BOUNDING LINEAR TIME VARYING HYBRID SYSTEMS WITH TIME EVENTS [1]

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Abstract: The problem of bounding the states of a linear time varying hybrid system at fixed transition times where the mode sequence is allowed to vary is considered. It is shown via an illustrative example that a simple decomposition algorithm produces weak bounds which get worse as the number of epochs increases. To address this issue, a novel algorithm is proposed, based on solving families of relaxed linear programming problems, which allows the incorporation of additional constraints derived from physical insight. This provides tighter bounds while avoiding explicit enumeration of all possible mode trajectories.

Keywords: varying mode sequence, exact state bounds, differential equations, optimization problems

1. INTRODUCTION

Continuous time hybrid systems have become the modeling framework of choice for a wide variety of applications that require detailed dynamic models with embedded discontinuities. In general, these time dependent, nonlinear models exhibit model switching and state jumps as a consequence of both time and state dependent events (Barton and Lee, 2002). Hybrid system models are important in many areas of science and engineering, including the analysis of digital circuits, signaling and decision making mechanisms in (biological) cells, robotic systems, air and ground traffic management systems, sequential operations, safety interlock systems, and embedded systems. Economic and safety considerations in these applications, such as the automated design of safe operating procedures and the formal verification of embedded systems, strongly motivate the development of algorithms and tools for the global optimization of hybrid systems.

Many modern, general methods for deterministic global optimization in Euclidean spaces rely on the notion of a convex relaxation of a nonconvex function (McCormick, 1976). This is a convex function which underestimates a nonconvex function on the set of interest. The convex programs that result from convex relaxation of all nonconvex objective and constraint functions in a problem formulation can (in principle) be solved to guaranteed global optimality, which, for example, can be used to generate rigorous lower bounds on the nonconvex problem for a branch and bound (B&B) algorithm (Horst and Tuy, 1993).

Recently, a convexity theory has been developed that enables well known symbolic convex relaxations on Euclidean spaces (McCormick, 1976; Adjiman *et al.*, 1998) to be harnessed in the construction of convex relaxations of general, nonconvex Bolza type functionals subject to an embedded linear time varying (LTV) hybrid system

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where the transition times are fixed, and the sequence of modes, T_μ, is known (Lee *et al.*, 2004). The construction of a set enclosing the image of the parameter space under the solution of the hybrid system, $\mathcal{X}^{(i)}$, is critical for obtaining tight (accurate) convex relaxations of the participating functionals. Note that $\mathcal{X}^{(i)}$ represents the state bounds for the embedded hybrid system for all values of the parameters. The better the estimate of $\mathcal{X}^{(i)}$ is, the tighter the relaxations obtained. Consequently, tighter lower bounds are obtained, increasing the efficiency of the global optimization algorithm.

In (Barton and Lee, 2003), a mixed-integer reformulation is proposed to deal with the problem when T_μ is allowed to vary and becomes an optimization parameter. This results in a nonconvex mixed-integer nonlinear programming (MINLP) problem. In particular, auxiliary optimization parameters, $\mathbf{Z}$, are introduced to represent the initial conditions for each epoch. In this case, $\mathcal{X}^{(i)}$ becomes a larger set containing the image of the parameter space under the solution of the hybrid system for all possible T_μ, and the bounds on $\mathbf{Z}$ are obtained from estimating $\mathcal{X}^{(i)}$ at the time events, i.e., the state bounds at the beginning of each epoch.

For analogous reasons to those presented above, it is very desirable to obtain tight bounds for $\mathbf{Z}$, as these bounds are needed to construct a convex relaxation of the nonconvex MINLP. Although the exact state bounds at the beginning of each epoch can be obtained with an explicit enumeration of all possible T_μ, the cost of doing so clearly becomes prohibitive (increases exponentially) as the number of epochs increases. To deal with this problem, a decomposition algorithm for estimating valid state bounds was proposed in (Barton and Lee, 2003).

In this paper, we formally present the decomposition algorithm, and show that it produces weak bounds which deteriorate as the number of epochs increases. To address this issue, a novel algorithm is proposed to obtain tighter state bounds, based on solving a family of relaxations of mixed-integer linear programming (MILP) problems as LP problems.

2. LTV HYBRID SYSTEMS

The modeling framework of (Barton and Lee, 2002) is used to define the LTV hybrid system of interest. The time horizon is partitioned into contiguous intervals called *epochs*. We define a *hybrid time trajectory*, T_τ, as a finite sequence of epochs $\{I_i\}$ terminating with epoch I_{n_e}, where n_e is fixed, and is the total number of epochs. Each epoch is a closed time interval $I_i = [\sigma_i, \tau_i] \subset \mathbb{R}$, $\sigma_i = \tau_{i-1}$ for $i = 2, \ldots, n_e$, $\sigma_1 \le \tau_1$, and $\tau_{i-1} \le \tau_i$ for all $i = 2, \ldots, n_e$. For epoch I_i, the system evolves continuously in time if $\sigma_i < \tau_i$, and it evolves discretely by making an instantaneous transition if $\sigma_i = \tau_i$. The continuous state subsystems are called *modes* and the corresponding sequence of modes for T_τ is called the *hybrid mode trajectory*, T_μ. At the end of epoch I_i, a transition is made from the *predecessor* mode in I_i to a *successor* mode in epoch I_{i+1}, also called an *event*, when the *transition condition* is satisfied.

Definition 1. The LTV ODE hybrid system of interest is defined by the following.

1. An index set of modes potentially visited along T_μ, $M = \{1, \ldots, n_m\}$, and a fixed T_τ with given time events (i.e., explicit transition times) $\sigma_1, \tau_1, \tau_2, \ldots, \tau_{n_e}$. It is clear that $T_\mu = \{m_i\}$, where $m_i \in M$. Henceforth, the superscript (m) will refer to any mode in M, while superscript (m_i) will refer to the active mode in epoch I_i;
2. An invariant structure system where the number of continuous state variables is constant between modes, $V = (\mathbf{x}(\mathbf{p}, T_\mu, t), \mathbf{p})$, where $\mathbf{p} \in P \subset \mathbb{R}^{n_p}$, and $\mathbf{x}(\mathbf{p}, T_\mu, t) \in \mathbb{R}^{n_x}$ for all $(\mathbf{p}, T_\mu, t) \in P \times M^{n_e} \times I_i$, $i = 1, \ldots, n_e$;
3. The LTV ODE system for each mode $m \in M$, which is given by
$$\dot{\mathbf{x}}(\mathbf{p}, T_\mu, t) = \mathbf{A}^{(m)}(t)\mathbf{x}(\mathbf{p}, T_\mu, t) + \mathbf{B}^{(m)}(t)\mathbf{p} + \mathbf{q}^{(m)}(t), \quad (1)$$
where $\mathbf{A}^{(m)}(t)$ is continuous on $[\sigma_1, \tau_{n_e}]$, $\mathbf{B}^{(m)}(t)$ and $\mathbf{q}^{(m)}(t)$ are piecewise continuous on $[\sigma_1, \tau_{n_e}]$ and defined at any point of discontinuity, for all $m \in M$;
4. The transition conditions for the transitions between epochs I_i and I_{i+1}, $i = 1, \ldots, n_e - 1$, which are explicit time events:
$$L^{(m_i)} := (t = \tau_i), \quad (2)$$
indicating the transition from mode m_i in epoch I_i to mode m_{i+1} in epoch I_{i+1} at time τ_i;
5. The system of transition functions, which is given by
$$\mathbf{x}(\mathbf{p}, T_\mu, \sigma_{i+1}) = \mathbf{D}_i\mathbf{x}(\mathbf{p}, T_\mu, \tau_i) + \mathbf{E}_i\mathbf{p} + \mathbf{k}_i, \quad \forall\, i = 1, \ldots, n_e - 1, \quad (3)$$
for the transition from mode m_i in epoch I_i to mode m_{i+1} in epoch I_{i+1}; and
6. A given initial condition for mode m_1,
$$\mathbf{x}(\mathbf{p}, T_\mu, \sigma_1) = \mathbf{E}_0\mathbf{p} + \mathbf{k}_0. \quad (4)$$

Definition 2. Let P be a nonempty compact convex subset of $\mathbb{R}^{n_p}$. Define the following sets for all $i = 1, \ldots, n_e$ where $\underline{t}$ denotes fixed t:
$$\mathcal{X}^{(i)}(\underline{t}) \equiv \left\{\mathbf{x}(\mathbf{p}, T_\mu, \underline{t}) \mid \mathbf{p} \in P, T_\mu \in M^{n_e}, \underline{t} \in I_i\right\}, \quad (5)$$

$$\mathcal{X}^{(i)} \equiv \bigcup_{\underline{t} \in I_i} \mathcal{X}^{(i)}(\underline{t}). \tag{6}$$

3. THE DECOMPOSITION ALGORITHM

Consider the following dynamic system,

$$\begin{aligned}\dot{\mathbf{x}}(\mathbf{p}, \tilde{\mathbf{z}}, t) = \mathbf{A}^{(m)}(t)\mathbf{x}(\mathbf{p}, \tilde{\mathbf{z}}, t) \\ + \mathbf{B}^{(m)}(t)\mathbf{p} + \mathbf{q}^{(m)}(t), \quad (7) \\ \mathbf{x}(\mathbf{p}, \tilde{\mathbf{z}}, \sigma) = \tilde{\mathbf{z}}, \quad (8)\end{aligned}$$

for some $m \in M$, where $\sigma < \tau, t \in T \equiv [\sigma, \tau]$, $\mathbf{p} \in P \subset \mathbb{R}^{n_p}$, $\tilde{\mathbf{z}} \in \tilde{Z} \subseteq \mathbb{R}^{n_x}$. Define the following set:

$$\mathcal{X}^a(\underline{t}) \equiv \left\{\mathbf{x}(\mathbf{p}, \tilde{\mathbf{z}}, \underline{t}) \mid \mathbf{p} \in P, \tilde{\mathbf{z}} \in \tilde{Z}, \underline{t} \ \in T\right\}. \tag{9}$$

Theorem 3. (Singer and Barton, 2003) Given $P \equiv [\mathbf{p}^L, \mathbf{p}^U]$ and $\tilde{Z} \equiv [\tilde{\mathbf{z}}^L, \tilde{\mathbf{z}}^U]$, the set $\mathcal{X}^a(\underline{t}) \equiv [\mathbf{x}^L(\underline{t}), \mathbf{x}^U(\underline{t})]$ for $\underline{t} \in T$ can be calculated point-wise in time from the following interval equation,

$$[\mathbf{x}](\underline{t}) = \mathbf{M}(\underline{t})[\mathbf{w}] + \mathbf{n}(\underline{t}), \tag{10}$$

where $\mathbf{w} = (\mathbf{p}, \tilde{\mathbf{z}})$, $\mathbf{w} \in W \equiv [\mathbf{w}^L, \mathbf{w}^U]$, $\mathbf{w}^L = (\mathbf{p}^L, \tilde{\mathbf{z}}^L)$, $\mathbf{w}^U = (\mathbf{p}^U, \tilde{\mathbf{z}}^U)$, and $\mathbf{M}(t)$ and $\mathbf{n}(t)$ are given by the solution of the following LTV system,

$$\dot{\mathbf{M}}(t) = \mathbf{A}^{(m)}(t)\mathbf{M}(t) + \mathbf{H}^{(m)}(t), \tag{11}$$

$$\dot{\mathbf{n}}(t) = \mathbf{A}^{(m)}(t)\mathbf{n}(t) + \mathbf{q}^{(m)}(t), \tag{12}$$

$$\mathbf{M}(\sigma) = \mathbf{L}, \tag{13}$$

$$\mathbf{n}(\sigma) = \mathbf{0}, \tag{14}$$

where $\mathbf{H}^{(m)}(t) = [\mathbf{B}^{(m)}(t) \ \mathbf{0}]$, $\mathbf{L} = [\mathbf{0} \ \mathbf{I}]$, and $\mathbf{I}$ is the identity matrix of rank n_x.

Remark 4. The functional form of the solution of the LTV system is affine in the parameters $\mathbf{w}$,

$$\mathbf{x}(\mathbf{w}, t) = \mathbf{M}(t)\mathbf{w} + \mathbf{n}(t). \tag{15}$$

The entries in $\mathbf{M}(t)$ are clearly the parametric sensitivities of the dynamic system, $\frac{\partial \mathbf{x}}{\partial \mathbf{w}}(t)$. Hence, (11) and (13) are simply the forward sensitivity equations of the embedded dynamic system in (7) and (8). We note that for problems where the number of parameters is much greater than the state variables, it might be more attractive to employ adjoint methods to calculate the required parametric sensitivities at the specified final time, i.e., calculating $\mathbf{M}(\tau)$ to construct $\mathcal{X}^a(\tau)$. However, it is beyond the scope of this paper to elaborate on this issue.

Remark 5. The bounds $\mathbf{x}^L(t)$ and $\mathbf{x}^U(t)$ from (10) are *exact* in the following sense. For any $i \in \{1, \ldots, n_x\}$, and any $\underline{t} \in T$, the following relationship holds,

$$\begin{aligned}x_i(\mathbf{w}^*, \underline{t}) = x_i^L(\underline{t}) \leq x_i(\mathbf{w}, \underline{t}) \leq \\ x_i^U(\underline{t}) = x_i(\mathbf{w}^\dagger, \underline{t}), \ \forall \ \mathbf{w} \in W, \quad (16)\end{aligned}$$

for some $\mathbf{w}^*, \mathbf{w}^\dagger \in W$.

From Remark 5, we know that exact bounds for $\mathbf{x}(\tau)$ can be constructed for each subproblem in the mixed-integer reformulation presented in (Barton and Lee, 2003) once the bounds for $\tilde{\mathbf{z}}$ are known. This suggests the following decomposition algorithm for estimating the bounds on $\mathbf{Z} \in Z$, where $\mathbf{z}_i$ represents the initial conditions for epoch I_i.

Algorithm 1. (A1).

(1) Initialize i=1.
(2) For $m = 1$ to n_m do:
    (a) Integrate the following system from σ_1 to τ_1, and store $\mathbf{M}_1^{(m)}(\tau_1)$ and $\mathbf{n}_1^{(m)}(\tau_1)$.

$$\dot{\mathbf{M}}_1^{(m)}(t) = \mathbf{A}^{(m)}(t)\mathbf{M}_1^{(m)}(t) + \mathbf{B}^{(m)}(t), \tag{17}$$

$$\dot{\mathbf{n}}_1^{(m)}(t) = \mathbf{A}^{(m)}(t)\mathbf{n}_1^{(m)}(t) + \mathbf{q}^{(m)}(t), \tag{18}$$

$$\mathbf{M}_1^{(m)}(\sigma_1) = \mathbf{E}_0, \tag{19}$$

$$\mathbf{n}_1^{(m)}(\sigma_1) = \mathbf{k}_0. \tag{20}$$

    (b) Calculate and store $[{\mathbf{x}^{(m)}}^L(\sigma_2)$, ${\mathbf{x}^{(m)}}^U(\sigma_2)]$ from

$$\begin{aligned}[\mathbf{x}^{(m)}](\sigma_2) = \Big(\mathbf{D}_1\mathbf{M}_1^{(m)}(\tau_1) + \mathbf{E}_1\Big)[\mathbf{p}] + \\ \mathbf{D}_1\mathbf{n}_1^{(m)}(\tau_1) + \mathbf{k}_1. \quad (21)\end{aligned}$$

(3) For $j = 1$ to n_x do:
    (a) Calculate and store the jth element of $[\mathbf{z}_{i+1}^L, \mathbf{z}_{i+1}^U]$ from

$$(\mathbf{z}_{i+1}^L)_j = \min_{m \in M} \ {x_j^{(m)}}^L(\sigma_{i+1}), \tag{22}$$

$$(\mathbf{z}_{i+1}^U)_j = \max_{m \in M} \ {x_j^{(m)}}^U(\sigma_{i+1}). \tag{23}$$

(4) For $i = 2$ to $(n_e - 1)$ do:
    (a) For $m = 1$ to n_m do:
        (i) Integrate the system (11), (12), (13) and (14) from $\sigma = \sigma_i$ to $\tau = \tau_i$, and store $\mathbf{M}_i^{(m)}(\tau_i) \leftarrow \mathbf{M}(\tau)$ and $\mathbf{n}_i^{(m)}(\tau_i) \leftarrow \mathbf{n}(\tau)$.
        (ii) Calculate and store $[{\mathbf{x}^{(m)}}^L(\sigma_{i+1})$, ${\mathbf{x}^{(m)}}^U(\sigma_{i+1})]$ from

$$\begin{aligned}[\mathbf{x}^{(m)}](\sigma_{i+1}) = \Big(\mathbf{D}_i\mathbf{M}_i^{(m)}(\tau_i) + \mathbf{L}_i\Big)[\mathbf{w}] + \\ \mathbf{D}_i\mathbf{n}_i^{(m)}(\tau_i) + \mathbf{k}_i. \quad (24)\end{aligned}$$

where $\mathbf{w}^L = (\mathbf{p}^L, \mathbf{z}_i^L)$, $\mathbf{w}^U = (\mathbf{p}^U, \mathbf{z}_i^U)$, and $\mathbf{L}_i = [\mathbf{E}_i \ \mathbf{0}]$.

    (b) Calculate and store $[\mathbf{z}_{i+1}^L, \mathbf{z}_{i+1}^U]$ as in Step (3) above.

Remark 6. The staggered corrector method can be used for efficient integration of the dynamic systems (Feehery *et al.*, 1997).

Remark 7. The system (11), (12), (13) and (14) is independent of the parameters $\mathbf{w}$, hence the values of $\mathbf{M}(\tau)$ and $\mathbf{n}(\tau)$ are also independent of $\mathbf{w}$. Hence, if the epochs are of equal duration, i.e., $\tau_i - \sigma_i$ is constant for all i, and we have a linear time invariant hybrid system, step (4ai) only needs to be executed once for $i = 2$.

Remark 8. Note that $\mathbf{M}_1$ is a $n_x \times n_p$ matrix, while $\mathbf{M}_{i\neq 1}$ is a $n_x \times (n_p + n_x)$ matrix.

Although Theorem 3 guarantees exact bounds for the system (7) and (8), the bounds obtained from implementing (A1) have no guarantee of being exact for $\mathbf{Z}$ past the first epoch. This arises because bounds for different elements of $[\mathbf{z}_i^L, \mathbf{z}_i^U]$, $i > 2$, could come from different predecessor modes I_{i-1}, and this is illustrated in the example presented below.

One way to obtain exact bounds is to solve the bounding equations (see (Lee *et al.*, 2004) for obtaining the exact bounds for fixed T_μ) for all possible combinations of T_μ. This method clearly suffers from exponential complexity in the number of epochs, and an alternative algorithm for computing tighter bounds for $\mathbf{Z}$ is needed.

4. THE RELAXED LP ALGORITHM

Consider the following problem.

Problem 9. (P1(α,β)).

$$\min_{\mathbf{p}\in P, \mathbf{Y}\in Y^b, \mathbf{Z}} \mathbf{e}_\beta^{\mathrm{T}} \mathbf{z}_{\alpha+1} \tag{25}$$

$$\text{s.t.} \sum_{m=1}^{n_m} y_{mi} = 1, \ \forall\, i = 1, \ldots, \alpha, \tag{26}$$

$$\mathbf{z}_{i+1} = \sum_{m=1}^{n_m} y_{mi}\Big(\mathbf{D}_i \mathbf{x}_{mi}(\mathbf{p}, \mathbf{Z}, \tau_i) + \mathbf{E}_i \mathbf{p} + \mathbf{k}_i\Big), \quad \forall\, i = 1, \ldots, \alpha, \tag{27}$$

$$\mathbf{z}_1 = \mathbf{E}_0 \mathbf{p} + \mathbf{k}_0, \tag{28}$$

where $Y^b \equiv \{0,1\}^{n_m \times \alpha} \subset Y \equiv [0,1]^{n_m \times \alpha}$, $\mathbf{Z} \in \mathbb{R}^{n_x \times (\alpha+1)}$, and the unit vector $\mathbf{e}_\beta$ is the βth column of the rank n_x identity matrix; $\mathbf{x}_{mi}(\mathbf{p}, \mathbf{Z}, t)$ are given by the solution of the following embedded LTV ODE systems for all $m \in M$, $i = 1, \ldots, \alpha$,

$$\dot{\mathbf{x}}_{mi}(\mathbf{p}, \mathbf{Z}, t) = \mathbf{A}^{(m)}(t)\mathbf{x}_{mi}(\mathbf{p}, \mathbf{Z}, t) + \mathbf{B}^{(m)}(t)\mathbf{p} + \mathbf{q}^{(m)}(t), \ \forall\, t \in I_i, \tag{29}$$

$$\mathbf{x}_{mi}(\mathbf{p}, \mathbf{Z}, \sigma_i) = \mathbf{z}_i. \tag{30}$$

Problem (P1) determines the exact lower bound for the βth component of $\mathbf{x}(\mathbf{p}, T_\mu, \sigma_{\alpha+1}) = \mathbf{z}_{\alpha+1}$. We can construct a convex relaxation for (P1) by treating the bilinear terms in (27) using the exact linearizations in (Glover, 1975). We can then formulate the following, equivalent, MILP.

Problem 10. (P2(α,β)).

$$\min_{\mathbf{p},\mathbf{Y},\mathbf{Z},\mathbf{V},\mathbf{W},\mathbf{S}} \mathbf{e}_\beta^{\mathrm{T}} \mathbf{z}_{\alpha+1} \tag{31}$$

$$\text{s.t.} \sum_{m=1}^{n_m} y_{mi} = 1, \ \forall\, i = 1, \ldots, \alpha, \tag{32}$$

$$\mathbf{z}_{i+1} = \sum_{m=1}^{n_m} \mathbf{s}_{mi}, \ \forall\, i = 1, \ldots, \alpha, \tag{33}$$

$$\mathbf{z}_1 = \mathbf{E}_0 \mathbf{p} + \mathbf{k}_0, \tag{34}$$

$$\mathbf{v}_{mi}^U (y_{mi} - 1) + \mathbf{v}_{mi} \leq \mathbf{s}_{mi} \leq \mathbf{v}_{mi}^L (y_{mi} - 1) + \mathbf{v}_{mi}, \ \forall\, m \in M, i = 1, \ldots, \alpha, \tag{35}$$

$$\mathbf{v}_{mi}^L y_{mi} \leq \mathbf{s}_{mi} \leq \mathbf{v}_{mi}^U y_{mi}, \ \forall\, m \in M, i = 1, \ldots, \alpha, \tag{36}$$

$$\mathbf{v}_{m1} = \Big(\mathbf{D}_1 \mathbf{M}_1^{(m)}(\tau_1) + \mathbf{E}_1\Big)\mathbf{p} + \mathbf{D}_1 \mathbf{n}_1^{(m)}(\tau_1) + \mathbf{k}_1, \ \forall\, m \in M, \tag{37}$$

$$\mathbf{v}_{mi} = \Big(\mathbf{D}_i \mathbf{M}_i^{(m)}(\tau_i) + \mathbf{L}_i\Big)\mathbf{w}_i + \mathbf{D}_i \mathbf{n}_i^{(m)}(\tau_i) + \mathbf{k}_i, \ \forall\, m \in M, i = 2, \ldots, \alpha, \tag{38}$$

$$\mathbf{w}_i = (\mathbf{p}, \mathbf{z}_i), \ \forall\, i = 2, \ldots, \alpha, \tag{39}$$

$$\mathbf{w}_1 = \mathbf{0}, \tag{40}$$

where $\mathbf{Y} \in Y^b \equiv \{0,1\}^{n_m \times \alpha} \subset Y \equiv [0,1]^{n_m \times \alpha}$, $\mathbf{Z} \in \mathbb{R}^{n_x \times (\alpha+1)}$, $\mathbf{V} \in V \subset \mathbb{R}^{n_x \times n_m \times \alpha}$, $\mathbf{W} \in \mathbb{R}^{(n_p+n_x) \times \alpha}$, $\mathbf{S} \in \mathbb{R}^{n_x \times n_m \times \alpha}$, and the unit vector $\mathbf{e}_\beta$ is the βth column of a rank n_x identity matrix; $\mathbf{L}_i = [\mathbf{E}_i \ \mathbf{0}]$; $\mathbf{M}_1^{(m)}(\tau_1)$ and $\mathbf{n}_1^{(m)}(\tau_1)$ are given by the solution of the system (17), (18), (19) and (20) from σ_1 to τ_1 for $m \in M$; and $\mathbf{M}_i^{(m)}(\tau_i)$ and $\mathbf{n}_i^{(m)}(\tau_i)$ are given by the solution of the system (11), (12), (13) and (14) from $\sigma = \sigma_i$ to $\tau = \tau_i$, for $m \in M$, $i = 2, \ldots, \alpha$.

The required bounds on the auxiliary variables $\mathbf{V}$ (see (35) and (36)) constitute the set V, and can be determined sequentially for each epoch (see algorithm below). The variables $\mathbf{Z}$, $\mathbf{W}$, $\mathbf{S}$ are left as free or unrestricted variables. While it is impractical to solve a family of MILPs (P2) to obtain the tightest bounds for $\mathbf{Z}$, it is much cheaper to solve (P2) on the relaxed space $\mathbf{Y} \in Y$, resulting in solving a family of relaxed LPs to provide valid (but not exact) bounds for $\mathbf{Z}$. This constitutes the following algorithm.

Algorithm 2. (A2).

(1) Execute steps (1), (2) and (3) in (A1).
(2) For $i = 2$ to $(n_e - 1)$ do:
  (a) For $m = 1$ to n_m do:
    (i) Integrate the system (11), (12), (13) and (14) from $\sigma = \sigma_i$ to $\tau = \tau_i$, and store $\mathbf{M}_i^{(m)}(\tau_i) \leftarrow \mathbf{M}(\tau)$ and $\mathbf{n}_i^{(m)}(\tau_i) \leftarrow \mathbf{n}(\tau)$.
    (ii) Calculate and store $[\hat{\mathbf{x}}^{(m)^L}(\sigma_{i+1}), \hat{\mathbf{x}}^{(m)^U}(\sigma_{i+1})]$ from

$$[\hat{\mathbf{x}}^{(m)}](\sigma_{i+1}) = \Big(\mathbf{D}_i \mathbf{M}_i^{(m)}(\tau_i) + \mathbf{L}_i\Big)[\mathbf{w}] + \mathbf{D}_i \mathbf{n}_i^{(m)}(\tau_i) + \mathbf{k}_i. \quad (41)$$

where $\mathbf{w}^L = (\mathbf{p}^L, \mathbf{z}_i^L)$, $\mathbf{w}^U = (\mathbf{p}^U, \mathbf{z}_i^U)$, and $\mathbf{L}_i = [\mathbf{E}_i \ \mathbf{0}]$.

  (b) For $m = 1$ to n_m do:
    (i) For $j = 1$ to n_x do:
      (A) Solve (P2(i,j)), with $[\mathbf{v}_{\lambda\theta}] = [\mathbf{x}^{(\lambda)}](\sigma_{\theta+1})$, $\theta = 1, \ldots, i-1$, and $[\mathbf{v}_{\lambda i}] = [\hat{\mathbf{x}}^{(\lambda)}](\sigma_{i+1})$, for all $\lambda \in M$, on the relaxed space Y, with the following constraint,

$$y_{mi} = 1, \quad (42)$$

and store $x_j^{(m)^L}(\sigma_{i+1}) \leftarrow$ objective.
      (B) Repeat step (A) as a maximization problem, and store $x_j^{(m)^U}(\sigma_{i+1}) \leftarrow$ objective.

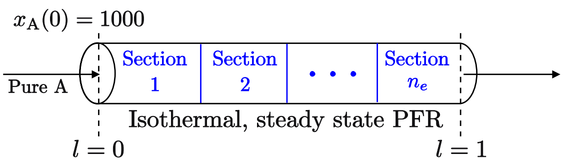
  (c) For $j = 1$ to n_x do:
    (i) Calculate and store the jth element of $[\mathbf{z}_{i+1}^L, \mathbf{z}_{i+1}^U]$ from

$$(\mathbf{z}_{i+1}^L)_j = \min_{m \in M} x_j^{(m)^L}(\sigma_{i+1}), \quad (43)$$

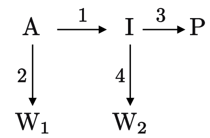
$$(\mathbf{z}_{i+1}^U)_j = \max_{m \in M} x_j^{(m)^U}(\sigma_{i+1}). \quad (44)$$

5. AN ILLUSTRATIVE EXAMPLE

Example 11. Consider an isothermal plug flow reactor (PFR) operating at steady state, and 3 possible choices of catalyst. The reaction scheme, initial conditions and associated rate constants are shown in Fig. 1, where x_i represents the molar concentration of component i (kmol m^{-3}) and k_j represents the rate constant of reaction j (h^{-1}). The PFR has a uniform cross-sectional area of 1 m^2, and a constant volumetric flow rate of 1 m^3 h^{-1}. In this example, the independent variable t is the length, l, of the reactor. Determine the bounds on the concentration of the reactant and products at the beginning of each reactor section.



Reaction scheme



Catalyst

	k_1	k_2	k_3	k_4
1	2.098	1.317	0.021	0.033
2	29.53	110.2	0.295	0.079
3	182.6	2325	1.826	0.143

Kinetics

$$\dot{x}_A = -(k_1 + k_2)x_A \qquad \dot{x}_I = k_1 x_A - (k_3 + k_4)x_I$$
$$\dot{x}_{W_1} = k_2 x_A \qquad \dot{x}_{W_2} = k_4 x_I$$
$$\dot{x}_P = k_3 x_I$$

Fig. 1. Chemical reaction scheme and kinetics for PFR example

Note that the choice of catalyst corresponds to the choice of the sequence of modes in a linear hybrid system with 3 modes (each mode corresponds to the choice of a different catalyst) and n_e epochs (each epoch corresponds to a section of the reactor), with state continuity at the transitions.

Tables 1 and 2 show the bounds obtained for $\mathbf{z}_8$ and $\mathbf{z}_{15}$ when $n_e = 15$ when explicit enumeration (EE) (which obtains the exact bounds), (A1) and (A2) are used. As can be seen, (A2) produces tighter bounds than (A1). When physical infor-

Table 1. Bounds for $\mathbf{z}_8$ where $n_e = 15$

Species	(EE) $\mathbf{z}_8^L$	(EE) $\mathbf{z}_8^U$	(A1) $\mathbf{z}_8^L$	(A1) $\mathbf{z}_8^U$
A	0.00	203.18	0.00	203.18
W_1	307.30	927.18	78.52	3628.49
I	29.08	493.23	29.08	735.13
W_2	1.48	12.68	0.76	29.59
P	2.98	139.37	0.49	373.51
Species	**(A2) $\mathbf{z}_8^L$**	**(A2) $\mathbf{z}_8^U$**	**(A2) with (45) $\mathbf{z}_8^L$**	**(A2) with (45) $\mathbf{z}_8^U$**
A	0.00	203.18	0.00	203.18
W_1	230.54	1734.62	307.30	959.02
I	29.08	493.23	29.08	493.23
W_2	1.19	16.16	1.19	16.16
P	1.26	190.19	1.28	180.97

Table 2. Bounds for $\mathbf{z}_{15}$ where $n_e = 15$

Species	(EE) $\mathbf{z}_{15}^L$	(EE) $\mathbf{z}_{15}^U$	(A1) $\mathbf{z}_{15}^L$	(A1) $\mathbf{z}_{15}^U$
A	0.00	41.28	0.00	41.28
W_1	369.73	927.18	78.52	4365.72
I	11.60	567.77	11.60	815.88
W_2	2.43	27.87	1.08	79.06
P	7.34	293.77	0.69	1005.21
Species	**(A2) $\mathbf{z}_{15}^L$**	**(A2) $\mathbf{z}_{15}^U$**	**(A2) with (45) $\mathbf{z}_{15}^L$**	**(A2) with (45) $\mathbf{z}_{15}^U$**
A	0.00	41.28	0.00	41.28
W_1	230.54	2030.39	321.03	981.59
I	11.60	567.77	11.60	567.77
W_2	1.54	44.77	1.54	44.77
P	1.51	544.39	1.53	451.06

mation from the problem can be used, e.g., conservation of molar species, we can add the following additional constraints to (P2),

$$\sum_{j=1}^{n_x} (\mathbf{s}_{mi})_j = 1000 y_{mi}, \ \forall\ m \in M, i = 1, \ldots, \alpha. \tag{45}$$

When this physical insight is employed, it can be seen that the bounds obtained from (A2) with (45) produces tighter bounds than using (A2) alone. The reason why (A2) itself does not produce bounds which obey this conservation law is that the linearizations of the bilinear terms in (27) are only exact on the space Y^b, and not on the space Y. Hence, we have to enforce the law with (45). Note that there is no way to incorporate additional constraints within (A1). For further illustration, the upper bound computed for species W_1 at the beginning of each section when $n_e = 10$ is shown in Table 3.

Table 4 shows the bounds obtained for W_1 when the algorithms are trivially extended to calculate the bounds at $l = 1$. It can be seen that the bounds obtained from (A1) and (A2) deteriorate significantly from the exact bounds as n_e increases. When physical insight (45) is employed in conjunction with (A2), much tighter bounds are obtained.

All calculations were performed on an AMD 1.2 GHz, 1 GB RAM machine using CPLEX 7.5 as the LP solver. All LPs were started cold, and we note that the computational times for (A2) would improve if the LPs were warm started where possible. The computation times for the algorithms are shown in Table 5, from which the exponential explosion of (EE) is clear.

6. CONCLUSION

The deterministic solution of global dynamic optimization problems with LTV hybrid systems embedded depends on the construction of convex relaxations of the participating functions. The quality of these relaxations in turn relies on the computation of tight state bounds. While the exact state bounds can be computed via explicit enumeration, this approach quickly becomes impractical as the number of epochs is increased. We show through an example that a simple and efficient decomposition approach based on calculating the exact state bounds for the subproblems of a mixed-integer reformulated problem produces weak bounds which deteriorate as the number of epochs increases. A novel algorithm is proposed based on the solution of families of MILPs as relaxed LPs. This algorithm is able to incorporate physical insight as additional constraints in the LPs, and produces significantly tighter bounds than the decomposition algorithm.

Table 3. Upper bound for W_1 ($n_e = 10$)

Section	(EE)	(A1)	(A2)	(A2) with (45)
2	927.18	927.18	927.18	927.18
3	927.18	1586.13	927.18	927.18
4	927.18	2054.45	1161.34	932.50
5	927.18	2387.29	1245.91	945.55
6	927.18	2623.83	1356.05	954.30
7	927.18	2791.95	1401.19	961.80
8	927.18	2911.43	1461.41	967.78
9	927.18	2996.34	1482.13	972.70
10	927.18	3056.69	1516.14	976.73

Table 4. Upper bound for W_1 at $l = 1$

n_e	(EE)	(A1)	(A2)	(A2) with (45)
5	927.18	1811.88	1094.46	967.02
10	927.18	3099.58	1523.92	980.04
15	927.18	4404.00	2052.69	983.43
20	927.18	5712.63	2605.73	984.89

Table 5. CPU times (s)

n_e	(EE)	(A1)	(A2)	(A2) with (45)
5	0.04	0.04	1.6	2.3
10	0.4	0.04	8.3	12.8
15	135	0.04	27.1	45.7
20	44227	0.04	50.7	86.7

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