)$ satisfies the required conditions, and therefore it is a barrier certificate.

- This can be solved using semidefinite programming, e.g. with the help of the software SOSTOOLS.

Extension: Three or More Measurements

- For brevity and w.l.o.g., assume now that measurements are performed at $t = 0, 1, 2$, indicating that

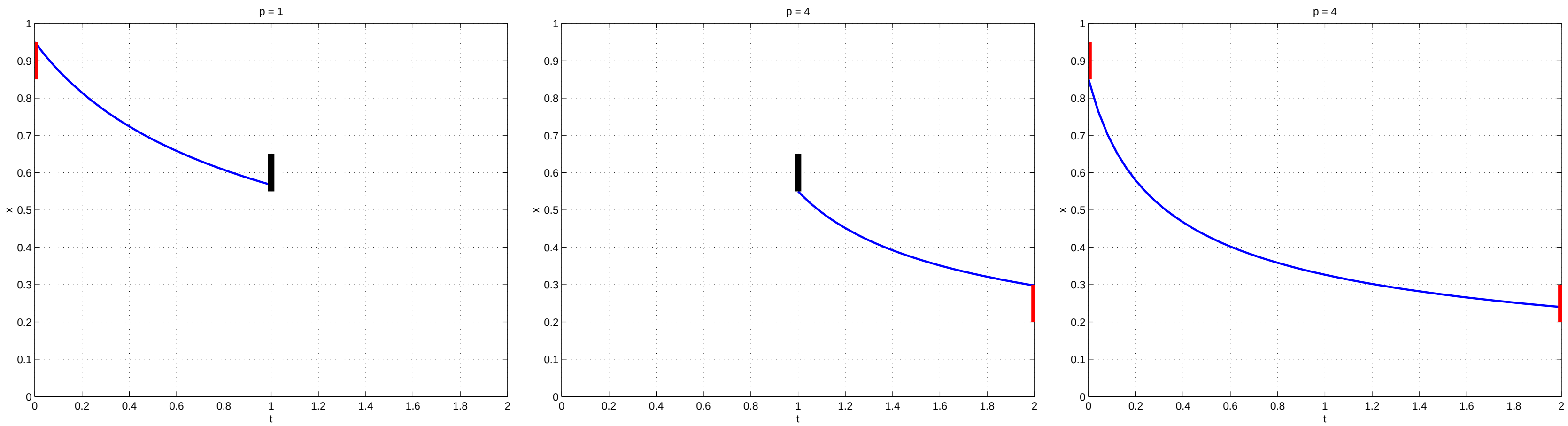
$$x(0) \in X_0, \quad x(1) \in X_1, \quad x(2) \in X_2.$$

- A direct, computationally less expensive way for invalidation is to consider the measurements pairwise.

- Unfortunately, it may give conservative results, because each pair of measurements may be consistent with the model, while the three measurements considered *simultaneously* yield inconsistency.

Example 2

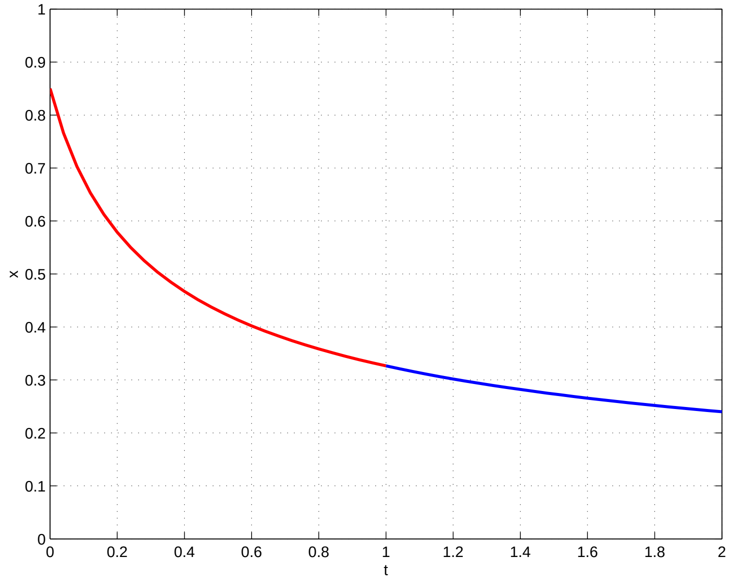
- Consider the system $\dot{x} = -px^3$, with $p \in P = [1, 4]$, and $X = \mathbb{R}$.
- Let $X_0 = [0.85, 0.95]$, $X_1 = [0.55, 0.65]$, $X_2 = [0.2, 0.3]$.
- Pairwise test will not be able to invalidate the model. In fact, each pair is consistent with the model.



Extended Method

- To avoid this conservatism, we need to take into account two factors:
  - two trajectory segments involved in this setting are generated using the *same* parameter.
  - there is *a coupling* between the two trajectory segments, namely

$$\lim_{t \to 1^-} x(t) = \lim_{t \to 1^+} x(t) = x(1).$$



- Use a model that captures the evolution of both segments simultaneously.

$$\dot{\tilde{x}} = \tilde{f}(\tilde{x}, p, t) = \begin{bmatrix} f(\tilde{x}_1, p, t) \\ f(\tilde{x}_2, p, t+1) \end{bmatrix},$$

where $\tilde{x} = (\tilde{x}_1, \tilde{x}_2)$, and $\tilde{x}_1, \tilde{x}_2 \in \mathbb{R}^n$ are the first and second segments.

- Also ask that $\tilde{x}_1(1) = \tilde{x}_2(0)$.

- **Theorem:** Suppose there exists $\tilde{B}(\tilde{x}, p, t)$ such that

$$\tilde{B}(\hat{x}_1, \hat{x}_2, p, 1) - \tilde{B}(\hat{x}_0, \hat{x}_1, p, 0) > 0 \quad \forall \hat{x}_i \in X_i, p \in P$$

$$\frac{\partial \tilde{B}}{\partial \tilde{x}} \tilde{f}(\tilde{x}, p, t) + \frac{\partial \tilde{B}}{\partial t}(\tilde{x}, p, t) \leq 0 \quad \forall t \in [0, 1], \tilde{x} \in X^2, p \in P.$$

Then the model and its parameter set P are inconsistent with the measurement data. Moreover, this test is always at least as powerful as the pairwise test.

Example 2 (Continued)

- The system is $\dot{x} = -px^3$, with $p \in P = [1, 4]$, and $X = \mathbb{R}$.
- $X_0 = [0.85, 0.95]$, $X_1 = [0.55, 0.65]$, $X_2 = [0.2, 0.3]$.
- Using the extended test, a barrier certificate can be found:

$$\begin{aligned} B(\tilde{x}, t) = 6.81\tilde{x}_1 - 57.9\tilde{x}_2 + 13.4\tilde{x}_1^2 - 50.3\tilde{x}_1\tilde{x}_2 \\ + 94.4\tilde{x}_2^2 - 3.66t + 2.53t\tilde{x}_1 + 9.05t\tilde{x}_2 \\ + .758t\tilde{x}_1^2 + 7.25t\tilde{x}_1\tilde{x}_2 - 25.9t\tilde{x}_2^2 \end{aligned}$$

- Thus the model and parameter set are inconsistent with the measurement data $\{X_0, X_1, X_2\}$.

Extension: Model with Constraints

- Consider the following model:

$$\begin{aligned} \dot{x} &= f(x, v, p, t), \\ 0 &= g(x, v, p, t), \\ 0 &\leq h(x, v, p, t), \\ 0 &\leq \int_0^T \phi(x, v, p, t) dt \quad \forall T \geq 0, \end{aligned}$$

  where $v \in V \subseteq \mathbb{R}^\ell$ are some auxiliary signals.

- This formulation includes a very large class of models, including differential-algebraic models, models with uncertain inputs, and models with memoryless and dynamic uncertainties.

- **Theorem:** Suppose there exist $B(x,p,t)$ and $\lambda_1(x,v,p,t)$, $\lambda_2(x,v,p,t)$, $\lambda_3(p)$ such that

$$B(x_T,p,T) - B(x_0,p,0) > 0 \qquad \forall x_T \in X_T, x_0 \in X_0, p \in P,$$

$$\frac{\partial B}{\partial x}(\cdot)f(\cdot) + \frac{\partial B}{\partial t}(\cdot) + \lambda_1^T(\cdot)g(\cdot) + \lambda_2^T(\cdot)h(\cdot) + \lambda_3^T(\cdot)\phi(\cdot) \le 0$$
$$\forall x \in X, v \in V, p \in P, t \in [0,T],$$

$$\lambda_2(\cdot) \ge 0 \quad \forall x \in X, v \in V, p \in P, t \in [0,T],$$

$$\lambda_3(\cdot) \ge 0 \quad \forall p \in P.$$

Then the model and its associated parameter set inconsistent with the measurement data.

Extension: Hybrid Model (Sketch)

- Consider the following model:

$$\dot{x} = f_{i(t)}(x,p,t),$$
$$i(t) = \phi(x(t), i(t^-)),$$

where i denotes the modes of the system.

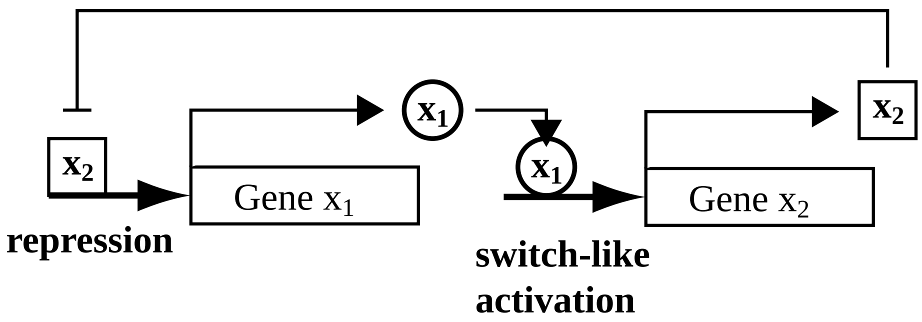
- For a hybrid model like this, a *piecewise differentiable* barrier certificate can be used to reduce conservatism:

$$B(x,p,t) = B_{i(t)}(x,p,t),$$

  – B_i satisfies the required conditions *only inside* the invariant of mode i.
  – $B_j(x,p,t) \leq B_i(x,p,t)$ during transition from mode i to mode j.

Biological Example: Genetic Circuit

- Consider a genetic regulatory circuit consisting of two transcription units in series.



- The product of the first gene, x_1, is a positive transcriptional activator of the second gene, and the product of the second gene, x_2, is a transcriptional repressor of the first gene.
- If the activation of the second gene by x_1 is highly cooperative, then the reaction can be modelled as a switch.

Mathematical Model

- Mathematically, we model the system as a switched system:

$$\dot{x}_1 = \frac{20u}{1+x_2} - kx_1, \qquad \dot{x}_2 = \begin{cases} -kx_2, & \text{if } x_1 < 1, \\ 10 - kx_2, & \text{if } x_1 \geq 1, \end{cases}$$

  where u is a signal from some signal transduction pathway.

- We will now do a toy experiment, with the non-hybrid equations

$$\dot{x}_1 = \frac{20u}{1+x_2} - kx_1, \qquad \dot{x}_2 = 10\frac{x_1^m}{1+x_1^m} - kx_2$$

  as the “real system”, and use them to generate some measurement data.

- When the Hill coefficient m in $\frac{x_1^m}{1+x_1^m}$ is not high enough, a switched model may be inadequate. Let us choose $m = 4$.

A Priori Knowledge

- Assume we know that the parameter ranges are

$$9.8 \le k \le 10.2,$$
$$1.4 \le u \le 1.6,$$

(say that the nominal values are 10 and 1.5).

- We also know possible values of the states:

$$0 \le x_1(t) \le 4,$$
$$0 \le x_2(t) \le 4,$$

(they can be neither negative nor too large, to be physically meaningful).

Measurement Data

- Our trajectory data are:

$$X_0: \quad 0 \le x_1(0) \le 0.1; \quad 0 \le x_2(0) \le 0.1$$
$$X_3: \quad 0 \le x_1(3) \le 4; \quad 0.85 \le x_2(3) \le 0.9.$$

  Interpretation:

  – The initial conditions are known quite accurately.

  – $x_2(3)$ is measured, therefore its uncertainty is small.

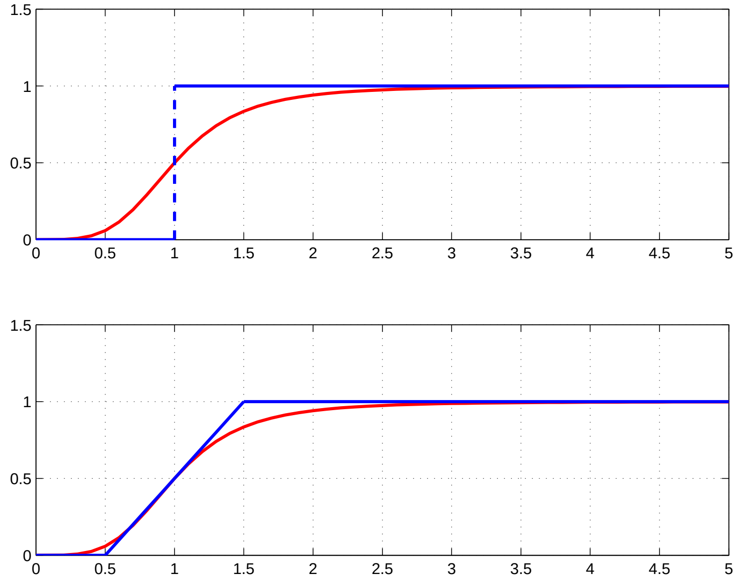
  – $x_1(3)$ is not measured. The uncertainty is big.

- We will show that these data cannot be generated by the hybrid model, by constructing a barrier certificate.

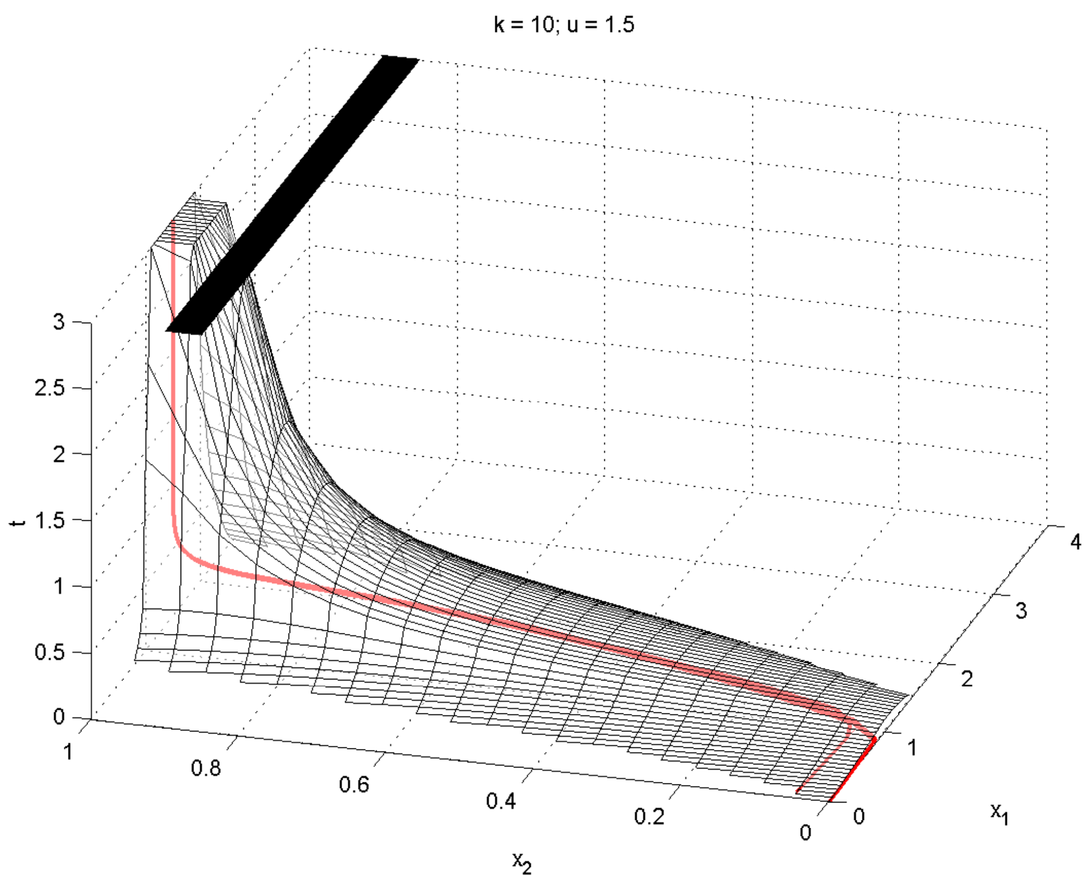
Invalidation

- Indeed, a piecewise polynomial barrier certificate can be found, showing that the measurement data is inconsistent with the hybrid model.

- This indicates that a model with switch is inadequate, and suggests that another model (e.g. with saturation function) is needed.



- The barrier certificate acts as a barrier in the space (x_1, x_2, k, u, t), separating measurement data from trajectories.



Conclusions

- We have presented a methodology for invalidation of nonlinear models using barrier certificates.
- Various sources of uncertainties can be taken into account.
- Construction of barrier certificates can be performed using the sum of squares decomposition and semidefinite programming.
- Many open research directions.

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