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Efficient polyhedral enclosures for the reachable set of nonlinear control systems

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Abstract This work presents a general theory for the construction of a polyhedral outer approximation of the reachable set (“polyhedral bounds”) of a dynamic system subject to time-varying inputs and uncertain initial conditions. This theory is inspired by the efficient methods for the construction of interval bounds based on comparison theorems. A numerically implementable instance of this theory leads to an auxiliary system of differential equations which can be solved with standard numerical integration methods. Meanwhile, the use of polyhedra provides greater flexibility in defining tight enclosures on the reachable set. These advantages are demonstrated with a few examples, which show that tight bounds can be efficiently computed for general, nonlinear systems. Further, it is demonstrated that the ability to use polyhedra provides a means to meaningfully distinguish between time-varying and constant, but uncertain, inputs.

Keywords control systems · reachability · linear programming · affine relaxations

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1 Introduction

This work considers estimating the reachable set of the initial value problem (IVP) in ordinary differential equations (ODEs)

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

where the initial condition is in some known set and the inputs \mathbf{u} vary in some known set (see Section 2 for notation and a formal problem statement). The time-varying inputs \mathbf{u} can model noise, disturbances, or control inputs; estimating the reachable set in these cases is critical to robust model predictive control (MPC) [2], fault detection [26] and global optimization of dynamic systems [43]. This work will focus on the construction of a time-varying (convex) polyhedral enclosure of the reachable set. Specifically, given a matrix \mathbf{A} , an auxiliary initial value problem in ordinary differential equations is constructed whose solution yields the function \mathbf{b} , such that the set $\{\mathbf{z} : \mathbf{Az} \leq \mathbf{b}(t)\}$ contains the values of the solutions of the dynamic system at all times t .

The major contribution of this work is as follows. First, the construction of the auxiliary system of bounding equations closely resembles the bounding method in [39] which produces interval bounds (i.e., component-wise upper and lower bounds) very quickly. The work in [39] is itself an extension of differential inequality-based comparison theorems in, for instance, [14]. The extension of these comparison theorems to the construction of polyhedral bounds is a significant improvement, allowing bounds with the increased flexibility of polyhedra (as opposed to intervals) to be calculated with powerful and efficient methods for numerical integration. The new theory in this work essentially permits the extension of the interval bounding methods in [16, 17] to the construction of polyhedral bounds. Although this extension is fairly straightforward once the theory is established, the subsequent analysis of the new algorithms to ensure that they remain numerically well behaved is nontrivial.

The general concept of previous implementations of polyhedron-based bounding methods, such as those in [1, 6, 8, 13], is to “move” the faces of the approximating polyhedra in accordance with the maximum value of the dynamics on that face, which is similar to the theory in this work. However, these previous methods manually implement the time-stepping, which contrasts with the proposed method, which takes advantage of established codes for numerical integration, and thus benefits from their handling of step size to control errors to a desired tolerance. The present work could be used to implement the step forward in time in these previous methods; however, the work presented here stands on its own as an effective method on the overall time scale of interest, as demonstrated by the numerical experiments in Section 5. Further, these examples provide new insight into “intelligent” choices for the matrix \mathbf{A} which defines the polyhedral approximation.

Another significant contribution of this work is its ability to distinguish meaningfully between time-varying inputs and constant, but unknown, parameters. This contrasts with the previous work involving comparison theorems,

such as in [16,22,35,38,39]. As noted in [39], comparison theorems in general take into account time-varying uncertainty, which can be an advantage or disadvantage depending on one's perspective or the model of interest. In contrast, methods based on parametric Taylor-models, such as in [5,25], intrinsically handle constant, but uncertain parameter inputs. Since the present work is inspired by comparison theorems, it is natural that it should be able to handle time-varying uncertainty. But the use of polyhedra allows one to propagate affine relaxations of the states with respect to the parameters by treating the unknown parameters as extra states, but with time derivatives equal to zero. This explicitly enforces these uncertain inputs to be constant, and as demonstrated by an example in Section 5.3, this leads to an improvement in the bounds.

Other work that should be mentioned involves the computation of the reachable set or an approximation of it through a level set that evolves in time, such as in [31]. However, this involves the solution of a Hamilton-Jacobi-type partial differential equation, and consequently is more computationally demanding than the comparison theorem based methods, including this work. This is noted in [19], in which the solution of matrix exponentials is favored over the solution of partial differential equations to obtain a polyhedral approximation of the reachable set of a dynamic system. However, that work only considers linear dependence on the inputs, and weakly nonlinear dynamics. Meanwhile, work dealing with differential inclusions is also related [9,21]. In particular, the work in [21] is theoretically more alike to the proposed work and has a numerical implementation that is based on validated or set-based numerical integrators (as in [33]). This class of methods have proven to be relevant numerical methods for calculating bounds.

The rest of this work is organized as follows. Section 2 gives notation and a rigorous problem statement. Section 3 is split into two subsections. Section 3.1 states and proves one of the main results of this work, Theorem 1. This theorem is a general result stating conditions under which a polyhedral-valued mapping is an enclosure of the reachable set. Section 3.2 provides a specific instance of this theory in Corollary 2, which states that the solution of an auxiliary initial value problem yields polyhedral bounds. This leads to a numerically implementable method for constructing polyhedral bounds discussed in Section 4. One of the main goals of Section 4 is to establish that the auxiliary problem satisfies basic assumptions to be amenable to solution with general classes of numerical integration methods. Section 5 demonstrates a numerical implementation of the proposed bounding method on a few examples. Section 6 concludes with some final remarks.

2 Problem Statement

Notation that is used in this work includes lowercase bold letters for vectors and uppercase bold letters for matrices. The transposes of a vector \mathbf{v} and matrix \mathbf{M} are denoted \mathbf{v}^T and \mathbf{M}^T , respectively. The exception is that $\mathbf{0}$ may

denote either a matrix or vector of zeros, but it should be clear from context what the appropriate dimensions are. Similarly, \mathbf{I} will denote the identity matrix whose dimensions should be clear from context. Inequalities between vectors hold componentwise. For $\mathbf{v}, \mathbf{w} \in \mathbb{R}^n$ such that $\mathbf{v} \leq \mathbf{w}$, $[\mathbf{v}, \mathbf{w}]$ denotes an interval in \mathbb{R}^n . A polyhedron is any subset of \mathbb{R}^n that can be expressed as $\{\mathbf{z} \in \mathbb{R}^n : \mathbf{M}\mathbf{z} \leq \mathbf{d}\}$, for some matrix $\mathbf{M} \in \mathbb{R}^{m \times n}$ and vector $\mathbf{d} \in \mathbb{R}^m$ (i.e., it is the intersection of a finite number of closed halfspaces). Consequently, it is clear that polyhedra are always closed, convex sets. The equivalence of norms on \mathbb{R}^n is used often; when a statement or result holds for any choice of norm, it is denoted $\|\cdot\|$. In some cases, it is useful to reference a specific norm, in which case it is subscripted; for instance, $\|\cdot\|_1$ denotes the 1-norm. The dual of a norm $\|\cdot\|$ is denoted $\|\cdot\|_*$. For $n \in \mathbb{N}$ and a set $T \subset \mathbb{R}$, denote the Lebesgue space $L^1(T, \mathbb{R}^n) \equiv \{(\mathbf{v} : T \rightarrow \mathbb{R}^n) : \int_T |v_i| < +\infty, \forall i\}$. That is, $\mathbf{v} \in L^1(T, \mathbb{R}^n)$ if each component of \mathbf{v} is in $L^1(T)$. For sets X, Y , a mapping S from X to the set of subsets of Y is denoted $S : X \rightrightarrows Y$. In a metric space, a neighborhood of a point x is denoted $N(x)$ and refers to an open ball centered at x with some nonzero radius. If this radius δ is important, it may be emphasized as a subscript, e.g. $N_\delta(x)$.

The problem statement follows. Let $n_x, n_u \in \mathbb{N}$, interval $T = [t_0, t_f] \subset \mathbb{R}$, $D_x \subset \mathbb{R}^{n_x}$, and $D_u \subset \mathbb{R}^{n_u}$ be given. For $U \subset D_u$, let the set of time-varying inputs be

$$\mathcal{U} = \{\mathbf{u} \in L^1(T, \mathbb{R}^{n_u}) : \mathbf{u}(t) \in U, a.e. t \in T\},$$

and let the set of possible initial conditions be $X_0 \subset D_x$. Given $\mathbf{f} : T \times D_u \times D_x \rightarrow \mathbb{R}^{n_x}$, the problem of interest is the IVP in ODEs

$$\dot{\mathbf{x}}(t, \mathbf{u}) = \mathbf{f}(t, \mathbf{u}(t), \mathbf{x}(t, \mathbf{u})), \quad a.e. t \in T, \quad \mathbf{x}(t_0, \mathbf{u}) \in X_0. \quad (1)$$

For given $\mathbf{u} \in \mathcal{U}$, a solution is an absolutely continuous mapping $\mathbf{x}(\cdot, \mathbf{u}) : T \rightarrow D_x$ which satisfies (1). The goal of this work is to construct a polyhedral-valued mapping $B : T \rightrightarrows \mathbb{R}^{n_x}$ such that for all $\mathbf{u} \in \mathcal{U}$ and any solution $\mathbf{x}(\cdot, \mathbf{u})$ (if one exists for this \mathbf{u}), $\mathbf{x}(t, \mathbf{u}) \in B(t)$, for all $t \in T$. Specifically, given a $m \in \mathbb{N}$ and a matrix $\mathbf{A} \in \mathbb{R}^{m \times n_x}$, the goal is to find $\mathbf{b} : T \rightarrow \mathbb{R}^m$ such that $B(t) = \{\mathbf{z} : \mathbf{A}\mathbf{z} \leq \mathbf{b}(t)\}$. This mapping B will be referred to as polyhedral bounds, or just bounds.

Assumption 1 For any $\mathbf{z} \in D_x$, there exists a neighborhood $N(\mathbf{z})$ and $\alpha \in L^1(T)$ such that for almost every $t \in T$ and every $\mathbf{p} \in U$

$$\|\mathbf{f}(t, \mathbf{p}, \mathbf{z}_1) - \mathbf{f}(t, \mathbf{p}, \mathbf{z}_2)\| \leq \alpha(t) \|\mathbf{z}_1 - \mathbf{z}_2\|,$$

for every $\mathbf{z}_1, \mathbf{z}_2 \in N(\mathbf{z}) \cap D_x$.

Assumption 1 is fairly critical to the following general theory. However, it is not restrictive at all. It is related to standard assumptions that general classes of numerical integration methods are applicable to the IVP (1). Further discussion along these lines is in Section 4.2. Furthermore, under Assumption 1 the solutions of IVP (1) for a given $\mathbf{u} \in \mathcal{U}$ and fixed initial condition are unique; see Theorem 2 in Section 1 of [10].

3 Bounding Theory

This section will give a general theorem for polyhedral bounds, which requires a specific assumption, then discuss how to satisfy this assumption.

3.1 General theory

First, two results from the literature. The first can be found as Theorem 3.1 in [45].

Lemma 1 *Let $T \subset \mathbb{R}$ be an interval. If $a : T \rightarrow \mathbb{R}$ is absolutely continuous and $\dot{a}(t) \leq 0$ for a.e. $t \in T$, then a is nonincreasing.*

The next result is Lemma 4 in [39].

Lemma 2 *Let $T \subset \mathbb{R}$ be an interval. For any $\gamma > 0$ and $\beta \in L^1(T)$, there exists an absolutely continuous, nondecreasing function $\rho : T \rightarrow \mathbb{R}$ satisfying $0 < \rho(t) \leq \gamma$, $\forall t \in T$, and $\dot{\rho}(t) > |\beta(t)|\rho(t)$ for a.e. $t \in T$.*

The following Assumption and Theorem provide the heart of the general bounding theory. The parallels between this theory and that in [39] should be fairly clear, but to emphasize a major difference, the current theory handles polyhedral bounds as opposed to intervals. However, before continuing, it is useful to note a definition of the matrix \mathbf{A} and mappings M_i required in Assumption 2 which yield the classic interval-based comparison theorem-type results in [14], for instance. This example provides an intuitive geometric interpretation to keep in mind while understanding the general theory. Interval bounds are obtained by letting $m = 2n_x$ and $\mathbf{A} = [-\mathbf{I} \ \mathbf{I}]^T$. Then for $i \in \{1, \dots, n_x\}$, let $M_i(t, \mathbf{d})$ be the i^{th} lower face of the interval $\{\mathbf{z} : \mathbf{A}\mathbf{z} \leq \mathbf{d}\}$ (assuming it is nonempty). Similarly, for $i \in \{n_x + 1, \dots, 2n_x\}$, let $M_i(t, \mathbf{d})$ be the $(i - n_x)^{\text{th}}$ upper face of the interval. One can check that these definitions satisfy Assumption 2.

A major component of Assumption 2 is a Lipschitz condition for the general set-valued mappings M_i . To allow flexibility and practical implementation, this assumption also allows that this Lipschitz condition only holds on some domain D_M satisfying certain conditions. Section 3.2 focuses on concrete definitions of M_i and D_M that satisfy Assumption 2, which will provide the basis for the following numerical developments. The reader may wish to consult the discussion in Section 3.2 to gain more insight into the nature of D_M and M_i .

Assumption 2 *Considering the problem stated in Section 2, for some $m \in \mathbb{N}$ and for $i \in \{1, \dots, m\}$, let $\mathbf{a}_i \in \mathbb{R}^{n_x}$. Assume*

$$\mathbf{A} = \begin{bmatrix} \mathbf{a}_1^T \\ \vdots \\ \mathbf{a}_m^T \end{bmatrix} \in \mathbb{R}^{m \times n_x},$$

$D_M \subset T \times \mathbb{R}^m$, and $M_i : D_M \rightrightarrows \mathbb{R}^{n_x}$ satisfy the following conditions for each $i \in \{1, \dots, m\}$:

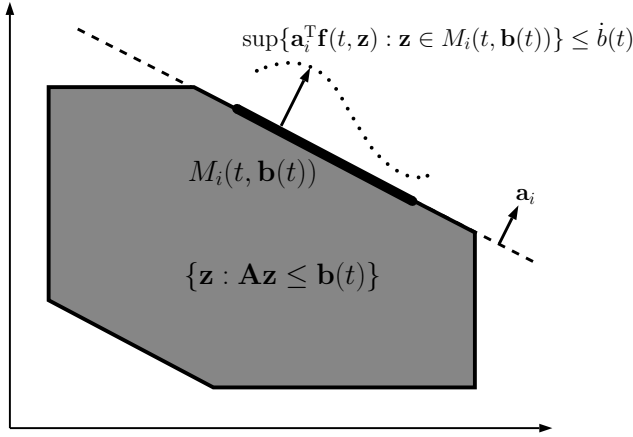


Fig. 1: Graphical representation of the basic idea of Theorem 1. In this case \mathbf{f} is independent of controls \mathbf{u} . Note that Assumption 2 allows M_i to be a strict subset of the i^{th} face of the polyhedron if external information is available, if a subset at all; see Figure 2 and Proposition 1.

1. For any $\mathbf{d} \in \mathbb{R}^m$, if there exists $(t, \mathbf{u}) \in T \times \mathcal{U}$ such that $\mathbf{A}\mathbf{x}(t, \mathbf{u}) \leq \mathbf{d}$ and $\mathbf{a}_i^T \mathbf{x}(t, \mathbf{u}) = d_i$ for some solution $\mathbf{x}(\cdot, \mathbf{u})$ of IVP (1), then $(t, \mathbf{d}) \in D_M$ and $\mathbf{x}(t, \mathbf{u}) \in M_i(t, \mathbf{d})$.
2. For any $(t, \mathbf{d}) \in D_M$, there exists a neighborhood $N(\mathbf{d})$ of \mathbf{d} , $t' > t$, and $L_M > 0$ such that for any $(s, \mathbf{d}_1), (s, \mathbf{d}_2) \in ([t, t'] \times N(\mathbf{d})) \cap D_M$ and $\mathbf{z}_1 \in M_i(s, \mathbf{d}_1)$, there exists a $\mathbf{z}_2 \in M_i(s, \mathbf{d}_2)$ such that

$$\|\mathbf{z}_1 - \mathbf{z}_2\| \leq L_M \|\mathbf{d}_1 - \mathbf{d}_2\|_1.$$

The main theorem follows. The hypothesis of most interest in this theorem is Hypothesis 4, which, for a practical implementation of this bounding theory, requires the overestimation of the dynamics on certain values of the M_i mappings. A conceptual representation of this hypothesis is given in Figure 1.

Theorem 1 *Let Assumptions 1 and 2 hold. If*

1. $\mathbf{b} : T \rightarrow \mathbb{R}^m$ is absolutely continuous and $B : T \ni t \mapsto \{\mathbf{z} : \mathbf{A}\mathbf{z} \leq \mathbf{b}(t)\}$,
2. $X_0 \subset B(t_0)$,
3. for almost every $t \in T$ and each $i \in \{1, \dots, m\}$, $(t, \mathbf{b}(t)) \in D_M$ and $M_i(t, \mathbf{b}(t)) \subset D_x$,
4. for almost every $t \in T$ and each $i \in \{1, \dots, m\}$,

$$\mathbf{a}_i^T \mathbf{f}(t, \mathbf{p}, \mathbf{z}) \leq \dot{b}_i(t), \quad \forall (\mathbf{p}, \mathbf{z}) \in U \times M_i(t, \mathbf{b}(t)),$$

then for all $\mathbf{u} \in \mathcal{U}$ and any solution $\mathbf{x}(\cdot, \mathbf{u})$ of IVP (1), $\mathbf{x}(t, \mathbf{u}) \in B(t)$, for all $t \in T$.

Proof Fix $\mathbf{u} \in \mathcal{U}$. If no solution of IVP (1) exists for this \mathbf{u} , then the conclusion of the theorem holds trivially. Otherwise, choose some solution and for convenience use the abbreviation $\mathbf{x}(t) \equiv \mathbf{x}(t, \mathbf{u})$. Let T_v be the set of $t \in T$ such that $\mathbf{a}_i^T \mathbf{x}(t) > b_i(t)$ for some i . For a contradiction, assume $T_v \neq \emptyset$.

Let $t_1 = \inf T_v$. By Hypothesis 2 and continuity, $\mathbf{Ax}(t_1) \leq \mathbf{b}(t_1)$ and $\mathbf{a}_i^T \mathbf{x}(t_1) = b_i(t_1)$ for some i . Note that by Condition 1 of Assumption 2, this implies $(t_1, \mathbf{b}(t_1)) \in D_M$. Further we must have $t_1 < t_f$.

Next, let $N_\delta(\mathbf{x}(t_1))$ and $\alpha \in L^1(T)$ satisfy Assumption 1 at the point $\mathbf{x}(t_1)$. Let $N_\epsilon(\mathbf{b}(t_1))$, $t_5 > t_1$, and $L_M > 0$ satisfy Condition 2 of Assumption 2 at $(t_1, \mathbf{b}(t_1))$ for each i . By continuity, we can choose $t_4 \in (t_1, t_5]$ so that

$$\|\mathbf{x}(t) - \mathbf{x}(t_1)\| < \delta/2, \quad (2)$$

$$\|\mathbf{b}(t) - \mathbf{b}(t_1)\|_\infty < \epsilon/2, \quad (3)$$

for all $t \in [t_1, t_4]$.

By definition of t_1 as the infimum of T_v , there exists a $t \in (t_1, t_4]$ such that for some i , $\mathbf{a}_i^T \mathbf{x}(t) > b_i(t) + \gamma$ for some $\gamma > 0$. Meanwhile, by Lemma 2, there exists an absolutely continuous and nondecreasing $\rho : [t_1, t_4] \rightarrow \mathbb{R}$ satisfying

$$\begin{aligned} 0 < \rho(t) &\leq \min\{\gamma, \epsilon/2, \delta/(2mL_M)\}, \quad \forall t \in [t_1, t_4], \\ \dot{\rho}(t) &> mL_M \max_i \{\|\mathbf{a}_i\|_*\} |\alpha(t)| \rho(t), \quad a.e. \ t \in [t_1, t_4]. \end{aligned} \quad (4)$$

Similarly to t_1 , let $t_3 = \inf\{s \in [t_1, t_4] : \exists i : \mathbf{a}_i^T \mathbf{x}(s) \geq b_i(s) + \rho(s)\}$. Since $\rho \leq \gamma$, we know that there exists a $t \in (t_1, t_4]$ such that $\mathbf{a}_i^T \mathbf{x}(t) > b_i(t) + \rho(t)$ for some i . Thus, t_3 is the infimum of a nonempty set. Since $\rho(t_1) > 0$, $\mathbf{Ax}(t_1) < \mathbf{b}(t_1) + \rho(t_1)\mathbf{1}$. Then, from continuity, we have $t_1 < t_3$ and $\mathbf{Ax}(t) < \mathbf{b}(t) + \rho(t)\mathbf{1}$, for all $t \in [t_1, t_3)$. Further, $\mathbf{a}_k^T \mathbf{x}(t_3) = b_k(t_3) + \rho(t_3)$ for some k . If not, we either have $\mathbf{a}_i^T \mathbf{x}(t_3) < b_i(t_3) + \rho(t_3)$ or $\mathbf{a}_i^T \mathbf{x}(t_3) > b_i(t_3) + \rho(t_3)$ for each i . If $\mathbf{a}_i^T \mathbf{x}(t_3) > b_i(t_3) + \rho(t_3)$ holds for any i , continuity contradicts t_3 as a lower bound. Meanwhile, continuity then contradicts t_3 as the greatest lower bound if $\mathbf{a}_i^T \mathbf{x}(t_3) < b_i(t_3) + \rho(t_3)$ holds for all i .

Now let $t_2 = \sup\{s \in [t_1, t_3] : \mathbf{a}_k^T \mathbf{x}(s) \leq b_k(s)\}$. By continuity, $t_2 < t_3$ and $\mathbf{a}_k^T \mathbf{x}(t_2) = b_k(t_2)$. The following has been established:

$$\mathbf{Ax}(t) < \mathbf{b}(t) + \rho(t)\mathbf{1}, \quad \forall t \in [t_1, t_3), \quad (5a)$$

$$b_k(t) < \mathbf{a}_k^T \mathbf{x}(t) < b_k(t) + \rho(t), \quad \forall t \in (t_2, t_3), \quad (5b)$$

$$\mathbf{a}_k^T \mathbf{x}(t_3) = b_k(t_3) + \rho(t_3), \quad (5c)$$

$$\mathbf{a}_k^T \mathbf{x}(t_2) = b_k(t_2). \quad (5d)$$

Let $\tilde{\mathbf{b}}$ be defined componentwise by $\tilde{b}_i : t \mapsto \max\{\mathbf{a}_i^T \mathbf{x}(t), b_i(t)\}$. Then, for any $t \in [t_2, t_3]$, $\mathbf{Ax}(t) \leq \tilde{\mathbf{b}}(t)$, and $\mathbf{a}_k^T \mathbf{x}(t) = \tilde{b}_k(t)$. Consequently, by Condition 1 of Assumption 2, $(t, \tilde{\mathbf{b}}(t)) \in D_M$ and $\mathbf{x}(t) \in M_k(t, \tilde{\mathbf{b}}(t))$ for all $t \in [t_2, t_3]$. By (5a), $\|\tilde{\mathbf{b}}(t) - \mathbf{b}(t)\|_\infty \leq \rho(t)$, so using the triangle inequality, Inequality (3),

and Inequality (4),

$$\begin{aligned} \left\| \tilde{\mathbf{b}}(t) - \mathbf{b}(t_1) \right\|_{\infty} &\leq \left\| \tilde{\mathbf{b}}(t) - \mathbf{b}(t) \right\|_{\infty} + \left\| \mathbf{b}(t) - \mathbf{b}(t_1) \right\|_{\infty} \\ &< \epsilon/2 + \epsilon/2. \end{aligned}$$

Thus, $\tilde{\mathbf{b}}(t)$ and $\mathbf{b}(t)$ are in $N_{\epsilon}(\mathbf{b}(t_1))$ for $t \in [t_2, t_3]$. And by Hypothesis 3, $(t, \mathbf{b}(t)) \in D_M$ for *a.e.* $t \in [t_2, t_3]$. So by Condition 2 of Assumption 2, there exists $\mathbf{z}_k(t) \in M_k(t, \mathbf{b}(t))$ such that

$$\left\| \mathbf{x}(t) - \mathbf{z}_k(t) \right\| \leq L_M \left\| \tilde{\mathbf{b}}(t) - \mathbf{b}(t) \right\|_1 \leq mL_M \rho(t) \leq \delta/2 \quad (6)$$

for *a.e.* $t \in [t_2, t_3]$. Combining this with the triangle inequality and Inequality (2),

$$\left\| \mathbf{z}_k(t) - \mathbf{x}(t_1) \right\| \leq \left\| \mathbf{z}_k(t) - \mathbf{x}(t) \right\| + \left\| \mathbf{x}(t) - \mathbf{x}(t_1) \right\| < \delta.$$

Thus $\mathbf{z}_k(t) \in N_{\delta}(\mathbf{x}(t_1))$ for *a.e.* $t \in [t_2, t_3]$.

Then for *a.e.* $t \in [t_2, t_3]$,

$$\begin{aligned} \mathbf{a}_k^{\top} \dot{\mathbf{x}}(t) &= \mathbf{a}_k^{\top} \mathbf{f}(t, \mathbf{u}(t), \mathbf{x}(t)) \\ &= \mathbf{a}_k^{\top} (\mathbf{f}(t, \mathbf{u}(t), \mathbf{x}(t)) - \mathbf{f}(t, \mathbf{u}(t), \mathbf{z}_k(t))) + \mathbf{a}_k^{\top} \mathbf{f}(t, \mathbf{u}(t), \mathbf{z}_k(t)) \\ &\leq \|\mathbf{a}_k\|_* \left\| \mathbf{f}(t, \mathbf{u}(t), \mathbf{x}(t)) - \mathbf{f}(t, \mathbf{u}(t), \mathbf{z}_k(t)) \right\| + \dot{b}_k(t), \end{aligned}$$

where the last inequality follows from Hypothesis 4 since $\mathbf{z}_k(t) \in M_k(t, \mathbf{b}(t))$. By Assumption 1 and Inequality (6), this leads to

$$\begin{aligned} \mathbf{a}_k^{\top} \dot{\mathbf{x}}(t) &\leq \|\mathbf{a}_k\|_* |\alpha(t)| \left\| \mathbf{x}(t) - \mathbf{z}_k(t) \right\| + \dot{b}_k(t) \\ &\leq \|\mathbf{a}_k\|_* |\alpha(t)| mL_M \rho(t) + \dot{b}_k(t). \end{aligned}$$

Using the properties of ρ , we have

$$\begin{aligned} \mathbf{a}_k^{\top} \dot{\mathbf{x}}(t) - \dot{\rho}(t) &\leq \|\mathbf{a}_k\|_* |\alpha(t)| mL_M \rho(t) - \dot{\rho}(t) + \dot{b}_k(t) \\ &< \dot{b}_k(t) \end{aligned}$$

for *a.e.* $t \in [t_2, t_3]$. Thus $\mathbf{a}_k^{\top} \mathbf{x} - \rho - b_k$ is nonincreasing on $[t_2, t_3]$ by Lemma 1; that is

$$\mathbf{a}_k^{\top} \mathbf{x}(t_2) - \rho(t_2) - b_k(t_2) \geq \mathbf{a}_k^{\top} \mathbf{x}(t_3) - \rho(t_3) - b_k(t_3).$$

But by (5), this means $-\rho(t_2) \geq 0$, which is a contradiction. \square

3.2 Implementation

This section describes how to construct the mappings M_i such that they satisfy Assumption 2 and lead to a numerically implementable bounding method.

The next result establishes “Lipschitz continuity” of the feasible sets, solution sets, and optimal objective value of certain parametric linear optimization problems. This result is from the literature; see for instance Theorem 2.4 of [28].

Lemma 3 *Let $m, n \in \mathbb{N}$. Let $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\mathbf{b} \in \mathbb{R}^m$, and $\mathbf{c} \in \mathbb{R}^n$. Consider the linear program*

$$q(\mathbf{b}) = \sup\{\mathbf{c}^T \mathbf{z} : \mathbf{A}\mathbf{z} \leq \mathbf{b}\}.$$

Let $P(\mathbf{b}) = \{\mathbf{z} : \mathbf{A}\mathbf{z} \leq \mathbf{b}\}$ (the feasible set), $S(\mathbf{b}) = \{\mathbf{z} \in P(\mathbf{b}) : \mathbf{c}^T \mathbf{z} = q(\mathbf{b})\}$ (the solution set), $F = \{\mathbf{b} : P(\mathbf{b}) \neq \emptyset\}$, and $F_S = \{\mathbf{b} : S(\mathbf{b}) \neq \emptyset\}$. Then

1. *there exists $L > 0$ such that for all $\mathbf{b}_1, \mathbf{b}_2 \in F$, for any $\mathbf{z}_1 \in P(\mathbf{b}_1)$, there exists a $\mathbf{z}_2 \in P(\mathbf{b}_2)$ with*

$$\|\mathbf{z}_1 - \mathbf{z}_2\|_\alpha \leq L \|\mathbf{b}_1 - \mathbf{b}_2\|_\beta,$$

2. *there exists $L_S > 0$ such that for all $\mathbf{b}_1, \mathbf{b}_2 \in F_S$, for any $\mathbf{z}_1 \in S(\mathbf{b}_1)$, there exists a $\mathbf{z}_2 \in S(\mathbf{b}_2)$ with*

$$\|\mathbf{z}_1 - \mathbf{z}_2\|_\alpha \leq L_S \|\mathbf{b}_1 - \mathbf{b}_2\|_\beta,$$

3. *and $q : F_S \rightarrow \mathbb{R}$ is Lipschitz continuous,*

for any choice of norms $\|\cdot\|_\alpha, \|\cdot\|_\beta$.

It is now possible to state a specific instance of the mappings which satisfy Assumption 2. Similar to the work in [37, 39], these mappings allow one to use a priori information about the solution set of (1) in the form of a polyhedral-valued mapping $G : T \rightrightarrows \mathbb{R}^{n_x}$ for which it is known that $\mathbf{x}(t, \mathbf{u}) \in G(t)$, for all $t \in T$ and $\mathbf{u} \in \mathcal{U}$ for which a solution exists. Figure 2 illustrates the definition of the M_i mappings given in Proposition 1. A valid definition of the M_i mapping would be to let it take the value of the i^{th} face of the bounds; however, if the a priori information $G(t)$ is available, it can be used to restrict the M_i mapping to a subset of the face. Some care must be taken to define M_i sensibly when $G(t)$ does not intersect the i^{th} face, or else somehow exclude this possibility through the definition of D_M . The specific conditions are formalized in the following assumption and subsequent result. The bounding methods from [16, 17] are special cases by defining \mathbf{A} to yield interval bounds and assuming that G is constant-valued.

Assumption 3 *For $m_g \in \mathbb{N}$, let $\mathbf{A}_G \in \mathbb{R}^{m_g \times n_x}$ and $\mathbf{b}_G : T \rightarrow \mathbb{R}^{m_g}$. Assume that for all $\mathbf{u} \in \mathcal{U}$ and any solution $\mathbf{x}(\cdot, \mathbf{u})$ of IVP (1), $\mathbf{A}_G \mathbf{x}(t, \mathbf{u}) \leq \mathbf{b}_G(t)$, for all $t \in T$.*

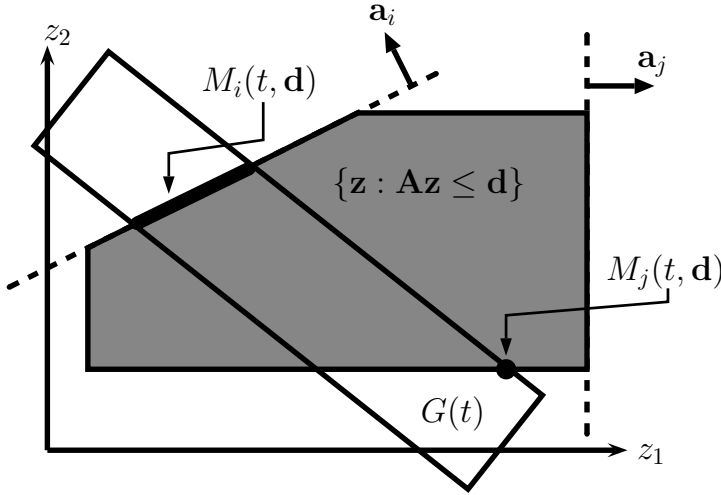


Fig. 2: Graphical representation of the definition of the M_i mappings which use the a priori information $G(t)$; see Proposition 1. Note that in this case, the j^{th} face does not intersect $G(t)$, however M_j is still well-defined.

Proposition 1 *Let Assumption 3 hold. For $m \in \mathbb{N}$, let $\mathbf{A} \in \mathbb{R}^{m \times n_x}$. Let*

$$P_M : (t, \mathbf{d}) \mapsto \{\mathbf{z} : \mathbf{A}\mathbf{z} \leq \mathbf{d}, \mathbf{A}_G\mathbf{z} \leq \mathbf{b}_G(t)\}. \quad (7)$$

Then \mathbf{A} ,

$$D_M = \{(t, \mathbf{d}) \in T \times \mathbb{R}^m : P_M(t, \mathbf{d}) \neq \emptyset\}, \text{ and} \quad (8)$$

$$M_i : (t, \mathbf{d}) \mapsto \arg \max \{\mathbf{a}_i^T \mathbf{z} : \mathbf{A}\mathbf{z} \leq \mathbf{d}, \mathbf{A}_G\mathbf{z} \leq \mathbf{b}_G(t)\}. \quad (9)$$

satisfy Assumption 2.

Proof To see that Condition 1 of Assumption 2 holds, choose any $i \in \{1, \dots, m\}$, $\mathbf{d} \in \mathbb{R}^m$, and $(t, \mathbf{u}) \in T \times \mathcal{U}$ such that $\mathbf{A}\mathbf{x}(t, \mathbf{u}) \leq \mathbf{d}$ and $\mathbf{a}_i^T \mathbf{x}(t, \mathbf{u}) = d_i$. Since $\mathbf{A}_G\mathbf{x}(t, \mathbf{u}) \leq \mathbf{b}_G(t)$, it holds that $\mathbf{x}(t, \mathbf{u}) \in P_M(t, \mathbf{d})$, and thus $(t, \mathbf{d}) \in D_M$. Further, since $\mathbf{a}_i^T \mathbf{x}(t, \mathbf{u}) = d_i$, and any \mathbf{z} such that $\mathbf{a}_i^T \mathbf{z} > d_i$ would be infeasible in LP (9), we must have $\mathbf{x}(t, \mathbf{u}) \in M_i(t, \mathbf{d})$.

Next, note that if $P_M(t, \mathbf{d})$ is nonempty, then $M_i(t, \mathbf{d})$ is nonempty for all i ($M_i(t, \mathbf{d})$ is the solution set of a linear program that must be feasible and bounded). Then to see that Condition 2 of Assumption 2 holds, choose any $(s, \mathbf{d}_1), (s, \mathbf{d}_2) \in D_M$. By definition of D_M and the previous observation, $M_i(s, \mathbf{d}_j)$ is nonempty for $i \in \{1, \dots, m\}$ and $j \in \{1, 2\}$. Applying Lemma 3, we have that there exists a $L > 0$ and for each $\mathbf{z}_1 \in M_i(s, \mathbf{d}_1)$, there exists a $\mathbf{z}_2 \in M_i(s, \mathbf{d}_2)$ such that

$$\|\mathbf{z}_1 - \mathbf{z}_2\| \leq L \|(\mathbf{d}_1, \mathbf{b}_G(s)) - (\mathbf{d}_2, \mathbf{b}_G(s))\|_1 = L \|\mathbf{d}_1 - \mathbf{d}_2\|_1.$$

□

Since there is no explicit requirement in Assumption 2 that M_i be nonempty-valued everywhere in D_M , one may be tempted to enlarge D_M and, for instance, make the definitions

$$D_M = T \times \mathbb{R}^m,$$

$$M_i : (t, \mathbf{d}) \mapsto \arg \max \{ \mathbf{a}_i^T \mathbf{z} : \mathbf{A} \mathbf{z} \leq \mathbf{d}, \mathbf{A}_G \mathbf{z} \leq \mathbf{b}_G(t) \},$$

rather than the definitions in Equations (8) and (9) above. The issue is that the Lipschitz condition (Condition 2 of Assumption 2) may be violated.

For example, consider what the definitions above mean for interval bounds; disregard the a priori information G (let G map to all of \mathbb{R}^{n_x} , for instance) and let $\mathbf{A} = [-\mathbf{I} \ \mathbf{I}]^T$ so that if $\mathbf{d} = (-\mathbf{v}, \mathbf{w})$ we have $\{\mathbf{z} : \mathbf{A} \mathbf{z} \leq \mathbf{d}\} = [\mathbf{v}, \mathbf{w}]$. For $\mathbf{d}_1 = (-\mathbf{v}_1, \mathbf{w}_1)$ with $\mathbf{v}_1 \leq \mathbf{w}_1$ and $v_{1,i} = w_{1,i}$ for some i , for all neighborhoods of \mathbf{d}_1 there exists a $\mathbf{d}_2 = (-\mathbf{v}_2, \mathbf{w}_2)$ in this neighborhood with $v_{2,i} > w_{2,i}$. It follows that (for any t) $M_i(t, \mathbf{d}_1)$ is nonempty while $M_i(t, \mathbf{d}_2)$ is empty (in fact, for all i , $M_i(t, \mathbf{d}_2)$ is empty since these are the faces of the empty interval $[\mathbf{v}_2, \mathbf{w}_2]$). It follows that Condition 2 of Assumption 2 cannot hold; there does not exist any $\mathbf{z}_2 \in M_i(t, \mathbf{d}_2)$ to satisfy the required inequality.

The following corollary establishes a useful topological property of the set D_M as well as the fact that it is non-trivial.

Corollary 1 *Let Assumption 3 hold. Assume that \mathbf{b}_G is continuous and that IVP (1) has a solution for some $\mathbf{u} \in \mathcal{U}$. Then for any choice of matrix \mathbf{A} , D_M defined in Equation (8) is nonempty and closed.*

Proof Let $P : (\mathbf{d}_1, \mathbf{d}_2) \mapsto \{\mathbf{z} : \mathbf{A} \mathbf{z} \leq \mathbf{d}_1, \mathbf{A}_G \mathbf{z} \leq \mathbf{d}_2\}$. Note that $F = \{(\mathbf{d}_1, \mathbf{d}_2) : P(\mathbf{d}_1, \mathbf{d}_2) \neq \emptyset\}$ is closed. This follows from Section 4.7 of [4]; the argument is that F is the projection of the polyhedron $\{(\mathbf{z}, \mathbf{d}_1, \mathbf{d}_2) : \mathbf{A} \mathbf{z} - \mathbf{d}_1 \leq \mathbf{0}, \mathbf{A}_G \mathbf{z} - \mathbf{d}_2 \leq \mathbf{0}\}$ and thus a polyhedron as well, and so closed.

We note that $P(\mathbf{d}, \mathbf{b}_G(t))$ is exactly $P_M(t, \mathbf{d})$ defined in Eqn. (7), and so D_M is the set of (t, \mathbf{d}) such that $(\mathbf{d}, \mathbf{b}_G(t)) \in F$. Since IVP (1) has a solution for $\mathbf{u} \in \mathcal{U}$, there exists $\mathbf{x}(\cdot, \mathbf{u})$ such that for each $t \in T$, $\mathbf{x}(t, \mathbf{u})$ is in $P(\mathbf{d}, \mathbf{b}_G(t))$, where $\mathbf{d} = \mathbf{A} \mathbf{x}(t, \mathbf{u})$. Therefore F and D_M are nonempty. Finally, note that the mapping $(t, \mathbf{d}) \mapsto (\mathbf{d}, \mathbf{b}_G(t))$ is continuous from $T \times \mathbb{R}^m$ to \mathbb{R}^{m+m_g} . Thus, the preimage of F under this mapping must be closed relative to $T \times \mathbb{R}^m$, and it is clear that this preimage must be D_M . And since $T \times \mathbb{R}^m$ is closed, a set which is closed relative to it must be closed relative to $\mathbb{R} \times \mathbb{R}^m$. \square

There are other possible choices for the definitions of D_M and the mappings M_i . For instance, the procedure for “tightening” an interval based on a set of linear constraints, given in Definition 4 of [39], provides a potential alternative. However, if this procedure is used, M_i would be interval-valued. In general, this interval would not be degenerate, and this loosely means that the dynamics must be overestimated on a much larger set, leading to more conservative bounds. In contrast, M_i in Proposition 1 takes the value of the face of a polyhedron (and thus is also polyhedral-valued), and therefore it is always a set in an affine subspace with a lower dimension. Thus, the dynamics are overestimated on a smaller set, leading to tighter bounds.

Further, in applications, the set of possible input values U is typically at least polyhedral (and more often an interval). Consequently, one notes that in practice, Hypothesis 4 of Theorem 1 requires that a linear combination of the dynamics is overestimated on a polyhedron. This observation shapes the following result, which combines Theorem 1 and Proposition 1 to obtain a system of differential equations; the solution of this system is \mathbf{b} , the right-hand sides of the polyhedral-valued bounds $B : t \mapsto \{\mathbf{z} : \mathbf{A}\mathbf{z} \leq \mathbf{b}(t)\}$. However, as noted, Hypothesis 4 requires that the dynamics of this system of differential equations overestimate potentially nonlinear optimization problems. Consequently, what is proposed in the following corollary is to solve parametric linear programming relaxations of these problems instead, which overall leads to a much more efficiently solved system. This forms the basis of the numerical method of the next section. Comparing with previous work, one could also use interval arithmetic to try to satisfy Hypothesis 4, similar to [38,39], however interval arithmetic in general would not be able to take advantage of the fact that the M_i mappings have values that are subsets of an affine subspace.

Corollary 2 *Let Assumptions 1 and 3 hold. For $m \in \mathbb{N}$ and $\mathbf{A} \in \mathbb{R}^{m \times n_x}$ define D_M and M_i , $i \in \{1, \dots, m\}$ as in Equations (8) and (9). For $i \in \{1, \dots, m\}$, let the mappings $\mathbf{c}_i \equiv (\mathbf{c}_i^u, \mathbf{c}_i^x) : D_M \rightarrow \mathbb{R}^{n_u} \times \mathbb{R}^{n_x}$ and $h_i : D_M \rightarrow \mathbb{R}$ be given. Assume the following:*

1. For some $m_u \in \mathbb{N}$, there exist $\mathbf{A}_U \in \mathbb{R}^{m_u \times n_u}$ and $\mathbf{b}_U \in \mathbb{R}^{m_u}$ such that $U = \{\mathbf{p} : \mathbf{A}_U \mathbf{p} \leq \mathbf{b}_U\}$ and is nonempty and compact.
2. For $i \in \{1, \dots, m\}$ and all $(t, \mathbf{d}) \in D_M$, $M_i(t, \mathbf{d})$ is compact and a subset of D_x .
3. For $i \in \{1, \dots, m\}$, for each $(t, \mathbf{d}) \in D_M$,

$$\mathbf{a}_i^T \mathbf{f}(t, \mathbf{p}, \mathbf{z}) \leq (\mathbf{c}_i^u(t, \mathbf{d}))^T \mathbf{p} + (\mathbf{c}_i^x(t, \mathbf{d}))^T \mathbf{z} + h_i(t, \mathbf{d}), \quad \forall (\mathbf{p}, \mathbf{z}) \in U \times M_i(t, \mathbf{d}).$$

4. The mapping $\mathbf{q} : D_M \rightarrow \mathbb{R}^m$ is defined componentwise by

$$q_i(t, \mathbf{d}) = \max_{(\mathbf{p}, \mathbf{z})} (\mathbf{c}_i^u(t, \mathbf{d}))^T \mathbf{p} + (\mathbf{c}_i^x(t, \mathbf{d}))^T \mathbf{z} + h_i(t, \mathbf{d}) \quad (10)$$

$$\text{s.t. } \begin{bmatrix} \mathbf{A}_U & \mathbf{0} \\ \mathbf{0} & \mathbf{A} \\ \mathbf{0} & \mathbf{A}_G \end{bmatrix} \begin{bmatrix} \mathbf{p} \\ \mathbf{z} \end{bmatrix} \leq \begin{bmatrix} \mathbf{b}_U \\ \mathbf{d} \\ \mathbf{b}_G(t) \end{bmatrix},$$

$$\mathbf{a}_i^T \mathbf{z} = \max\{\mathbf{a}_i^T \mathbf{y} : \mathbf{A}\mathbf{y} \leq \mathbf{d}, \mathbf{A}_G \mathbf{y} \leq \mathbf{b}_G(t)\}.$$

5. The mapping $\mathbf{b} : T \rightarrow \mathbb{R}^m$ is any solution of the initial value problem in ordinary differential equations

$$\dot{\mathbf{b}}(t) = \mathbf{q}(t, \mathbf{b}(t)), \quad \text{a.e. } t \in T, \quad (11)$$

with initial conditions that satisfy $X_0 \subset \{\mathbf{z} : \mathbf{A}\mathbf{z} \leq \mathbf{b}(t_0)\}$.

Then for all $\mathbf{u} \in U$ and any solution $\mathbf{x}(\cdot, \mathbf{u})$ of IVP (1), $\mathbf{A}\mathbf{x}(t, \mathbf{u}) \leq \mathbf{b}(t)$, for all $t \in T$.

Proof First, it is clear that the feasible set of the linear program (10) which defines $q_i(t, \mathbf{d})$ is the nonempty compact set $U \times M_i(t, \mathbf{d})$. It follows that $q_i(t, \mathbf{d})$ is well defined for each $(t, \mathbf{d}) \in D_M$. Next, by assumption, Assumption 1 is satisfied. Further, if D_M and M_i are defined as in Equations (8) and (9), then by Proposition 1, Assumption 2 is satisfied. Let \mathbf{b} be any solution of the IVP (11). Then it is clear that \mathbf{b} must be absolutely continuous. Let $B : t \mapsto \{\mathbf{z} : \mathbf{A}\mathbf{z} \leq \mathbf{b}(t)\}$. Then by the assumption on the initial conditions of \mathbf{b} , $X_0 \subset B(t_0)$. Thus, the first two hypotheses of Theorem 1 are satisfied. Further, if \mathbf{b} is a solution of IVP (11), then $(t, \mathbf{b}(t)) \in D_M$ for almost every $t \in T$, since otherwise \mathbf{q} would not be defined and Equation (11) could not be satisfied almost every $t \in T$. Consequently, by Hypothesis 2, Hypothesis 3 of Theorem 1 is satisfied. Finally, by assumption on \mathbf{c}_i and h_i and construction of the linear programming relaxation \mathbf{q} , for all $(t, \mathbf{d}) \in D_M$

$$q_i(t, \mathbf{d}) \geq \sup\{\mathbf{a}_i^T \mathbf{f}(t, \mathbf{p}, \mathbf{z}) : (\mathbf{p}, \mathbf{z}) \in U \times M_i(t, \mathbf{d})\}.$$

Therefore, \mathbf{b} must satisfy $\dot{b}_i(t) \geq \mathbf{a}_i^T \mathbf{f}(t, \mathbf{p}, \mathbf{z})$, for all $(\mathbf{p}, \mathbf{z}) \in U \times M_i(t, \mathbf{b}(t))$, for each $i \in \{1, \dots, m\}$ and almost every t . Thus, all the assumptions and hypotheses of Theorem 1 are satisfied and so B must bound all solutions of IVP (1). \square

4 Numerical Implementation

The goals of this section are to state an algorithm to compute \mathbf{q} defining IVP (11), and in specific, a method to compute the affine relaxations (\mathbf{c}_i, h_i) required in Hypothesis 3 of Corollary 2. Furthermore, it is established that, with these definitions, \mathbf{q} satisfies an appropriate Lipschitz continuity condition to ensure that IVP (11) is amenable to numerical solution.

4.1 Computing affine relaxations and the dynamics

To implement a bounding method based on Corollary 2, specific affine relaxations are needed. Affine relaxations (of certain classes of functions) on intervals can be obtained in a number of ways; subgradients to convex and concave relaxations [32] and first-order Taylor models [27] are two possibilities. However, in the next subsection, some specific parameterization properties of these relaxations are required. To simplify the discussion, the following assumption is made. Appendix A considers a way to construct affine relaxations on intervals which satisfy Assumption 4. With this assumption, one only needs to calculate an interval enclosure of $M_i(t, \mathbf{d})$ to establish Hypothesis 3 of Corollary 2.

Assumption 4 Let $D_x^{\mathbb{I}} = \{(\mathbf{v}, \mathbf{w}) \in \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} : \mathbf{v} \leq \mathbf{w}, [\mathbf{v}, \mathbf{w}] \subset D_x\}$. Assume that for each $i \in \{1, \dots, m\}$, there exist continuous $\tilde{\mathbf{c}}_i \equiv (\tilde{\mathbf{c}}_i^u, \tilde{\mathbf{c}}_i^x) : T \times D_x^{\mathbb{I}} \rightarrow \mathbb{R}^{n_u} \times \mathbb{R}^{n_x}$ and continuous $\tilde{h}_i : T \times D_x^{\mathbb{I}} \rightarrow \mathbb{R}$ such that for each $(\mathbf{v}, \mathbf{w}) \in D_x^{\mathbb{I}}$ and $t \in T$,

$$\mathbf{a}_i^T \mathbf{f}(t, \mathbf{p}, \mathbf{z}) \leq (\tilde{\mathbf{c}}_i^u(t, \mathbf{v}, \mathbf{w}))^T \mathbf{p} + (\tilde{\mathbf{c}}_i^x(t, \mathbf{v}, \mathbf{w}))^T \mathbf{z} + \tilde{h}_i(t, \mathbf{v}, \mathbf{w}),$$

for all $(\mathbf{p}, \mathbf{z}) \in U \times [\mathbf{v}, \mathbf{w}]$. Further, for all $(\mathbf{v}, \mathbf{w}) \in D_x^{\mathbb{I}}$, there exists a neighborhood $N^i(\mathbf{v}, \mathbf{w})$ and $\tilde{L}_i > 0$ such that for all $(t, \mathbf{v}_1, \mathbf{w}_1), (t, \mathbf{v}_2, \mathbf{w}_2) \in T \times N^i(\mathbf{v}, \mathbf{w}) \cap D_x^{\mathbb{I}}$

$$\begin{aligned} \|\tilde{\mathbf{c}}_i(t, \mathbf{v}_1, \mathbf{w}_1) - \tilde{\mathbf{c}}_i(t, \mathbf{v}_2, \mathbf{w}_2)\| &\leq \tilde{L}_i \|(\mathbf{v}_1, \mathbf{w}_1) - (\mathbf{v}_2, \mathbf{w}_2)\|, \\ \left| \tilde{h}_i(t, \mathbf{v}_1, \mathbf{w}_1) - \tilde{h}_i(t, \mathbf{v}_2, \mathbf{w}_2) \right| &\leq \tilde{L}_i \|(\mathbf{v}_1, \mathbf{w}_1) - (\mathbf{v}_2, \mathbf{w}_2)\|. \end{aligned}$$

At this point, a specific algorithm for computing \mathbf{q} defining the dynamics in IVP (11) can be stated. See Algorithm 1. In Step 1 of Algorithm 1, an interval enclosure of $M_i(t, \mathbf{d})$ is given by $[\mathbf{v}^i(t, \mathbf{d}), \mathbf{w}^i(t, \mathbf{d})]$. This step uses the procedure for “tightening” an interval, given a set of linear constraints, from Definition 4 in [39]. The essential operation is repeated in Algorithm 2; this algorithm defines the operation I_t , which tightens an interval $[\mathbf{v}, \mathbf{w}]$ by excluding points which cannot satisfy a given linear constraint $\mathbf{m}^T \mathbf{z} \leq d$. Specifically, the discussion in Section 5.2 of [39] establishes that the tightened interval $I_t(\mathbf{v}, \mathbf{w}, d; \mathbf{m})$ satisfies $[\mathbf{v}, \mathbf{w}] \supset I_t(\mathbf{v}, \mathbf{w}, d; \mathbf{m}) \supset \{\mathbf{z} \in [\mathbf{v}, \mathbf{w}] : \mathbf{m}^T \mathbf{z} \leq d\}$.

Thus, Algorithm 1 recursively applies the tightening operation I_t to some interval enclosure of the overall polyhedron $\{\mathbf{z} : \mathbf{A}\mathbf{z} \leq \mathbf{d}, \mathbf{A}_G \mathbf{z} \leq \mathbf{b}_G(t)\}$. In the algorithm, this initial enclosure is taken as the interval hull. However, this means that none of the constraints defining the overall polyhedron will result in a reduction of the size of the interval when applying the tightening operation. Thus, what should be noted is that the first inequality used in tightening is the one unique to the definition of $M_i(t, \mathbf{d})$: $-\mathbf{a}_i^T \mathbf{z} \leq -b_i^*(t, \mathbf{d})$. Intuitively, using this constraint first results in the most significant reduction in the size of the interval.

4.2 Lipschitz continuity of the dynamics

This section establishes a kind of Lipschitz continuity condition on \mathbf{q} defined in Algorithm 1. Theoretically, this condition ensures that if a solution exists, then it must be unique; see Theorem 1.10 of Chapter II of [29] or Theorem 2 in Section 1 of [10]. Further, a similar condition establishes that many numerical integration methods, including Runge-Kutta and linear multistep methods, are convergent for problem (11); see, for instance, Theorem 1.1 of Section 1.4 of [23], and Definition 1.6 of Section II.1 and the convergence analyses in Section III.3 and Section VII.4 of [29]. It should be noted that the domain of \mathbf{q} defined in Algorithm 1 is D_M . Unfortunately, this is not necessarily an open set, which can often cause numerical issues [15]. However, in the experience of the authors, the Lipschitz condition on \mathbf{q} is sufficient for the successful solution of IVP (11) with most numerical integration methods.

The following result helps establish this Lipschitz continuity condition. It appears in various forms in the literature; see for instance Theorem 14 in [46] and Proposition 3 in [16].

Algorithm 1 Calculation of dynamics \mathbf{q} of bounding IVP (11)**Require:** $(t, \mathbf{d}) \in D_M$ Calculate $\mathbf{b}^*(t, \mathbf{d})$ by $b_i^*(t, \mathbf{d}) = \max\{\mathbf{a}_i^T \mathbf{z} : \mathbf{A}\mathbf{z} \leq \mathbf{d}, \mathbf{A}_G \mathbf{z} \leq \mathbf{b}_G(t)\}$.Calculate $[\mathbf{v}^*(t, \mathbf{d}), \mathbf{w}^*(t, \mathbf{d})]$ by

$$v_j^*(t, \mathbf{d}) = \min\{z_j : \mathbf{A}\mathbf{z} \leq \mathbf{d}, \mathbf{A}_G \mathbf{z} \leq \mathbf{b}_G(t)\},$$

$$w_j^*(t, \mathbf{d}) = \max\{z_j : \mathbf{A}\mathbf{z} \leq \mathbf{d}, \mathbf{A}_G \mathbf{z} \leq \mathbf{b}_G(t)\}.$$

for $i \in \{1, \dots, m\}$ **do**1. Calculate $[\mathbf{v}^i(t, \mathbf{d}), \mathbf{w}^i(t, \mathbf{d})]$ by the following:

- (a) Set $[\widehat{\mathbf{v}}, \widehat{\mathbf{w}}] = [\mathbf{v}^*(t, \mathbf{d}), \mathbf{w}^*(t, \mathbf{d})]$.
- (b) Set $[\widehat{\mathbf{v}}, \widehat{\mathbf{w}}] = I_t(\widehat{\mathbf{v}}, \widehat{\mathbf{w}}, -b_i^*(t, \mathbf{d}); -\mathbf{a}_i)$.
- (c) For $k \in \{1, \dots, m\}$, set $[\widehat{\mathbf{v}}, \widehat{\mathbf{w}}] = I_t(\widehat{\mathbf{v}}, \widehat{\mathbf{w}}, b_k^*(t, \mathbf{d}); \mathbf{a}_k)$.
- (d) For $k \in \{1, \dots, m_g\}$, set $[\widehat{\mathbf{v}}, \widehat{\mathbf{w}}] = I_t(\widehat{\mathbf{v}}, \widehat{\mathbf{w}}, b_{G,k}(t); \mathbf{a}_{G,k})$.
- (e) Set $[\mathbf{v}^i(t, \mathbf{d}), \mathbf{w}^i(t, \mathbf{d})] = [\widehat{\mathbf{v}}, \widehat{\mathbf{w}}]$.

2. Calculate $\mathbf{c}_i^u(t, \mathbf{d}) = \widetilde{\mathbf{c}}_i^u(t, \mathbf{v}^i(t, \mathbf{d}), \mathbf{w}^i(t, \mathbf{d}))$, $\mathbf{c}_i^x(t, \mathbf{d}) = \widetilde{\mathbf{c}}_i^x(t, \mathbf{v}^i(t, \mathbf{d}), \mathbf{w}^i(t, \mathbf{d}))$, and $h_i(t, \mathbf{d}) = \widetilde{h}_i(t, \mathbf{v}^i(t, \mathbf{d}), \mathbf{w}^i(t, \mathbf{d}))$ (See Assumption 4 and Appendix A).

3. Calculate

$$q_i(t, \mathbf{d}) = \max_{(\mathbf{p}, \mathbf{z})} (\mathbf{c}_i^u(t, \mathbf{d}))^T \mathbf{p} + (\mathbf{c}_i^x(t, \mathbf{d}))^T \mathbf{z} + h_i(t, \mathbf{d})$$

$$\text{s.t. } \begin{bmatrix} \mathbf{A}_U & \mathbf{0} \\ \mathbf{0} & \mathbf{A} \\ \mathbf{0} & \mathbf{A}_G \end{bmatrix} \begin{bmatrix} \mathbf{p} \\ \mathbf{z} \end{bmatrix} \leq \begin{bmatrix} \mathbf{b}_U \\ \mathbf{d} \\ \mathbf{b}_G(t) \end{bmatrix},$$

$$\mathbf{a}_i^T \mathbf{z} = b_i^*(t, \mathbf{d}).$$

end for**return** $\mathbf{q}(t, \mathbf{d})$ **Algorithm 2** Definition of the interval-tightening operator I_t **Require:** $\mathbf{m} \in \mathbb{R}^{n_x}$, $d \in \mathbb{R}$, $(\mathbf{v}, \mathbf{w}) \in \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$, $\mathbf{v} \leq \mathbf{w}$ $(\widehat{\mathbf{v}}, \widehat{\mathbf{w}}) \leftarrow (\mathbf{v}, \mathbf{w})$ **for** $j \in \{1, \dots, n_x\}$ **do****if** $m_j \neq 0$ **then**

$$\gamma \leftarrow \text{median} \left\{ \widehat{v}_j, \widehat{w}_j, 1/m_j (d + \sum_{k \neq j} \max\{-m_k \widehat{v}_k, -m_k \widehat{w}_k\}) \right\}$$

if $m_j > 0$ **then**

$$\widehat{w}_j \leftarrow \gamma$$

end if**if** $m_j < 0$ **then**

$$\widehat{v}_j \leftarrow \gamma$$

end if**end if****end for****return** $I_t(\mathbf{v}, \mathbf{w}, d; \mathbf{m}) \leftarrow [\widehat{\mathbf{v}}, \widehat{\mathbf{w}}]$

Lemma 4 Given $m, n \in \mathbb{N}$ and a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$, let the polyhedron $P(\mathbf{d}) = \{\mathbf{z} : \mathbf{A}\mathbf{z} \leq \mathbf{d}\}$ for $\mathbf{d} \in \mathbb{R}^m$. Let $F = \{\mathbf{d} : P(\mathbf{d}) \neq \emptyset\}$. Assume $P(\mathbf{d})$ is bounded (i.e. compact) for all $\mathbf{d} \in F$. Then $\hat{q} : \mathbb{R}^n \times F \rightarrow \mathbb{R}$ defined by

$$\hat{q}(\mathbf{c}, \mathbf{d}) = \max\{\mathbf{c}^T \mathbf{z} : \mathbf{A}\mathbf{z} \leq \mathbf{d}\}$$

is locally Lipschitz continuous.

The following lemma helps establish that the affine relaxations (\mathbf{c}_i, h_i) defined in Algorithm 1 have the appropriate continuity properties required in Theorem 2 below.

Lemma 5 Let Assumptions 3 and 4 hold. For $m \in \mathbb{N}$ and $\mathbf{A} \in \mathbb{R}^{m \times n_x}$ define D_M as in Equation (8). Assume the following:

1. \mathbf{b}_G is continuous on T .
2. For $i \in \{1, \dots, m\}$ and all $(t, \mathbf{d}) \in D_M$, $\mathbf{v}^i, \mathbf{w}^i : D_M \rightarrow \mathbb{R}^{n_x}$ defined by Step 1 in Algorithm 1 satisfy $[\mathbf{v}^i(t, \mathbf{d}), \mathbf{w}^i(t, \mathbf{d})] \subset D_x$.
3. For $i \in \{1, \dots, m\}$, define $\mathbf{c}_i = (\mathbf{c}_i^u, \mathbf{c}_i^x) : D_M \rightarrow \mathbb{R}^{n_u} \times \mathbb{R}^{n_x}$ and $h_i : D_M \rightarrow \mathbb{R}$ by Step 2 in Algorithm 1; i.e.

$$\begin{aligned} \mathbf{c}_i^u(t, \mathbf{d}) &= \tilde{\mathbf{c}}_i^u(t, \mathbf{v}^i(t, \mathbf{d}), \mathbf{w}^i(t, \mathbf{d})), & \mathbf{c}_i^x(t, \mathbf{d}) &= \tilde{\mathbf{c}}_i^x(t, \mathbf{v}^i(t, \mathbf{d}), \mathbf{w}^i(t, \mathbf{d})), \\ h_i(t, \mathbf{d}) &= \tilde{h}_i(t, \mathbf{v}^i(t, \mathbf{d}), \mathbf{w}^i(t, \mathbf{d})). \end{aligned}$$

Then for $i \in \{1, \dots, m\}$, \mathbf{c}_i and h_i are continuous, and for all $(t, \mathbf{d}) \in D_M$, there exists a neighborhood $N^i(\mathbf{d})$ of \mathbf{d} and $L_i > 0$ such that for all $(t', \mathbf{d}_1), (t', \mathbf{d}_2) \in (T \times N^i(\mathbf{d})) \cap D_M$

$$\begin{aligned} \|\mathbf{c}_i(t', \mathbf{d}_1) - \mathbf{c}_i(t', \mathbf{d}_2)\| &\leq L_i \|\mathbf{d}_1 - \mathbf{d}_2\|, \\ |h_i(t', \mathbf{d}_1) - h_i(t', \mathbf{d}_2)| &\leq L_i \|\mathbf{d}_1 - \mathbf{d}_2\|. \end{aligned}$$

Proof By Lemma 3 and the fact that \mathbf{b}_G is continuous, \mathbf{v}^* , \mathbf{w}^* , and \mathbf{b}^* defined in Algorithm 1 are continuous, and that there exists a $L > 0$ such that for any $(t, \mathbf{d}_1), (t, \mathbf{d}_2) \in D_M$

$$\|\mathbf{v}^*(t, \mathbf{d}_1) - \mathbf{v}^*(t, \mathbf{d}_2)\| \leq L \|\mathbf{d}_1 - \mathbf{d}_2\|,$$

and similarly for \mathbf{w}^* and \mathbf{b}^* . Next, it should be clear that the I_t operation defined in Algorithm 2 is a well-defined Lipschitz continuous mapping on $D_{it} = \{(\mathbf{v}, \mathbf{w}, d) \in \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \times \mathbb{R} : \mathbf{v} \leq \mathbf{w}\}$ (that is, the endpoints of the interval defining I_t are Lipschitz continuous with respect to its first three arguments). Consequently, an inductive argument shows that \mathbf{v}^i and \mathbf{w}^i are continuous and must satisfy

$$\|\mathbf{v}^i(t, \mathbf{d}_1) - \mathbf{v}^i(t, \mathbf{d}_2)\|_1 \leq L_{v,i} \|\mathbf{d}_1 - \mathbf{d}_2\|, \quad (12)$$

$$\|\mathbf{w}^i(t, \mathbf{d}_1) - \mathbf{w}^i(t, \mathbf{d}_2)\|_1 \leq L_{w,i} \|\mathbf{d}_1 - \mathbf{d}_2\|. \quad (13)$$

for some $L_{v,i} > 0$ and all $(t, \mathbf{d}_1), (t, \mathbf{d}_2) \in D_M$.

Choose $(t, \mathbf{d}) \in D_M$. By Hypothesis 2, $(\mathbf{v}^i(t, \mathbf{d}), \mathbf{w}^i(t, \mathbf{d})) \in D_x^{\mathbb{I}}$ (as defined in Assumption 4). Let $N^i(\mathbf{v}^i(t, \mathbf{d}), \mathbf{w}^i(t, \mathbf{d}))$ be the open neighborhood

of $(\mathbf{v}^i(t, \mathbf{d}), \mathbf{w}^i(t, \mathbf{d}))$ assumed to exist by Assumption 4. Assume without loss of generality that $N^i(\mathbf{v}^i(t, \mathbf{d}), \mathbf{w}^i(t, \mathbf{d})) = N_\delta(\mathbf{v}^i(t, \mathbf{d})) \times N_\delta(\mathbf{w}^i(t, \mathbf{d}))$. By Inequalities (12) and (13), if $(t, \mathbf{d}') \in D_M$ satisfies that $\|\mathbf{d} - \mathbf{d}'\| < \delta/L_{v,i} = \varepsilon_i$, it follows that $(\mathbf{v}^i(t, \mathbf{d}'), \mathbf{w}^i(t, \mathbf{d}')) \in N^i(\mathbf{v}^i(t, \mathbf{d}), \mathbf{w}^i(t, \mathbf{d}))$. Consequently, for any $(t, \mathbf{d}_1), (t, \mathbf{d}_2) \in (T \times N_{\varepsilon_i}(\mathbf{d})) \cap D_M$,

$$\begin{aligned} & \|\tilde{\mathbf{c}}_i(t, \mathbf{v}^i(t, \mathbf{d}_1), \mathbf{w}^i(t, \mathbf{d}_1)) - \tilde{\mathbf{c}}_i(t, \mathbf{v}^i(t, \mathbf{d}_2), \mathbf{w}^i(t, \mathbf{d}_2))\| \\ & \leq \tilde{L}_i \|(\mathbf{v}^i(t, \mathbf{d}_1), \mathbf{w}^i(t, \mathbf{d}_1)) - (\mathbf{v}^i(t, \mathbf{d}_2), \mathbf{w}^i(t, \mathbf{d}_2))\|_1 \\ & \leq \tilde{L}_i (L_{v,i} \|\mathbf{d}_1 - \mathbf{d}_2\| + L_{w,i} \|\mathbf{d}_1 - \mathbf{d}_2\|) \\ & = 2\tilde{L}_i L_{v,i} \|\mathbf{d}_1 - \mathbf{d}_2\|. \end{aligned}$$

This establishes that \mathbf{c}_i is continuous and satisfies the Lipschitz condition. A similar argument establishes that h_i is continuous and satisfies this condition as well. \square

Theorem 2 below shows that \mathbf{q} defined in Algorithm 1 satisfies the desired Lipschitz continuity assumption of many numerical integration methods, and thus that IVP (11) is amenable to numerical solution.

Theorem 2 *Let Assumptions 3 and 4 hold. For $m \in \mathbb{N}$ and $\mathbf{A} \in \mathbb{R}^{m \times n_x}$ define D_M as in Equation (8). In addition, assume the following.*

1. *For some $m_u \in \mathbb{N}$, there exist $\mathbf{A}_U \in \mathbb{R}^{m_u \times n_u}$ and $\mathbf{b}_U \in \mathbb{R}^{m_u}$ such that $U = \{\mathbf{p} : \mathbf{A}_U \mathbf{p} \leq \mathbf{b}_U\}$ and is nonempty and compact.*
2. *\mathbf{b}_G is continuous on T .*
3. *IVP (1) has a solution for some $\mathbf{u} \in U$.*
4. *For $i \in \{1, \dots, m\}$ and all $(t, \mathbf{d}) \in D_M$, $\mathbf{v}^i, \mathbf{w}^i : D_M \rightarrow \mathbb{R}^{n_x}$ defined by Step 1 in Algorithm 1 satisfy $[\mathbf{v}^i(t, \mathbf{d}), \mathbf{w}^i(t, \mathbf{d})] \subset D_x$.*

Then the mapping \mathbf{q} defined in Algorithm 1 is continuous, and for all $(t, \mathbf{d}) \in D_M$, there exists a neighborhood $N^q(\mathbf{d})$ of \mathbf{d} and $L_q > 0$ such that for all $(t', \mathbf{d}_1), (t', \mathbf{d}_2) \in (T \times N^q(\mathbf{d})) \cap D_M$

$$\|\mathbf{q}(t', \mathbf{d}_1) - \mathbf{q}(t', \mathbf{d}_2)\| \leq L_q \|\mathbf{d}_1 - \mathbf{d}_2\|.$$

Proof For $i \in \{1, \dots, m\}$, define $b_i^* : D_M \rightarrow \mathbb{R}$ by $b_i^*(t, \mathbf{d}) = \max\{\mathbf{a}_i^T \mathbf{y} : \mathbf{A} \mathbf{y} \leq \mathbf{d}, \mathbf{A}_G \mathbf{y} \leq \mathbf{b}_G(t)\}$. It is clear that b_i^* is well defined (i.e. the maximum is indeed attained for any $(t, \mathbf{d}) \in D_M$). Furthermore, since \mathbf{b}_G is continuous and by Lemma 3 the optimal objective value of an LP is continuous with respect to the right-hand side of its constraints, b_i^* is continuous. Applying Lemma 3 again, we have that there exists a $L_i^* > 0$ such that

$$\begin{aligned} |b_i^*(t_1, \mathbf{d}_1) - b_i^*(t_2, \mathbf{d}_2)| & \leq L_i^* \|(\mathbf{d}_1, \mathbf{b}_G(t_1)) - (\mathbf{d}_2, \mathbf{b}_G(t_2))\|_1 \\ & = L_i^* \|\mathbf{d}_1 - \mathbf{d}_2\|_1 + L_i^* \|\mathbf{b}_G(t_1) - \mathbf{b}_G(t_2)\|_1 \end{aligned}$$

for all $(t_1, \mathbf{d}_1), (t_2, \mathbf{d}_2) \in D_M$. Let $\hat{m} = m_u + m + m_g + 2$. Let $\hat{\mathbf{b}}_i : D_M \rightarrow \mathbb{R}^{\hat{m}}$ be given by $\hat{\mathbf{b}}_i(t, \mathbf{d}) = (\mathbf{b}_U, \mathbf{d}, \mathbf{b}_G(t), b_i^*(t, \mathbf{d}), -b_i^*(t, \mathbf{d}))$. Again, $\hat{\mathbf{b}}_i$ is the

composition of continuous functions and so is continuous. We also have

$$\begin{aligned} & \left\| \widehat{\mathbf{b}}_i(t_1, \mathbf{d}_1) - \widehat{\mathbf{b}}_i(t_2, \mathbf{d}_2) \right\|_1 \\ &= \|\mathbf{d}_1 - \mathbf{d}_2\|_1 + \|\mathbf{b}_G(t_1) - \mathbf{b}_G(t_2)\|_1 + 2|b_i^*(t_1, \mathbf{d}_1) - b_i^*(t_2, \mathbf{d}_2)| \\ &\leq (2L_i^* + 1)(\|\mathbf{d}_1 - \mathbf{d}_2\|_1 + \|\mathbf{b}_G(t_1) - \mathbf{b}_G(t_2)\|_1) \end{aligned}$$

for all $(t_1, \mathbf{d}_1), (t_2, \mathbf{d}_2) \in D_M$. From this inequality, there exists a $\widehat{L}_i > 0$ such that

$$\left\| \widehat{\mathbf{b}}_i(t, \mathbf{d}_1) - \widehat{\mathbf{b}}_i(t, \mathbf{d}_2) \right\|_1 \leq \widehat{L}_i \|\mathbf{d}_1 - \mathbf{d}_2\|_1$$

for all $(t, \mathbf{d}_1), (t, \mathbf{d}_2) \in D_M$. Further, since \mathbf{b}_G is continuous on compact T it is also bounded, and for any $(t, \mathbf{d}) \in D_M$ and (bounded) neighborhood $N(\mathbf{d})$ of \mathbf{d} , there exists a finite $k \geq 0$ such that

$$\left\| \widehat{\mathbf{b}}_i(t_1, \mathbf{d}_1) - \widehat{\mathbf{b}}_i(t_2, \mathbf{d}_2) \right\| \leq k$$

for all $(t_1, \mathbf{d}_1), (t_2, \mathbf{d}_2) \in (T \times N(\mathbf{d})) \cap D_M$, which is to say that the image of $(T \times N(\mathbf{d})) \cap D_M$ under $\widehat{\mathbf{b}}_i$ is bounded.

For $i \in \{1, \dots, m\}$, define $\mathbf{c}_i = (\mathbf{c}_i^u, \mathbf{c}_i^x) : D_M \rightarrow \mathbb{R}^{n_u} \times \mathbb{R}^{n_x}$ and $h_i : D_M \rightarrow \mathbb{R}$ as in Step 2 in Algorithm 1 (the same definition in Lemma 5). Then by Lemma 5 each \mathbf{c}_i (and h_i) are continuous, and so a similar boundedness condition holds for each \mathbf{c}_i : For any $(t, \mathbf{d}) \in D_M$ and bounded neighborhood $N(\mathbf{d})$ of \mathbf{d} , denote the closure of $N(\mathbf{d})$ by $\overline{N(\mathbf{d})}$. Then $T \times \overline{N(\mathbf{d})}$ is compact. By Corollary 1, D_M is nonempty and closed, so $(T \times \overline{N(\mathbf{d})}) \cap D_M$ is compact, and so its image under \mathbf{c}_i is compact and thus bounded.

Let

$$\widehat{\mathbf{A}}_i = \begin{bmatrix} \mathbf{A}_U & \mathbf{0} \\ \mathbf{0} & \mathbf{A} \\ \mathbf{0} & \mathbf{A}_G \\ \mathbf{0} & \mathbf{a}_i^T \\ \mathbf{0} & -\mathbf{a}_i^T \end{bmatrix}.$$

For $\mathbf{d} \in \mathbb{R}^{\widehat{m}}$, let $P_i(\mathbf{d}) = \{\mathbf{y} : \widehat{\mathbf{A}}_i \mathbf{y} \leq \mathbf{d}\}$. Let $F_i = \{\mathbf{d} : P_i(\mathbf{d}) \neq \emptyset\}$. F_i is a closed set, by a similar argument as in Corollary 1. Let $\widehat{q}_i : \mathbb{R}^{n_u+n_x} \times F_i \rightarrow \mathbb{R}$ be given by $\widehat{q}_i(\mathbf{c}, \mathbf{d}) = \max\{\mathbf{c}^T \mathbf{y} : \widehat{\mathbf{A}}_i \mathbf{y} \leq \mathbf{d}\}$. We note that

$$P_i(\widehat{\mathbf{b}}_i(t, \mathbf{d})) = U \times \arg \max\{\mathbf{a}_i^T \mathbf{z} : \mathbf{A} \mathbf{z} \leq \mathbf{d}, \mathbf{A}_G \mathbf{z} \leq \mathbf{b}_G(t)\}.$$

By the definition of D_M and Hypothesis 1, $P_i(\widehat{\mathbf{b}}_i(t, \mathbf{d}))$ is nonempty for each $(t, \mathbf{d}) \in D_M$. By Hypothesis 4 and the discussion in Section 4.1,

$$[\mathbf{v}^i(t, \mathbf{d}), \mathbf{w}^i(t, \mathbf{d})] \supset \arg \max\{\mathbf{a}_i^T \mathbf{z} : \mathbf{A} \mathbf{z} \leq \mathbf{d}, \mathbf{A}_G \mathbf{z} \leq \mathbf{b}_G(t)\}$$

and so along with Hypothesis 1, $P_i(\widehat{\mathbf{b}}_i(t, \mathbf{d}))$ is also compact for each $(t, \mathbf{d}) \in D_M$. This also establishes that $\widehat{\mathbf{b}}_i(t, \mathbf{d}) \in F_i$ for each $(t, \mathbf{d}) \in D_M$. Applying

Lemma 3, we note that there exists a $L > 0$ such that for all $\mathbf{d}_1, \mathbf{d}_2 \in F_i$, for each $\mathbf{y}_1 \in P_i(\mathbf{d}_1)$, there exists a $\mathbf{y}_2 \in P_i(\mathbf{d}_2)$ such that

$$\|\mathbf{y}_1 - \mathbf{y}_2\| \leq L \|\mathbf{d}_1 - \mathbf{d}_2\|.$$

Since $P_i(\widehat{\mathbf{b}}_i(t, \mathbf{d}'))$ is nonempty and compact for all $(t, \mathbf{d}') \in D_M$, there exists a finite $k(t, \mathbf{d}') \geq 0$ such that for all $\mathbf{y}'_1, \mathbf{y}'_2 \in P_i(\widehat{\mathbf{b}}_i(t, \mathbf{d}'))$,

$$\|\mathbf{y}'_1 - \mathbf{y}'_2\| \leq k(t, \mathbf{d}').$$

Thus, for any $\mathbf{d} \in F_i$, and for any $\mathbf{y}_1, \mathbf{y}_2 \in P_i(\mathbf{d})$, we can fix $(t, \mathbf{d}') \in D_M$ and $\mathbf{y}'_1, \mathbf{y}'_2 \in P_i(\widehat{\mathbf{b}}_i(t, \mathbf{d}'))$ such that

$$\begin{aligned} \|\mathbf{y}_1 - \mathbf{y}_2\| &\leq \|\mathbf{y}_1 - \mathbf{y}'_1\| + \|\mathbf{y}'_1 - \mathbf{y}'_2\| + \|\mathbf{y}'_2 - \mathbf{y}_2\| \\ &\leq 2L \left\| \mathbf{d} - \widehat{\mathbf{b}}_i(t, \mathbf{d}') \right\| + k(t, \mathbf{d}') < +\infty. \end{aligned}$$

Consequently, $P_i(\mathbf{d})$ is compact for each $\mathbf{d} \in F_i$. It follows that \widehat{q}_i is finite and well-defined on $\mathbb{R}^{n_u+n_x} \times F_i$, and further by Lemma 4 it is locally Lipschitz continuous.

Finally, note that $q_i(t, \mathbf{d}) = \widehat{q}_i(\mathbf{c}_i(t, \mathbf{d}), \widehat{\mathbf{b}}_i(t, \mathbf{d})) + h_i(t, \mathbf{d})$. We have that q_i is continuous, since \widehat{q}_i , \mathbf{c}_i , $\widehat{\mathbf{b}}_i$, and h_i are continuous. Now choose $(t, \mathbf{d}) \in D_M$. By Lemma 5 there exists a neighborhood $N^i(\mathbf{d})$ of \mathbf{d} and $L_i > 0$ such that for all $(t', \mathbf{d}_1), (t', \mathbf{d}_2) \in (T \times N^i(\mathbf{d})) \cap D_M$

$$\begin{aligned} \|\mathbf{c}_i(t', \mathbf{d}_1) - \mathbf{c}_i(t', \mathbf{d}_2)\| &\leq L_i \|\mathbf{d}_1 - \mathbf{d}_2\|, \\ |h_i(t', \mathbf{d}_1) - h_i(t', \mathbf{d}_2)| &\leq L_i \|\mathbf{d}_1 - \mathbf{d}_2\|. \end{aligned}$$

Let K_i be the image of $(T \times N^i(\mathbf{d})) \cap D_M$ under $(\mathbf{c}_i, \widehat{\mathbf{b}}_i)$. As established earlier, \mathbf{c}_i and $\widehat{\mathbf{b}}_i$ are bounded on $(T \times N^i(\mathbf{d})) \cap D_M$, and so it follows that K_i is bounded and so its closure is a compact subset of $\mathbb{R}^{n_u+n_x} \times F_i$. Since \widehat{q}_i is locally Lipschitz continuous, it is Lipschitz continuous on K_i , and so there exists $\widehat{L}_q > 0$ such that

$$\begin{aligned} |q_i(t', \mathbf{d}_1) - q_i(t', \mathbf{d}_2)| &\leq \widehat{L}_q \|\mathbf{c}_i(t', \mathbf{d}_1) - \mathbf{c}_i(t', \mathbf{d}_2)\|_1 + \\ &\quad \widehat{L}_q \left\| \widehat{\mathbf{b}}_i(t', \mathbf{d}_1) - \widehat{\mathbf{b}}_i(t', \mathbf{d}_2) \right\|_1 + \\ &\quad |h_i(t', \mathbf{d}_1) - h_i(t', \mathbf{d}_2)| \end{aligned}$$

for all $(t', \mathbf{d}_1), (t', \mathbf{d}_2) \in (T \times N^i(\mathbf{d})) \cap D_M$. Then, applying the properties of \mathbf{c}_i , $\widehat{\mathbf{b}}_i$ and h_i , we have that

$$|q_i(t', \mathbf{d}_1) - q_i(t', \mathbf{d}_2)| \leq (\widehat{L}_q L_i + \widehat{L}_q \widehat{L}_i + L_i) \|\mathbf{d}_1 - \mathbf{d}_2\|,$$

for all $(t', \mathbf{d}_1), (t', \mathbf{d}_2) \in (T \times N^i(\mathbf{d})) \cap D_M$, applying the equivalence of norms on \mathbb{R}^n as necessary. Since this holds for each $i \in \{1, \dots, m\}$, the desired conclusion holds. \square

5 Numerical Examples

This section considers the performance of a numerical implementation of the bounding method established in Corollary 2, using the definition of \mathbf{q} in Algorithm 1. This implementation is a C/C++ code which solves the IVP (11) with the implementation of the Backwards Differentiation Formulae (BDF) in the CVODE component of the SUNDIALS suite [18] (<http://computation.llnl.gov/casc/sundials/main.html>). Newton’s method is used for the corrector iteration. CPLEX [20] version 12.4 is used to solve the linear programs required to define the dynamics in Algorithm 1. Further, all LPs are solved with advanced starting information (“warm-started”) with dual simplex. This results in a fairly significant speedup of the code, as Phase I simplex typically can be skipped. The feasibility and optimality tolerances used to solve the LPs and the integration tolerances are given below for each individual example. It should be noted that for these values of the tolerances, an infeasible LP is never encountered in these examples. All numerical studies were performed on a 64-bit Linux virtual machine allocated a single core of a 3.07 GHz Intel Xeon processor.

5.1 Lotka-Volterra problem

The Lotka-Volterra problem is a classic problem in the study of nonlinear dynamic systems and often serves as a benchmark for numerical methods. It is thought of as a model for the evolution in time of the populations of a predator and a prey species, and the solution is asymptotically periodic. The equations describing this system are

$$\dot{x}_1(t) = u_1(t)x_1(t)(1 - x_2(t)), \quad (14)$$

$$\dot{x}_2(t) = u_2(t)x_2(t)(x_1(t) - 1). \quad (15)$$

For this study the initial conditions are $\mathbf{x}(0) = (1.2, 1.1)$. The goal is to compute enclosures of the solutions for any value of the inputs $\mathbf{u} \in \mathcal{U}$, where $U = [2.99, 3.01] \times [0.99, 1.01]$. These are the same input ranges and initial conditions used in [25], which demonstrates the performance of the code VSPODE, an implementation of a Taylor model based bounding procedure.

For this example, one could claim that since x_1 and x_2 represent the populations of species, they should always be nonnegative, and consequently one could set $\mathbf{A}_G = -\mathbf{I}$ and $\mathbf{b}_G : t \mapsto \mathbf{0}$. However, for what will be considered “meaningful” bounds, this kind of a priori enclosure does not make a difference. Consequently, for the purpose of applying the theory, the vacuous enclosure given by $\mathbf{A}_G = [0, 0]$ and $\mathbf{b}_G : t \mapsto 0$ is used, although in the implementation this information is unnecessary and is easily omitted.

In [25], VSPODE manages to propagate upper and lower bounds on the solution which remain a subset of the interval in state space $[0.5, 1.5] \times [0.5, 1.5]$ on the time interval $T = [0, 10]$. This is used as a metric to determine whether the calculated bounds are “meaningful.” First, interval bounds are calculated,

which is to say that the matrix $\mathbf{A} = [-\mathbf{I} \ \mathbf{I}]^T$ is used. Unfortunately, despite the use of affine relaxations to improve the estimate of the dynamics, the upper and lower bounds for each species calculated using the above \mathbf{A} matrix cease to be a subset of the interval $[0.5, 1.5] \times [0.5, 1.5]$ before $t = 4$, or before the completion of one full cycle. This, of course, is one of the drawbacks of pure interval enclosures, and what has motivated the development of Taylor model bounding methods. It should be noted that although the bounds are meaninglessly loose in this case, there is no associated numerical “breakdown” before $t = 10$; the solution of the linear programs defining the dynamics and the numerical integration method still proceed without error.

However, using the polyhedral bounding theory discussed in the present work, it is possible to obtain much better upper and lower bounds, which remain a subset of the interval $[0.5, 1.5] \times [0.5, 1.5]$ for all $t \in T$. This can be achieved by letting the i^{th} row \mathbf{a}_i^T of the matrix $\mathbf{A} \in \mathbb{R}^{16 \times 2}$ be given by

$$\mathbf{a}_i^T = [\cos((i/16)2\pi), \sin((i/16)2\pi)]. \quad (16)$$

Each row of \mathbf{A} merely represents the normal of a face of a 16-sided polygon. Lower and upper bounds on each component can be chosen from these bounding hyperplanes. The results are plotted in Figure 3. The upper and lower bounds resulting from \mathbf{A} in Equation (16) are superior, and indeed are a subset of $[0.5, 1.5] \times [0.5, 1.5]$ for all $t \in [0, 10]$. In effect, the use of the current theory more than doubles the time interval over which meaningful bounds can be calculated.

Using LP feasibility and optimality tolerances of 10^{-5} and 10^{-6} , respectively, and absolute and relative integration tolerances of 10^{-6} , the CPU time required to solve the bounding system is 0.050s (with \mathbf{A} defined in Equation (16)). For comparison, the purely interval bounds require 0.020s, while the time required by VSPODE (on a processor with a comparable clock speed) reported in [25] is 0.59s. Although the enclosure obtained from VSPODE is tighter, it is solving an intrinsically different problem; namely, one in which the inputs u_1 and u_2 are *constant* functions on T . That is, for all $t \in T$, $\mathbf{u}(t) \equiv \hat{\mathbf{u}}$ for some $\hat{\mathbf{u}} \in U$.

5.2 Stirred-tank reactor

This next example demonstrates that, in contrast to the previous example, a brute-force approach to constructing polyhedral bounds is not necessary in all cases. For the following class of engineering-relevant problems, an intelligent choice of bounds is available. Furthermore, much of the justification that the choice is intelligent does not have anything to do with the idea that it “wraps” the reachable set in an intelligent manner, which is the typical geometric justification of many bounding methods. Rather, it relates to the idea that the quantities that must be estimated to construct these bounds can be estimated well with tools such as interval arithmetic.

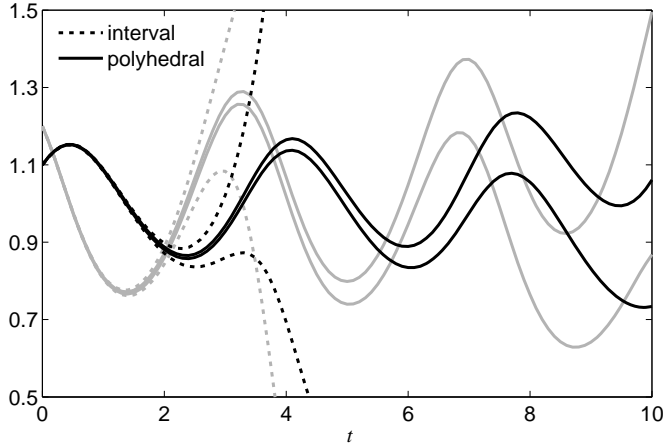


Fig. 3: Upper and lower bounds on the components of the solution of the Lotka-Volterra problem versus time; x_1 is in gray, while x_2 is in black. Results from polyhedral bounds using \mathbf{A} as in Equation (16) are solid lines, while results from purely interval bounds are dashed.

The general form of the material balance equations for a homogeneous, constant-density, stirred-tank reactor with constant material volume is

$$\dot{\mathbf{x}}(t) = \mathbf{S}\mathbf{r}(t, \mathbf{x}(t)) + (1/V) (\mathbf{C}_{in}(t)\mathbf{v}_{in}(t) - v_{out}(t)\mathbf{x}(t)), \quad \mathbf{x}(t_0) = \mathbf{x}_0, \quad (17)$$

where $\mathbf{x}(t)$ is the vector of the n_x species concentrations at time t , $\mathbf{S} \in \mathbb{R}^{n_x \times n_r}$ and \mathbf{r} are the stoichiometry matrix and vector of n_r rate functions, respectively, V is the constant reactor volume, $\mathbf{v}_{in}(t) \in \mathbb{R}^p$ is the vector of the volumetric flow rates of the p inlets to the reactor at t , the j^{th} column of $\mathbf{C}_{in}(t) \in \mathbb{R}^{n_x \times p}$ is the vector of species concentrations in the j^{th} inlet, and $\mathbf{1}^T \mathbf{v}_{in}(t) = v_{out}(t)$ is the volumetric flow rate of the single outlet from the reactor, where $\mathbf{1}$ denotes a vector of ones in \mathbb{R}^p .

For a system of this form, a linear transformation yields a system in terms of reaction “variants” and “invariants” [44]. For instance, if \mathbf{S} is full column rank, the rows of \mathbf{N} are left null vectors of \mathbf{S} , and \mathbf{S}^+ is the Moore-Penrose pseudoinverse of \mathbf{S} (see Chapter 1 of [3]), then letting $\mathbf{y}_1 = \mathbf{S}^+ \mathbf{x}$ and $\mathbf{y}_2 = \mathbf{N}\mathbf{x}$ one obtains

$$\dot{\mathbf{y}}_1(t) = \mathbf{r}_y(t, \mathbf{y}(t)) + (1/V) (\mathbf{S}^+ \mathbf{C}_{in}(t)\mathbf{v}_{in}(t) - v_{out}(t)\mathbf{y}_1(t)), \quad \mathbf{y}_1(t_0) = \mathbf{S}^+ \mathbf{x}_0, \quad (18)$$

$$\dot{\mathbf{y}}_2(t) = (1/V) (\mathbf{N}\mathbf{C}_{in}(t)\mathbf{v}_{in}(t) - v_{out}(t)\mathbf{y}_2(t)), \quad \mathbf{y}_2(t_0) = \mathbf{N}\mathbf{x}_0,$$

where the subscript y on \mathbf{r} denotes that \mathbf{r}_y is considered a function of the transformed variables. If the system has no inlets or outlets, i.e. is a batch reactor, then $\dot{\mathbf{y}}_2(t) = \mathbf{0}$ for all t , and so is constant. From the perspective of

the original system, the solution must obey the affine constraints $\mathbf{N}\mathbf{x}(t) = \mathbf{N}\mathbf{x}_0$ for all t . This forms the basis of the a priori enclosures used in [16, 38, 39].

However, the addition of inlets and outlets complicates this kind of a priori enclosure. It is possible to salvage this enclosure, by noting that the linear transformation partially decouples the system of equations. If \mathbf{C}_{in} and \mathbf{v}_{in} are known, simple functions or are constant parameters, then an analytical solution for \mathbf{y}_2 can be obtained fairly easily. The result is that the a priori enclosure is now time-varying; specifically, the solution must obey $\mathbf{N}\mathbf{x}(t) = \mathbf{y}_2(t)$, where again \mathbf{y}_2 is now known explicitly. This kind of information still satisfies Assumption 3, and could be used in the current bounding theory. But again, matters are more complicated if, for instance, the values of \mathbf{C}_{in} or \mathbf{v}_{in} are subject to some unknown, but bounded time-varying disturbance.

Instead, the approach taken here will be to use a bounding polyhedron that will implicitly enforce this time-varying enclosure, without the need to determine explicitly \mathbf{y}_2 , or some other functions that take the role of \mathbf{b}_G . Since the solution \mathbf{x} describes concentrations, the components must be nonnegative, and so for this example the only a priori enclosure used is given by these nonnegativity constraints. In general, the bounding matrix is given by

$$\mathbf{A} = \begin{bmatrix} -\mathbf{I} \\ \mathbf{I} \\ -\mathbf{D}^+ \\ \mathbf{D}^+ \\ -\mathbf{N} \\ \mathbf{N} \end{bmatrix}, \quad (19)$$

where \mathbf{D}^+ is the Moore-Penrose pseudoinverse of \mathbf{D} , a matrix formed from a maximal set of linearly independent columns of \mathbf{S} , and the rows of \mathbf{N} are linearly independent and span the left null space of \mathbf{S} .

Before considering the specifics of the example, the merits of this form of polyhedral bounds, as determined by the matrix \mathbf{A} above, are discussed. It helps to write the dynamics of the system (17) in the following general form:

$$\mathbf{f}(t, \mathbf{p}, \mathbf{z}) = [\mathbf{S} \ \mathbf{I}] \begin{bmatrix} \mathbf{r}_p(t, \mathbf{p}, \mathbf{z}) \\ \mathbf{g}_1(t, \mathbf{p}) - g_2(t, \mathbf{p})\mathbf{z} \end{bmatrix} = \widehat{\mathbf{S}}\widehat{\mathbf{r}}(t, \mathbf{p}, \mathbf{z}),$$

where the functions \mathbf{g}_1 and g_2 take into account the possibility that the inlet flow rates and concentrations are modeled as controls, parameters, or disturbances, and \mathbf{r}_p takes into account that the reaction kinetics might not be known exactly. In general, the more rows that the matrix \mathbf{A} has, the tighter the bounds. Of course, too many superfluous rows slows down the calculation and does little to improve the bounds. To a certain extent, the bounds on the individual components (that is, the interval bounds) are improved the most when linear combinations of the states that are “estimated well” are included in the bounds. Inspired by the previous discussion, the linear combinations $\mathbf{y}_2 = \mathbf{N}\mathbf{z}$, which no longer depend on the reaction rates, are a good candidate. Part of this relates to the specifics of how the affine overestimators of the dynamics are constructed. The affine relaxation method described in Appendix A requires interval arithmetic, and it is well known that the effectiveness of interval arithmetic is diminished by the dependency problem (see

for instance Section 1.4 in [34]). As a general observation, the “simpler” the expression, the more effective interval arithmetic is at generating a tight estimate of its range. Thus, the quantities \mathbf{y}_2 , whose dynamics no longer depend on the potentially nonlinear rate function \mathbf{r}_p , have a good chance of being estimated well by interval arithmetic and the affine relaxation method. Further, the dynamics for \mathbf{y}_2 are decoupled. This is significant since the value of $\mathbf{a}_i^T \mathbf{z}$ is unique for $\mathbf{z} \in M_i(t, \mathbf{d})$, and it is over $M_i(t, \mathbf{d})$ which the dynamics must be estimated. This means that if \mathbf{a}_i is the j^{th} row of \mathbf{N} , then $\mathbf{a}_i^T \mathbf{z} = y_{2,j}$ and $\mathbf{a}_i^T \mathbf{f}(t, \mathbf{p}, \mathbf{z}) = \mathbf{a}_i^T \mathbf{g}_1(t, \mathbf{p}) - g_2(t, \mathbf{p})y_{2,j}$. In a loose sense, uncertainty with respect to the states has been removed, and overestimating the dynamics in this case only requires overestimation with respect to the inputs.

Similar reasoning supports why the quantities $\mathbf{y}_1 = \mathbf{D}^+ \mathbf{z}$ also are estimated well. If \mathbf{S} is full column rank, one can choose $\mathbf{D} = \mathbf{S}$ and then $\mathbf{D}^+ = \mathbf{S}^+$, and so $\mathbf{D}^+ \mathbf{S} = \mathbf{I}$. The result is that the dynamics of these quantities \mathbf{y}_1 only depend on a single component of the rate function \mathbf{r}_p (in fact, in a batch system, this motivates their interpretation as “extents of reaction”). As before, the simpler the expression, the more likely it is to be estimated well via the affine relaxation procedure. If \mathbf{S} is not full column rank, for instance $\mathbf{S} = [\mathbf{D} \ \mathbf{E}]$, then $\mathbf{D}^+ \mathbf{S} = [\mathbf{I} \ \mathbf{D}^+ \mathbf{E}]$, and again, the expression for the dynamics of the quantities \mathbf{y}_1 is potentially simplified.

At this point it is reasonable to wonder why not apply an interval-based bounding method to the transformed system (18). The complicating fact is that this requires explicitly rewriting the rate function in terms of the transformed variables to obtain \mathbf{r}_y . In general, this is not a trivial task. Although it is possible to automate the evaluation of \mathbf{r}_y , since the transformation from \mathbf{x} to \mathbf{y} is invertible in certain cases [44], it is likely that extending this evaluation to interval arithmetic will suffer from dependency issues. For this reason, explicitly bounding the original variables, in terms of which the rate function is originally written, helps reduce the overestimation of the original variables, and in turn reduce the overestimation of the range of the rate function on the various sets it must be estimated. Finally, as upper and lower bounds on the original variables are most likely the ultimate goal of estimating the reachable set of this system, there is little reason to exclude bounding them in the definition of \mathbf{A} .

Now, consider the specifics of the example. Let the components of the solution be $\mathbf{x} = (x_A, x_B, x_C, x_D)$, which are the concentration profiles (in M) of the four chemical species A, B, C, and D, respectively. Let

$$\dot{\mathbf{x}}(t, \mathbf{u}) = \begin{bmatrix} -1 & -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_3(t)x_A(t, \mathbf{u})x_B(t, \mathbf{u}) \\ k_2x_A(t, \mathbf{u})x_C(t, \mathbf{u}) \\ (1/V)(u_1(t)v_A - x_A(t, \mathbf{u})(v_A + v_B)) \\ (1/V)(u_2(t)v_B - x_B(t, \mathbf{u})(v_A + v_B)) \\ (1/V)(-x_C(t, \mathbf{u})(v_A + v_B)) \\ (1/V)(-x_D(t, \mathbf{u})(v_A + v_B)) \end{bmatrix}. \quad (20)$$

The known parameters are $V = 20$ (L), $k_2 = 0.4$ ($\text{M}^{-1}\text{min}^{-1}$), $v_A = v_B = 1$ ($\text{L}(\text{min})^{-1}$). The time-varying uncertainties are the inlet concentration of

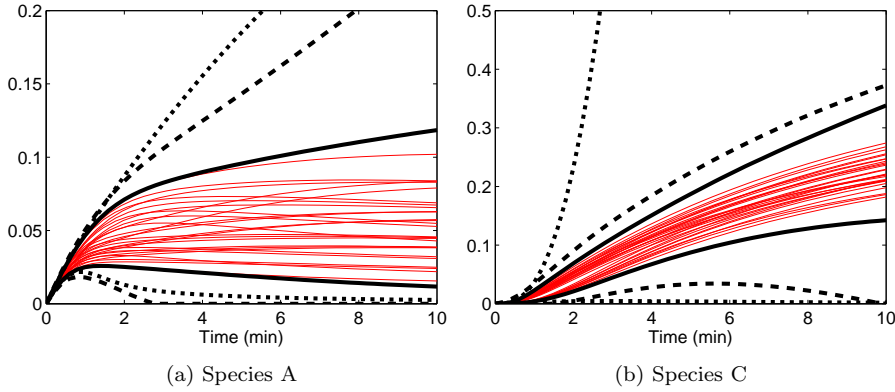


Fig. 4: Interval hull of enclosures versus time for the stirred-tank reactor (Equation (20)). Solution trajectories for various constant inputs are thin solid lines. Results from \mathbf{A} in Equation (19) are solid black lines, while results from \mathbf{A}' and \mathbf{A}'' as in Equation (21) are dotted lines and dashed lines, respectively.

species A, $u_1(t) \in [0.9, 1.1]$ (M), the inlet concentration of species B, $u_2(t) \in [0.8, 1.0]$ (M), and the rate constant of the first reaction, $u_3(t) \in [10, 50]$ ($\text{M}^{-1}\text{min}^{-1}$). Initially, the concentration of each species is zero, and at $t = 0$, A and B begin to flow in. The time period of interest is $T = [0, 10]$ (min). The first two columns of the matrix in Equation (20) correspond to the stoichiometry matrix \mathbf{S} . Its columns are linearly independent, and so let

$$\mathbf{D}^+ = \mathbf{S}^+ = \begin{bmatrix} -1/3 & -1/3 & 1/3 & 0 \\ -1/3 & 0 & -1/3 & 1/3 \end{bmatrix} \text{ and } \mathbf{N} = \begin{bmatrix} -1 & 2 & 1 & 0 \\ 1 & -1 & 0 & 1 \end{bmatrix}.$$

Results for two representative species are in Figure 4. For comparison, the interval hull of the enclosures that result from using

$$\mathbf{A}' = \begin{bmatrix} -\mathbf{I} \\ \mathbf{I} \end{bmatrix} \text{ or } \mathbf{A}'' = \begin{bmatrix} -\mathbf{D}^+ \\ \mathbf{D}^+ \\ -\mathbf{N} \\ \mathbf{N} \end{bmatrix} \quad (21)$$

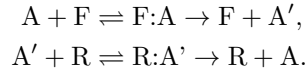
as the matrix that defines the polyhedral enclosure are included. These are interval bounds on the original system (17), and (roughly) the transformed system (18), respectively. The interval hull of the polyhedral enclosures are calculated in a post-processing step for the purpose of comparing the different results on an equal footing. It is clear that the bounds that result from using \mathbf{A} in Equation (19) are superior, and much tighter than just the intersection of the bounds resulting from the other enclosures. Finally, with LP feasibility and optimality tolerances of 10^{-5} and 10^{-6} , respectively, and absolute and relative integration tolerances of 10^{-6} , the CPU time required to solve the bounding system is 0.030s.

5.3 Piecewise affine relaxations

An interesting application of this theory is to the construction of piecewise affine relaxations of the solutions of initial value problems in parametric ordinary differential equations. The initial value problem in parametric ordinary differential equations is a special case of the problem of interest (1), when the uncertainty is fixed, i.e. not time-varying. Certainly, the theory as it stands can handle this case already, but intuitively the bounds produced may not be as tight as those produced by a method that explicitly takes advantage of the fact that the uncertain inputs have a constant value in time, such as the Taylor-model methods described in [25].

The idea is fairly straightforward; the fixed uncertain parameters are treated as extra state variables with zero time derivatives and an uncertain set of initial values. Of course, nothing is gained from this reformulation if one can only propagate interval bounds on the states, but if one propagates polyhedral bounds the reformulation is meaningful.

To demonstrate this, an example adapted from Example 2 in [39] is considered, involving the following enzymatic reaction network:



The dynamic equations governing the evolution of the species concentrations $\mathbf{x} = (x_{\text{A}}, x_{\text{F}}, x_{\text{F:A}}, x_{\text{A}'}, x_{\text{R}}, x_{\text{R:A}'})$ in a closed system are

$$\begin{aligned} \dot{x}_{\text{A}} &= -k_1 x_{\text{F}} x_{\text{A}} + k_2 x_{\text{F:A}} + k_6 x_{\text{R:A}'}, \\ \dot{x}_{\text{F}} &= -k_1 x_{\text{F}} x_{\text{A}} + k_2 x_{\text{F:A}} + k_3 x_{\text{F:A}}, \\ \dot{x}_{\text{F:A}} &= k_1 x_{\text{F}} x_{\text{A}} - k_2 x_{\text{F:A}} - k_3 x_{\text{F:A}}, \\ \dot{x}_{\text{A}'} &= k_3 x_{\text{F:A}} - k_4 x_{\text{A}'} x_{\text{R}} + k_5 x_{\text{R:A}'}, \\ \dot{x}_{\text{R}} &= -k_4 x_{\text{A}'} x_{\text{R}} + k_5 x_{\text{R:A}'} + k_6 x_{\text{R:A}'}, \\ \dot{x}_{\text{R:A}'} &= k_4 x_{\text{A}'} x_{\text{R}} - k_5 x_{\text{R:A}'} - k_6 x_{\text{R:A}'}. \end{aligned} \tag{22}$$

The time interval of interest is $T = [0, 0.04]$ (s). For the original states \mathbf{x} , the initial conditions are $\mathbf{x}_0 = (34, 20, 0, 0, 16, 0)$ (M). Let the uncertain, but constant, parameters be $(p_1, p_2) = (k_1, k_6) \in [0.1, 1] \times [0.3, 3] = P$. The other k_i are known: $(k_2, k_3, k_4, k_5) = (0.1815, 88, 27.5, 2.75)$. To obtain the reformulated system, append the equations $\dot{\mathbf{p}} = \mathbf{0}$ to Equations (22) and now for the reformulated system, the initial conditions are uncertain: $(\mathbf{x}(0), \mathbf{p}(0)) \in \{\mathbf{x}_0\} \times P$. As in [39], the following a priori enclosure is available for the reformulated system:

$$\begin{aligned} G &\equiv \{(\mathbf{z}, \mathbf{r}) \in \mathbb{R}^6 \times \mathbb{R}^2 : \mathbf{0} \leq \mathbf{z} \leq \bar{\mathbf{x}}, \mathbf{N}\mathbf{z} = \mathbf{N}\mathbf{x}_0, \mathbf{r} \in P\}, \quad \text{with} \\ \mathbf{N} &= \begin{bmatrix} 0 & -1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & -1 \\ 1 & -1 & 0 & 1 & -1 & 0 \end{bmatrix}, \\ \bar{\mathbf{x}} &= (34, 20, 20, 34, 16, 16). \end{aligned}$$

The bounding matrix \mathbf{A} used in this example is

$$\mathbf{A} = \begin{bmatrix} -\mathbf{I} & \mathbf{0} \\ \mathbf{I} & \mathbf{0} \\ -\mathbf{I} & \mathbf{M} \\ \mathbf{I} & -\mathbf{M} \end{bmatrix}$$

where \mathbf{M} is the matrix whose columns are (approximately) the sensitivities of \mathbf{x} with respect to each p_i , evaluated at the final time $t_f = 0.04$ and at the midpoint of the interval P . These sensitivities, as calculated numerically with CVODES, are

$$\begin{bmatrix} -14.4 & -3.12 & 3.12 & 1.99 & -9.28 & 9.28 \\ 0.105 & -0.00577 & 0.00577 & -0.00748 & 0.103 & -0.103 \end{bmatrix}^T,$$

however, any value with magnitude less than 10^{-2} is set to zero to construct \mathbf{M} . The reasoning behind this form of \mathbf{A} is that the first half of its rows give interval bounds, while the second half of its rows give affine under- and over-estimators of each original state with respect to \mathbf{p} , and specifically, these should be “good” estimators at the final time point t_f .

Figure 5 shows the piecewise affine underestimator (maximum of the lower bound and affine underestimator) and overestimator (minimum of the upper bound and affine overestimator) for a certain concentration on the set P . When only interval bounds are propagated, the interval bound on the state $x_{F:A}$ at t_f is $[0.517, 4.79]$, while the use of the affine relaxations reduces this to $[0.582, 4.09]$, corresponding to an 18% reduction in the width of the enclosure. Thus, using the extra bounds in the form of affine under and overestimators also improves the interval bounds. This contrasts with the methods in [40] and [42], where the benefit is one-way; relaxations with respect to the parameters cannot improve the interval bounds.

With LP feasibility and optimality tolerances of 10^{-5} and 10^{-6} , respectively, and absolute and relative integration tolerances of 10^{-6} , the CPU time required to solve the bounding system is 0.15s. In comparison, the methods for constructing convex and concave relaxations of the solutions of parametric ordinary differential equations presented in [40, 41] also involve the solution of an auxiliary dynamic system, but this system must be solved at each parameter value of interest to determine the value of the relaxations. The current method only requires that the auxiliary dynamic system is solved once to obtain the value of the relaxation on the entire parameter range.

6 Conclusions

This work has presented a general theory, as well as an efficient numerical implementation, for the construction of polyhedral bounds on the reachable set of a dynamic system subject to time-varying inputs and uncertain initial conditions. Some more fine-tuning of the current numerical implementation of

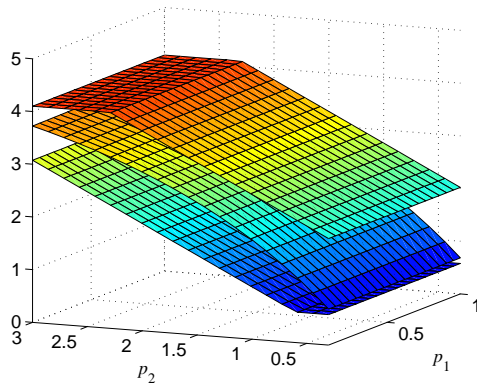


Fig. 5: Piecewise affine under and overestimators of $x_{F:A}$ at t_f on P ; the sampled parametric solution surface is in the middle.

the bounding method is a subject for future research. For instance, the function \mathbf{q} defining the dynamics of the bounding system is nonsmooth, and it may be beneficial to supply approximate or “locked” Jacobian information to the numerical integrator. As mentioned in Section 4.2, to ensure that one does not run into viability issues, the reformulation in [11] could be used. Alternative implementations of the theory are also a subject for future research; that is, defining the general mappings M_i differently provides avenues for different numerical implementations. These different numerical implementations might avoid some of the cost of the solution of the linear programs, and provide a slightly faster method, although potentially at the cost of producing more conservative bounds. Nevertheless, the present work as is stands as an effective method.

Other future work might include using the proposed method in the reachability analysis of hybrid systems [7, 30, 36]. In such an analysis, bounds are required for the continuous dynamics, which could be obtained by the methods in the present work. It should be noted that the work in this area often focuses on the case that the continuous dynamics of the hybrid system are linear or affine, as demonstrated by the recent thesis [24]. In this case, certain properties of linear systems (such as the fact that they preserve convexity of sets under the “flow” of the dynamics [12]) can be used, of which the present method does not explicitly take advantage.

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A Parametric Affine Relaxations

This section discusses a method for constructing affine relaxations of the dynamics which satisfy Assumption 4. The method relies on Proposition 5.1 in [17], which is repeated below. It is a general result, and to implement it, one needs specific relaxations of various arithmetic operations. Such operations are listed in Table 1 below.

Proposition 2 (Proposition 5.1 in [17]) *Let $m, n \in \mathbb{N}$. Let $Z \subset \mathbb{R}^n$ be a nonempty open set, and let $Y \subset \mathbb{R}^m$. Let $\mathbf{g} : Z \rightarrow \mathbb{R}^m$ and $f : Y \rightarrow \mathbb{R}$. Define $Z^{\mathbb{I}} = \{(\mathbf{v}, \mathbf{w}) \in \mathbb{R}^n \times \mathbb{R}^m : \mathbf{v} \leq \mathbf{w}, [\mathbf{v}, \mathbf{w}] \subset Z\}$, and similarly define $Y^{\mathbb{I}}$. For $i \in \{1, \dots, m\}$, let \mathbf{g}_i^{al} and \mathbf{g}_i^{au} be locally Lipschitz continuous mappings $Z^{\mathbb{I}} \rightarrow \mathbb{R}^n$ and $g_i^{bl}, g_i^{bu}, g_i^L, g_i^U$ be locally Lipschitz continuous mappings $Z^{\mathbb{I}} \rightarrow \mathbb{R}$ which satisfy*

$$\begin{aligned} \mathbf{g}_i^{al}(\mathbf{v}, \mathbf{w})^T \mathbf{z} + g_i^{bl}(\mathbf{v}, \mathbf{w}) &\leq g_i(\mathbf{z}) \leq \mathbf{g}_i^{au}(\mathbf{v}, \mathbf{w})^T \mathbf{z} + g_i^{bu}(\mathbf{v}, \mathbf{w}), \quad \forall \mathbf{z} \in [\mathbf{v}, \mathbf{w}], \\ g_i^L(\mathbf{v}, \mathbf{w}) &\leq g_i(\mathbf{z}) \leq g_i^U(\mathbf{v}, \mathbf{w}), \quad \forall \mathbf{z} \in [\mathbf{v}, \mathbf{w}], \\ [\mathbf{g}^L(\mathbf{v}, \mathbf{w}), \mathbf{g}^U(\mathbf{v}, \mathbf{w})] &\subset Y, \end{aligned}$$

for all $(\mathbf{v}, \mathbf{w}) \in Z^{\mathbb{I}}$. Let \mathbf{f}^{al} and \mathbf{f}^{au} and be locally Lipschitz continuous mappings $Y^{\mathbb{I}} \rightarrow \mathbb{R}^m$ and f^{bl} and f^{bu} be locally Lipschitz continuous mappings $Y^{\mathbb{I}} \rightarrow \mathbb{R}$ which satisfy

$$\mathbf{f}^{al}(\mathbf{v}', \mathbf{w}')^T \mathbf{y} + f^{bl}(\mathbf{v}', \mathbf{w}') \leq f(\mathbf{y}) \leq \mathbf{f}^{au}(\mathbf{v}', \mathbf{w}')^T \mathbf{y} + f^{bu}(\mathbf{v}', \mathbf{w}'), \quad \forall \mathbf{y} \in [\mathbf{v}', \mathbf{w}'],$$

for all $(\mathbf{v}', \mathbf{w}') \in Y^{\mathbb{I}}$.

Let $h : Z \rightarrow \mathbb{R}$ be defined by $h(\mathbf{z}) = f(\mathbf{g}(\mathbf{z}))$. For $i \in \{1, \dots, m\}$, let

$$\begin{aligned} \mathbf{h}_i^{al}(\mathbf{v}, \mathbf{w}) &= \begin{cases} \mathbf{f}_i^{al}(\mathbf{g}^L(\mathbf{v}, \mathbf{w}), \mathbf{g}^U(\mathbf{v}, \mathbf{w})) \mathbf{g}_i^{al}(\mathbf{v}, \mathbf{w}) & \text{if } f_i^{al}(\mathbf{g}^L(\mathbf{v}, \mathbf{w}), \mathbf{g}^U(\mathbf{v}, \mathbf{w})) \geq 0, \\ \mathbf{f}_i^{al}(\mathbf{g}^L(\mathbf{v}, \mathbf{w}), \mathbf{g}^U(\mathbf{v}, \mathbf{w})) \mathbf{g}_i^{au}(\mathbf{v}, \mathbf{w}) & \text{otherwise,} \end{cases} \\ \mathbf{h}_i^{bl}(\mathbf{v}, \mathbf{w}) &= \begin{cases} \mathbf{f}_i^{al}(\mathbf{g}^L(\mathbf{v}, \mathbf{w}), \mathbf{g}^U(\mathbf{v}, \mathbf{w})) g_i^{bl}(\mathbf{v}, \mathbf{w}) & \text{if } f_i^{al}(\mathbf{g}^L(\mathbf{v}, \mathbf{w}), \mathbf{g}^U(\mathbf{v}, \mathbf{w})) \geq 0, \\ \mathbf{f}_i^{al}(\mathbf{g}^L(\mathbf{v}, \mathbf{w}), \mathbf{g}^U(\mathbf{v}, \mathbf{w})) g_i^{bu}(\mathbf{v}, \mathbf{w}) & \text{otherwise,} \end{cases} \\ \mathbf{h}_i^{au}(\mathbf{v}, \mathbf{w}) &= \begin{cases} \mathbf{f}_i^{au}(\mathbf{g}^L(\mathbf{v}, \mathbf{w}), \mathbf{g}^U(\mathbf{v}, \mathbf{w})) \mathbf{g}_i^{au}(\mathbf{v}, \mathbf{w}) & \text{if } f_i^{au}(\mathbf{g}^L(\mathbf{v}, \mathbf{w}), \mathbf{g}^U(\mathbf{v}, \mathbf{w})) \geq 0, \\ \mathbf{f}_i^{au}(\mathbf{g}^L(\mathbf{v}, \mathbf{w}), \mathbf{g}^U(\mathbf{v}, \mathbf{w})) \mathbf{g}_i^{al}(\mathbf{v}, \mathbf{w}) & \text{otherwise,} \end{cases} \\ \mathbf{h}_i^{bu}(\mathbf{v}, \mathbf{w}) &= \begin{cases} \mathbf{f}_i^{au}(\mathbf{g}^L(\mathbf{v}, \mathbf{w}), \mathbf{g}^U(\mathbf{v}, \mathbf{w})) g_i^{bu}(\mathbf{v}, \mathbf{w}) & \text{if } f_i^{au}(\mathbf{g}^L(\mathbf{v}, \mathbf{w}), \mathbf{g}^U(\mathbf{v}, \mathbf{w})) \geq 0, \\ \mathbf{f}_i^{au}(\mathbf{g}^L(\mathbf{v}, \mathbf{w}), \mathbf{g}^U(\mathbf{v}, \mathbf{w})) g_i^{bl}(\mathbf{v}, \mathbf{w}) & \text{otherwise.} \end{cases} \end{aligned}$$

Let $\mathbf{h}^{al}, \mathbf{h}^{au} : Z^{\mathbb{I}} \rightarrow \mathbb{R}^n$ and $h^{bl}, h^{bu} : Z^{\mathbb{I}} \rightarrow \mathbb{R}$ be defined by

$$\begin{aligned} \mathbf{h}^{al}(\mathbf{v}, \mathbf{w}) &= \sum_i \mathbf{h}_i^{al}(\mathbf{v}, \mathbf{w}), & h^{bl}(\mathbf{v}, \mathbf{w}) &= f^{bl}(\mathbf{g}^L(\mathbf{v}, \mathbf{w}), \mathbf{g}^U(\mathbf{v}, \mathbf{w})) + \sum_i h_i^{bl}(\mathbf{v}, \mathbf{w}), \\ \mathbf{h}^{au}(\mathbf{v}, \mathbf{w}) &= \sum_i \mathbf{h}_i^{au}(\mathbf{v}, \mathbf{w}), & h^{bu}(\mathbf{v}, \mathbf{w}) &= f^{bu}(\mathbf{g}^L(\mathbf{v}, \mathbf{w}), \mathbf{g}^U(\mathbf{v}, \mathbf{w})) + \sum_i h_i^{bu}(\mathbf{v}, \mathbf{w}). \end{aligned}$$

Then $\mathbf{h}^{al}, \mathbf{h}^{au}, h^{bl}, h^{bu}$ are locally Lipschitz continuous mappings on $Z^{\mathbb{I}}$ which satisfy

$$\mathbf{h}^{al}(\mathbf{v}, \mathbf{w})^T \mathbf{z} + h^{bl}(\mathbf{v}, \mathbf{w}) \leq h(\mathbf{z}) \leq \mathbf{h}^{au}(\mathbf{v}, \mathbf{w})^T \mathbf{z} + h^{bu}(\mathbf{v}, \mathbf{w}), \quad \forall \mathbf{z} \in [\mathbf{v}, \mathbf{w}],$$

for all $(\mathbf{v}, \mathbf{w}) \in Z^{\mathbb{I}}$.

Constructing relaxations which satisfy Assumption 4 proceeds by recursively applying Proposition 2, illustrated by the following example.

Example 1 This example demonstrates how to construct affine relaxations for a simple function (in fact, this function is part of the dynamics of the Lotka-Volterra problem in Section 5.1). Let $f : \mathbb{R} \times \mathbb{R}^2 \ni (p, \mathbf{z}) \mapsto pz_1(1 - z_2)$. As in the Lotka-Volterra problem, p is an uncertain parameter. The goal is to construct, for any $p \in [p^L, p^U]$ such that $p^L > 0$,

Table 1: Some arithmetic operations f and their parameterized affine relaxations on $[\mathbf{y}^L, \mathbf{y}^U]$

Underestimators

f	$\mathbf{f}^{al}(\mathbf{y}^L, \mathbf{y}^U)$	$f^{bl}(\mathbf{y}^L, \mathbf{y}^U)$
$s \in \mathbb{R}, y \mapsto sy$	s	0
$s \in \mathbb{R}, y \mapsto y + s$	1	s
$(y_1, y_2) \mapsto y_1 + y_2$	$(1, 1)$	0
$(y_1, y_2) \mapsto y_1 - y_2$	$(1, -1)$	0
$(y_1, y_2) \mapsto y_1 y_2$	$\left(\frac{y_2^L + y_2^U}{2}, \frac{y_1^L + y_1^U}{2}\right)$	$-1/2(y_1^L y_2^L + y_1^U y_2^U)$
$y > 0, y \mapsto 1/y$	$-(y^U)^{-2}$	$2/y^U$

Overestimators

f	$\mathbf{f}^{au}(\mathbf{y}^L, \mathbf{y}^U)$	$f^{bu}(\mathbf{y}^L, \mathbf{y}^U)$
$s \in \mathbb{R}, y \mapsto sy$	s	0
$s \in \mathbb{R}, y \mapsto y + s$	1	s
$(y_1, y_2) \mapsto y_1 + y_2$	$(1, 1)$	0
$(y_1, y_2) \mapsto y_1 - y_2$	$(1, -1)$	0
$(y_1, y_2) \mapsto y_1 y_2$	$\left(\frac{y_2^L + y_2^U}{2}, \frac{y_1^L + y_1^U}{2}\right)$	$-1/2(y_1^U y_2^L + y_1^L y_2^U)$
$y > 0, y \mapsto 1/y$	$-1/(y^L y^U)$	$(1/(y^L y^U))y^L + 1/y^L$

affine relaxations of $f(p, \cdot)$ on any interval $[\mathbf{z}^L, \mathbf{z}^U]$ such that $z_1^L > 0$ and $z_2^L > 1$ (in the context of Assumption 4, obtaining a nontrivial $\tilde{\mathbf{c}}_i^u$ is beneficial only when U is not an interval). Furthermore, one desires that these relaxations are locally Lipschitz continuous with respect to $(\mathbf{z}^L, \mathbf{z}^U)$.

The process resembles the construction of an interval enclosure of the range of f via interval arithmetic, and indeed part of the method involves interval arithmetic. Evaluation of f is broken down into a sequence of auxiliary variables called ‘‘factors,’’ which can be expressed as simple arithmetic operations on previously computed factors. An interval enclosure and affine relaxation of each factor can also be computed, and following the rules in Proposition 2 and Table 1, the affine relaxations will also be locally Lipschitz continuous in the manner desired. See Table 2 for the factored expression. Note that factor v_3 , corresponding to the parameter p , is initialized with the trivial affine relaxations $\mathbf{0}^T \mathbf{z} + p^L \leq p \leq \mathbf{0}^T \mathbf{z} + p^U$. This ensures that the final relaxations obtained are valid for all $p \in [p^L, p^U]$. Also, note that the restrictions $z_1^L > 0$, $z_2^L > 1$, and $p^L > 0$, simplify the evaluation and preclude the need to consider the different ‘‘branches’’ when constructing the affine relaxations for factors v_5 and v_6 , as indicated in Proposition 2 (for example, this implies that $1/2(v_4^L + v_4^U) < 0$). Although in general, the different cases must be taken into account.

The final factor, v_6 , gives the value of f , and thus one also has

$$(\mathbf{v}_6^{al})^T \mathbf{z} + v_6^{bl} \leq f(p, \mathbf{z}) \leq (\mathbf{v}_6^{au})^T \mathbf{z} + v_6^{bu}$$

for all $(p, \mathbf{z}) \in [p^L, p^U] \times [\mathbf{z}^L, \mathbf{z}^U]$. However, by virtue of Proposition 2, \mathbf{v}_6^{al} , \mathbf{v}_6^{au} , v_6^{bl} , v_6^{bu} can be considered locally Lipschitz continuous functions with respect to $(\mathbf{z}^L, \mathbf{z}^U)$.

More generally, Assumption 4 requires parametric relaxations which are continuous on $T \times D_x^{\mathbb{I}}$. To include dependence on t , one could construct relaxations with respect to t as well, over the degenerate interval $[t, t]$. Then it is clear that the final relaxations would be locally Lipschitz continuous on $(T \times D_x)^{\mathbb{I}}$. The following lemmata show that this yields the desired properties.

Lemma 6 *Assume $m, n, p \in \mathbb{N}$. Let $C \subset \mathbb{R}^m$ be nonempty and compact and $D \subset \mathbb{R}^n$ be nonempty. Let $\mathbf{g} : C \times D \rightarrow \mathbb{R}^p$ be locally Lipschitz continuous. Then for all $\mathbf{z} \in D$, there exists a neighborhood $N(\mathbf{z})$ and $L > 0$ such that for all $(\mathbf{y}, \mathbf{z}_1), (\mathbf{y}, \mathbf{z}_2) \in C \times N(\mathbf{z}) \cap D$*

$$\|\mathbf{g}(\mathbf{y}, \mathbf{z}_1) - \mathbf{g}(\mathbf{y}, \mathbf{z}_2)\| \leq L \|\mathbf{z}_1 - \mathbf{z}_2\|.$$

Table 2: Factored expression, corresponding interval enclosures, and corresponding affine relaxations for Example 1

Factor	Value	Lower bound	Upper Bound
v_1	z_1	$v_1^L = z_1^L$	$v_1^U = z_1^U$
v_2	z_2	$v_2^L = z_2^L$	$v_2^U = z_2^U$
v_3	p	$v_3^L = p^L$	$v_3^U = p^U$
v_4	$1 - v_2$	$v_4^L = 1 - v_2^U$	$v_4^U = 1 - v_2^L$
v_5	$v_1 v_4$	$v_5^L = \min\{v_1^L v_4^L, v_1^L v_4^U, v_1^U v_4^L, v_1^U v_4^U\}$	$v_5^U = \max\{v_1^L v_4^L, v_1^L v_4^U, v_1^U v_4^L, v_1^U v_4^U\}$
v_6	$v_3 v_5$	$v_6^L = \min\{v_3^L v_5^L, v_3^L v_5^U, v_3^U v_5^L, v_3^U v_5^U\}$	$v_6^U = \max\{v_3^L v_5^L, v_3^L v_5^U, v_3^U v_5^L, v_3^U v_5^U\}$
Factor	Underestimator	Overestimator	
v_1	$\mathbf{v}_1^{al} = (1, 0), v_1^{bl} = 0$	$\mathbf{v}_1^{au} = (1, 0), v_1^{bu} = 0$	
v_2	$\mathbf{v}_2^{al} = (0, 1), v_2^{bl} = 0$	$\mathbf{v}_2^{au} = (0, 1), v_2^{bu} = 0$	
v_3	$\mathbf{v}_3^{al} = (0, 0), v_3^{bl} = p^L$	$\mathbf{v}_3^{au} = (0, 0), v_3^{bu} = p^U$	
v_4	$\mathbf{v}_4^{al} = -\mathbf{v}_2^{au}, v_4^{bl} = 1 - v_2^{bu}$	$\mathbf{v}_4^{au} = -\mathbf{v}_2^{al}, v_4^{bu} = 1 - v_2^{bl}$	
v_5	$\mathbf{v}_5^{al} = 1/2(v_4^L + v_4^U)\mathbf{v}_1^{au} + 1/2(v_1^L + v_1^U)\mathbf{v}_4^{al},$ $v_5^{bl} = -1/2(v_1^L v_4^L + v_1^U v_4^U) + 1/2(v_4^L + v_4^U)v_1^{bu} + 1/2(v_1^L + v_1^U)v_4^{bl}$	$\mathbf{v}_5^{au} = 1/2(v_4^L + v_4^U)\mathbf{v}_1^{al} + 1/2(v_1^L + v_1^U)\mathbf{v}_4^{au},$ $v_5^{bu} = -1/2(v_1^U v_4^L + v_1^L v_4^U) + 1/2(v_4^L + v_4^U)v_1^{bl} + 1/2(v_1^L + v_1^U)v_4^{bu}$	
v_6	$\mathbf{v}_6^{al} = 1/2(v_5^L + v_5^U)\mathbf{v}_3^{au} + 1/2(v_3^L + v_3^U)\mathbf{v}_5^{al},$ $v_6^{bl} = -1/2(v_3^L v_5^L + v_3^U v_5^U) + 1/2(v_5^L + v_5^U)v_3^{bu} + 1/2(v_3^L + v_3^U)v_5^{bl}$	$\mathbf{v}_6^{au} = 1/2(v_5^L + v_5^U)\mathbf{v}_3^{al} + 1/2(v_3^L + v_3^U)\mathbf{v}_5^{au},$ $v_6^{bu} = -1/2(v_3^U v_5^L + v_3^L v_5^U) + 1/2(v_5^L + v_5^U)v_3^{bl} + 1/2(v_3^L + v_3^U)v_5^{bu}$	

Proof Choose $\mathbf{z} \in D$. For each $\mathbf{y} \in C$, let $N(\mathbf{y}, \mathbf{z})$ be a neighborhood of (\mathbf{y}, \mathbf{z}) such that \mathbf{g} is Lipschitz continuous on $N(\mathbf{y}, \mathbf{z}) \cap (C \times D)$, with corresponding Lipschitz constant $L(\mathbf{y})$. However, this collection of open sets form an open cover of $C \times \{\mathbf{z}\}$, which is compact, and thus we can choose a finite number of these neighborhoods $\{N(\mathbf{y}_i, \mathbf{z}) : 1 \leq i \leq k\}$, such that their union, \tilde{N} , contains $C \times \{\mathbf{z}\}$. Let L be the (finite) maximum of the corresponding Lipschitz constants (i.e. $L = \max\{L(\mathbf{y}_i) : 1 \leq i \leq k\}$). Note that \tilde{N} is an open set, and \mathbf{g} is Lipschitz continuous on $\tilde{N} \cap (C \times D)$ with Lipschitz constant L .

We claim that there exists a $\delta > 0$ such that $C \times N_\delta(\mathbf{z}) \subset \tilde{N}$ (where $N_\delta(\mathbf{z})$ is viewed as a subset of \mathbb{R}^n). This follows from, for instance, Lemma 1 in Section 5 of [10]. The argument is that the complement of \tilde{N} , \tilde{N}^C , is closed and disjoint from $C \times \{\mathbf{z}\}$, and so there exists a $\delta > 0$ such that the distance between any point in $C \times \{\mathbf{z}\}$ and any point in \tilde{N}^C is greater than δ . This implies that $C \times N_\delta(\mathbf{z})$ is disjoint from \tilde{N}^C , which in turn implies $C \times N_\delta(\mathbf{z}) \subset \tilde{N}$. The result follows from Lipschitz continuity on $(C \times N_\delta(\mathbf{z})) \cap (C \times D) = C \times N_\delta(\mathbf{z}) \cap D$. \square

Lemma 7 Assume $n, p \in \mathbb{N}$. Let $T \subset \mathbb{R}$ be nonempty and compact and $D \subset \mathbb{R}^n$ be nonempty. Define $(T \times D)^{\mathbb{I}} = \{(s, \mathbf{v}, t, \mathbf{w}) : s \leq t, \mathbf{v} \leq \mathbf{w}, [s, t] \times [\mathbf{v}, \mathbf{w}] \subset T \times D\}$ and define $D^{\mathbb{I}}$ similarly. Let $\tilde{\mathbf{g}} : (T \times D)^{\mathbb{I}} \rightarrow \mathbb{R}^p$ be locally Lipschitz continuous. Define $\mathbf{g} : T \times D^{\mathbb{I}} \rightarrow \mathbb{R}^p$ by $\mathbf{g}(t, \mathbf{v}, \mathbf{w}) = \tilde{\mathbf{g}}(t, \mathbf{v}, t, \mathbf{w})$. Then \mathbf{g} is continuous, and for all $(\mathbf{v}, \mathbf{w}) \in D^{\mathbb{I}}$ there exists a neighborhood $N(\mathbf{v}, \mathbf{w})$ and $L > 0$ such that for all $(t, \mathbf{v}_1, \mathbf{w}_1), (t, \mathbf{v}_2, \mathbf{w}_2) \in T \times N(\mathbf{v}, \mathbf{w}) \cap D^{\mathbb{I}}$

$$\|\mathbf{g}(t, \mathbf{v}_1, \mathbf{w}_1) - \mathbf{g}(t, \mathbf{v}_2, \mathbf{w}_2)\| \leq L \|(\mathbf{v}_1, \mathbf{w}_1) - (\mathbf{v}_2, \mathbf{w}_2)\|.$$

Proof The mapping $\mathbf{h} : (t, \mathbf{v}, \mathbf{w}) \mapsto (t, \mathbf{v}, t, \mathbf{w})$ is Lipschitz continuous, and so \mathbf{g} , as the composition of locally Lipschitz $\bar{\mathbf{g}}$ and \mathbf{h} is locally Lipschitz continuous on $T \times D^2$. Applying Lemma 6 we obtain the desired result. \square

References

1. Althoff, M., Stursberg, O., Buss, M.: Reachability analysis of nonlinear systems with uncertain parameters using conservative linearization. In: Proceedings of the 47th IEEE Conference on Decision and Control, pp. 4042–4048 (2008)
2. Bemporad, A., Morari, M.: Robust Model Predictive Control: A Survey. In: A. Garulli, A. Tesi (eds.) Robustness in Identification and Control, Lecture Notes in Control and Information Sciences, pp. 207–226. Springer London (1999)
3. Ben-Israel, A., Greville, T.N.E.: Generalized Inverses: Theory and Applications, second edn. Springer, New York (2003)
4. Bertsimas, D., Tsitsiklis, J.N.: Introduction to Linear Optimization. Athena Scientific, Belmont, Massachusetts (1997)
5. Chachuat, B., Villanueva, M.: Bounding the solutions of parametric ODEs: When Taylor models meet differential inequalities. In: I.D.L. Bogle, M. Fairweather (eds.) Proceedings of the 22nd European Symposium on Computer Aided Process Engineering, pp. 17–20 (2012)
6. Chutinan, A., Krogh, B.H.: Computing polyhedral approximations to flow pipes for dynamic systems. In: Proceedings of the 37th IEEE Conference on Decision and Control, vol. 2, pp. 2089–2094 (1998)
7. Chutinan, A., Krogh, B.H.: Computational techniques for hybrid system verification. IEEE Transactions on Automatic Control **48**(1), 64–75 (2003)
8. Dang, T., Maler, O.: Reachability Analysis via Face Lifting. In: T. Henzinger, S. Sastry (eds.) Hybrid Systems: Computation and Control, pp. 96–109. Springer Berlin Heidelberg (1998)
9. Dontchev, A.L., Lempio, F.: Difference methods for differential inclusions: A survey. SIAM Review **34**(2), 263–294 (1992)
10. Filippov, A.F.: Differential Equations with Discontinuous Righthand Sides. Kluwer Academic, Boston (1988)
11. Gomez, J.A., Höffner, K., Barton, P.I.: DFBAlab: a fast and reliable MATLAB code for dynamic flux balance analysis. BMC Bioinformatics **15**(409), 1–10 (2014)
12. Greenstreet, M.R., Mitchell, I.: Integrating Projections. In: T. Henzinger, S. Sastry (eds.) Hybrid Systems: Computation and Control, pp. 159–174. Springer Berlin Heidelberg (1998)
13. Greenstreet, M.R., Mitchell, I.: Reachability Analysis Using Polygonal Projections. In: F.W. Vaandrager, J.H. van Schuppen (eds.) Hybrid Systems: Computation and Control, Lecture Notes in Computer Science, pp. 103–116. Springer Berlin Heidelberg (1999)
14. Harrison, G.W.: Dynamic models with uncertain parameters. In: X.J.R. Avula (ed.) Proceedings of the First International Conference on Mathematical Modeling, vol. 1, pp. 295–304. University of Missouri Rolla (1977)
15. Harwood, S.M., Höffner, K., Barton, P.I.: Efficient solution of ordinary differential equations with a parametric lexicographic linear program embedded. Numerische Mathematik (accepted)
16. Harwood, S.M., Scott, J.K., Barton, P.I.: Bounds on reachable sets using ordinary differential equations with linear programs embedded. In: S. Tarbouriech, M. Krstic (eds.) Nonlinear Control Systems, vol. 9, pp. 62–67 (2013)
17. Harwood, S.M., Scott, J.K., Barton, P.I.: Bounds on reachable sets using ordinary differential equations with linear programs embedded. IMA Journal of Mathematical Control and Information (in press)
18. Hindmarsh, A.C., Brown, P.N., Grant, K.E., Lee, S.L., Serban, R., Shumaker, D.E., Woodward, C.S.: SUNDIALS: Suite of Nonlinear and Differential/Algebraic Equation Solvers. ACM Transactions on Mathematical Software **31**(3), 363–396 (2005)

19. Hwang, I., Stipanovic, D.M., Tomlin, C.J.: Applications of polytopic approximations of reachable sets to linear dynamic games and a class of nonlinear systems. In: Proceedings of the American Control Conference, 2003, vol. 6, pp. 4613–4619 (2003)
20. IBM: IBM ILOG CPLEX: High performance mathematical programming solver. <http://www-01.ibm.com/software/commerce/optimization/cplex-optimizer/> (2014)
21. Kapela, T., Zgliczyński, P.: A Lohner-type algorithm for control systems and ordinary differential inclusions. *Discrete and Continuous Dynamical Systems Series B* **11**(2), 365–385 (2009)
22. Kieffer, M., Walter, E.: Guaranteed nonlinear state estimator for cooperative systems. *Numerical Algorithms* **37**(1-4), 187–198 (2004)
23. Lambert, J.D.: *Numerical Methods for Ordinary Differential Systems: The Initial Value Problem*. John Wiley & Sons, New York (1991)
24. Le Guernic, C.: *Reachability Analysis of Hybrid Systems with Linear Continuous Dynamics*. Ph.D. thesis, Université Joseph-Fourier (2009)
25. Lin, Y., Stadtherr, M.A.: Validated solutions of initial value problems for parametric ODEs. *Applied Numerical Mathematics* **57**(10), 1145–1162 (2007)
26. Lin, Y., Stadtherr, M.A.: Fault detection in nonlinear continuous-time systems with uncertain parameters. *AIChE Journal* **54**(9), 2335–2345 (2008)
27. Makino, K., Berz, M.: Remainder Differential Algebras and Their Applications. In: M. Berz, C. Bischof, G. Corliss, A. Griewank (eds.) *Computational Differentiation: Techniques, Applications, and Tools*, chap. 5, pp. 63–75. SIAM (1996)
28. Mangasarian, O.L., Shiau, T.H.: Lipschitz Continuity of Solutions of Linear Inequalities, Programs, and Complementarity Problems. *SIAM Journal on Control and Optimization* **25**(3), 583–595 (1987)
29. Mattheij, R., Molenaar, J.: *Ordinary Differential Equations in Theory and Practice*. SIAM, Philadelphia (2002)
30. Mitchell, I., Tomlin, C.J.: Level Set Methods for Computation in Hybrid Systems. In: N. Lynch, B.H. Krogh (eds.) *Hybrid Systems: Computation and Control*, pp. 310–323. Springer Berlin Heidelberg (2000)
31. Mitchell, I.M., Bayen, A.M., Tomlin, C.J.: A time-dependent Hamilton-Jacobi formulation of reachable sets for continuous dynamic games. *IEEE Transactions on Automatic Control* **50**(7), 947–957 (2005)
32. Mitsos, A., Chachuat, B., Barton, P.I.: McCormick-based relaxations of algorithms. *SIAM Journal on Optimization* **20**(2), 573–601 (2009)
33. Nedialkov, N.S.: *Computing Rigorous Bounds on the Solution of an Initial Value Problem for an Ordinary Differential Equation*. Ph.D. thesis, University of Toronto (1999)
34. Neumaier, A.: *Interval Methods for Systems of Equations*. Cambridge University Press, New York (1990)
35. Ramdani, N., Meslem, N., Candau, Y.: A hybrid bounding method for computing an over-approximation for the reachable set of uncertain nonlinear systems. *IEEE Transactions on Automatic Control* **54**(10), 2352–2364 (2009)
36. Ramdani, N., Nedialkov, N.S.: Computing reachable sets for uncertain nonlinear hybrid systems using interval constraint-propagation techniques. *Nonlinear Analysis: Hybrid Systems* **5**, 149–162 (2011)
37. Scott, J.K.: *Reachability Analysis and Deterministic Global Optimization of Differential-Algebraic Systems*. Ph.D. thesis, Massachusetts Institute of Technology (2012)
38. Scott, J.K., Barton, P.I.: Tight, efficient bounds on the solutions of chemical kinetics models. *Computers & Chemical Engineering* **34**(5), 717–731 (2010)
39. Scott, J.K., Barton, P.I.: Bounds on the reachable sets of nonlinear control systems. *Automatica* **49**(1), 93–100 (2013)
40. Scott, J.K., Barton, P.I.: Improved relaxations for the parametric solutions of ODEs using differential inequalities. *Journal of Global Optimization* **57**, 143–176 (2013)
41. Scott, J.K., Chachuat, B., Barton, P.I.: Nonlinear convex and concave relaxations for the solutions of parametric ODEs. *Optimal Control Applications and Methods* **34**(2), 145–163 (2013)
42. Singer, A.B., Barton, P.I.: Bounding the Solutions of Parameter Dependent Nonlinear Ordinary Differential Equations. *SIAM Journal on Scientific Computing* **27**(6), 2167–2182 (2006)

-
43. Singer, A.B., Barton, P.I.: Global Optimization with Nonlinear Ordinary Differential Equations. *Journal of Global Optimization* **34**(2), 159–190 (2006)
 44. Srinivasan, B., Amrhein, M., Bonvin, D.: Reaction and Flow Variants/Invariants in Chemical Reaction Systems with Inlet and Outlet Streams. *AIChE Journal* **44**(8), 1858–1867 (1998)
 45. Szarski, J.: *Differential Inequalities*. Polish Scientific Publishers, Warszawa, Poland (1965)
 46. Wets, R.J.B.: On the continuity of the value of a linear program and of related polyhedral-valued multifunctions. *Mathematical Programming Study* **24**, 14–29 (1985)