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Bounds on reachable sets using ordinary differential equations with linear programs embedded

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This work considers the computation of rigorous componentwise time-varying bounds on the states of a non-linear control system. This work develops a new implementation of an existing bounding theory that exploits physical information to produce tight bounds. It is shown that the solution of a certain initial value problem in ordinary differential equations (ODEs) depending on parametric linear programs (LPs) (which are said to be 'embedded') yields componentwise bounds. To ensure the numerical tractability of such a formulation, some properties of the resulting system of ODEs with LPs embedded are discussed. Finally, the tightness of the bounds are demonstrated for models of reacting chemical systems with uncertain rate parameters.

Keywords: reachable states; uncertain dynamic systems; affine relaxations.

1. Introduction

The problem of interest is the computation of time-varying enclosures of the reachable sets of the initial value problem (IVP)

$$\begin{aligned} \dot{\mathbf{x}}(t, \mathbf{u}, \mathbf{x}_0) &= \mathbf{f}(t, \mathbf{u}(t), \mathbf{x}(t, \mathbf{u}, \mathbf{x}_0)), \\ \mathbf{x}(t_0, \mathbf{u}, \mathbf{x}_0) &= \mathbf{x}_0, \end{aligned} \tag{1.1}$$

where $\mathbf{u}$ and $\mathbf{x}_0$ take values in some set of permissible controls and initial conditions, respectively. Using a bounding theory recently developed in Scott & Barton (2013), this work demonstrates that tight component-wise upper and lower bounds, called state bounds, can be computed by solving numerically a related IVP depending on parametric LPs. To this end, this work also analyses the IVP in ordinary differential equations (ODEs) with parametric linear programs (LPs) 'embedded.' The fundamental nature of 'ODEs with LPs embedded' is an IVP in ODEs, where the vector field depends on the optimal objective values of parametric LPs that are in turn parametrized in the right-hand side of their constraints and/or objective functions by the differential states. The LPs are then said to be 'embedded'.

Reachability analysis refers to estimating the set of possible states that a dynamic system may achieve for a range of parameter values or controls. This is an important task in state and parameter estimation (Jaulin, 2002; Raïssi *et al.*, 2004; Kieffer *et al.*, 2006; Singer *et al.*, 2006; Kieffer & Walter, 2011), uncertainty propagation (Harrison, 1977), safety verification and quality assurance (Huang *et al.*, 2002; Lin & Stadtherr, 2008), and as well global dynamic optimization (Singer & Barton, 2006b). This problem traces back as far as the work in Bertsekas & Rhodes (1971), however, some of the more recent

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applicable references are Althoff *et al.* (2008), Lin & Stadtherr (2007), Mitchell *et al.* (2005), Singer & Barton (2006a). Meanwhile, the goal of this work is to introduce a new implementation of the theory developed in Scott & Barton (2013). This theory provides a way to incorporate an '*a priori* enclosure' of the reachable sets to improve the estimates computed. As in Section 4.1, this is an enclosure of the reachable set based on mathematical manipulations of Equation (1.1). This type of information is conceptually distinct from continuous-time measurements of a physical system that (1.1) models. This type of information serves as a basis to improve the bounds obtained in Meslem & Ramdani (2011) and Moisan & Bernard (2005), for instance, which constructs bounds based on observers. Further, the bounding methods in Meslem & Ramdani (2011) and Moisan & Bernard (2005), still depend on an application of the classic 'Müller theorem,' of which the result in Scott & Barton (2013) is an extension.

The theory in Scott & Barton (2013) relies on differential inequalities, which in essence yields an IVP derived from (1.1) but involving parametric optimization problems. The implementation in Scott & Barton (2013) uses interval analysis to estimate the solutions of these optimization problems. This work will construct LPs to estimate the solutions of the necessary optimization problems. An added benefit of this is that the implementation developed in this work can handle, in a meaningful way, a polytopal set of admissible control values, which contrasts with the previous implementation in Scott & Barton (2013), and related work such as Singer & Barton (2006a), for example, which employed interval arithmetic and so could only meaningfully handle an interval set of admissible control values.

The rest of the article is as follows. Section 2 introduces notation and establishes the formal problem statement concerning the reachable set estimation. Section 3 establishes a few Lipschitz continuity results concerning parametric LPs which are useful in subsequent sections. Section 4 returns to the state bounding problem and demonstrates that estimates of the reachable set can be obtained from the solution of an IVP in ODEs with LPs embedded. Section 5 considers numerical aspects of the solution of ODEs with LPs embedded. In specific, Section 5.2 demonstrates how to construct appropriately parameterized affine relaxations to use in the embedded LPs. Section 6 applies this formulation to calculate state bounds for reacting chemical systems. Section 7 concludes with some final remarks.

2. Preliminaries and problem statement

The set of non-empty compact subsets of a metric space (X, d) is denoted $\mathbb{K}X$. Define the distance from a point x to a set Y in a metric space (X, d) by $d(x, Y) \equiv \inf_{y \in Y} d(x, y)$. The Hausdorff distance d_H between two sets Y, Z in the metric space (X, d) is given by

$$d_H(Y, Z) = \max\{\sup\{d(y, Z) : y \in Y\}, \sup\{d(z, Y) : z \in Z\}\}.$$

It is clear that if for all $y \in Y$ there exists a $z \in Z$ such that $d(y, z) \leqslant \delta$ and vice versa, then $d_H(Y, Z) \leqslant \delta$. The image of a set $S \subset X$ under a mapping $g : X \to Y$ is denoted $g(S)$. An open neighbourhood of a point x will typically be denoted $N(x)$; an open ϵ-ball around x will be denoted $B_\epsilon(x)$. For vectors $\mathbf{v}, \mathbf{w} \in \mathbb{R}^n$, the notation $\mathbf{v} \leqslant \mathbf{w}$ means that the inequality holds component-wise. Thus, given $\mathbf{v} \leqslant \mathbf{w}$, let $[\mathbf{v}, \mathbf{w}] = [v_1, w_1] \times \cdots \times [v_n, w_n]$ be an interval in $\mathbb{R}^n$. A vector of zeros will be denoted $\mathbf{0}$. A set-valued mapping S from the set X to the set of subsets of Y is denoted $S : X \rightrightarrows Y$. Statements which hold almost everywhere on a measurable set $T \subset \mathbb{R}$, i.e. except on a subset of Lebesgue measure zero, are abbreviated a.e. $t \in T$. For a measurable set $T \subset \mathbb{R}$, let $L^1(T)$ denote the set of Lebesgue-integrable functions $u : T \to \mathbb{R}$. Let $(L^1(T))^n$ denote the set of vector-valued functions $\mathbf{u} : T \to \mathbb{R}^n$ for which each of the components satisfy $u_i \in L^1(T)$.

The formal problem statement is as follows. Let $[t_0, t_f] = T \subset \mathbb{R}$, open $D_u \subset \mathbb{R}^{n_u}$, open $D \subset \mathbb{R}^{n_x}$, compact $U \subset D_u$, compact $X_0 \subset D$ and $\mathbf{f}: T \times D_u \times D \to \mathbb{R}^{n_x}$ be given. The goal is to compute functions $\mathbf{x}^L, \mathbf{x}^U : T \to \mathbb{R}^{n_x}$ such that $\mathbf{x}(t, \mathbf{u}, \mathbf{x}_0) \in [\mathbf{x}^L(t), \mathbf{x}^U(t)]$, $\forall (t, \mathbf{u}, \mathbf{x}_0) \in T \times \mathscr{U} \times X_0$, where $\mathscr{U} = \{\mathbf{u} \in (L^1(T))^{n_u} : \mathbf{u}(t) \in U, \text{a.e. } t \in T\}$ and $\mathbf{x}$ is a solution of

$$\begin{aligned} \dot{\mathbf{x}}(t, \mathbf{u}, \mathbf{x}_0) &= \mathbf{f}(t, \mathbf{u}(t), \mathbf{x}(t, \mathbf{u}, \mathbf{x}_0)), \quad \text{a.e. } t \in T, \\ \mathbf{x}(t_0, \mathbf{u}, \mathbf{x}_0) &= \mathbf{x}_0. \end{aligned} \tag{2.1}$$

Such a $\mathbf{x}^L$ and $\mathbf{x}^U$ are called state bounds, as in Scott & Barton (2013); the intervals $[\mathbf{x}^L(t), \mathbf{x}^U(t)]$ can also be thought of as enclosures of the reachable sets of the ODE system (2.1).

3. Parametric optimization

This section establishes Lipschitz continuity properties of parametric optimization problems that are necessary to satisfy the hypotheses of the bounding theory in Scott & Barton (2013). These results will also be useful to establish that the implementation is numerically tractable.

The following result, a form of which appears as Lemma 1 in Klatte & Kummer (1985), helps prove the main result of this section.

LEMMA 3.1 Let (X, d_X) and (Y, d_Y) be metric spaces. Assume $f : X \times Y \to \mathbb{R}$ and $M : Y \rightrightarrows X$ are mappings such that

1. M is non-empty valued,
2. $f(\cdot, y)$ attains its infimum on $M(y)$ for each $y \in Y$,
3. there exists $L_f > 0$ such that for all $(x_1, y_1), (x_2, y_2) \in X \times Y$, f satisfies $|f(x_1, y_1) - f(x_2, y_2)| \leqslant L_f(d_X(x_1, x_2) + d_Y(y_1, y_2))$,
4. there exists $L_M > 0$ such that for all y_1, y_2 in Y and for all $x_1 \in M(y_1)$, there exists $x_2 \in M(y_2)$ such that $d_X(x_1, x_2) \leqslant L_M d_Y(y_1, y_2)$.

Then $f_{\min} : Y \ni y \mapsto \min\{f(x, y) : x \in M(y)\}$ is Lipschitz continuous.

The following lemma concerns a Lipschitz property of polytopes with respect to perturbations of the right-hand side of the constraints. This is a well-established result in the literature (see Mangasarian & Shiau, 1987).

LEMMA 3.2 Let $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\mathbf{d} \in \mathbb{R}^m$, and

$$P(\mathbf{d}) = \{\mathbf{v} \in \mathbb{R}^n : \mathbf{A}\mathbf{v} \leqslant \mathbf{d}\}, \tag{3.1}$$

$$F = \{\mathbf{d} \in \mathbb{R}^m : P(\mathbf{d}) \neq \emptyset\}. \tag{3.2}$$

Then there exists $L_P \geqslant 0$ such that for all $\mathbf{d}_1, \mathbf{d}_2 \in F$ and all $\mathbf{v}_1 \in P(\mathbf{d}_1)$, there exists a $\mathbf{v}_2 \in P(\mathbf{d}_2)$ such that

$$\|\mathbf{v}_1 - \mathbf{v}_2\|_\infty \leqslant L_P \|\mathbf{d}_1 - \mathbf{d}_2\|$$

(for any norm $\|\cdot\|$).

Since the Hausdorff distance is a metric on $\mathbb{K}X$ (for some metric space (X,d)), when P defined in (3.1) is compact-valued, it follows from Lemma 3.2 that $P : F \to \mathbb{K}\mathbb{R}^n$ is Lipschitz continuous, with F defined in (3.2).

Finally, the following result concerning the local Lipschitz continuity of the optimal objective value of certain parametric optimization problems is established. See Appendix A for its proof.

PROPOSITION 3.1 Let P and F be defined as in Equations (3.1) and (3.2), respectively. Assume that $P(\mathbf{d})$ is bounded for all $\mathbf{d} \in F$. Let $I = \{1, \ldots, p\}$, and $\mathbf{c}_i \in \mathbb{R}^n$ for all $i \in I$. Let $\mathbf{c} = (\mathbf{c}_1, \ldots, \mathbf{c}_p) \in \mathbb{R}^{pn}$ and $\mathbf{h} = (h_1, \ldots, h_p) \in \mathbb{R}^p$. Define $\hat{q} : F \times \mathbb{R}^{pn} \times \mathbb{R}^p \to \mathbb{R}$ by

$$\begin{aligned} \hat{q}(\mathbf{d},\mathbf{c},\mathbf{h}) = \min_{\mathbf{v}\in\mathbb{R}^n} \max_{i\in I} \quad & \{\mathbf{c}_i^\top \mathbf{v} + h_i\} \\ \text{s.t.} \quad & \mathbf{A}\mathbf{v} \leqslant \mathbf{d}. \end{aligned} \tag{3.3}$$

Then $\hat{q}$ is locally Lipschitz continuous, i.e. for all $(\mathbf{d},\mathbf{c},\mathbf{h}) \in F \times \mathbb{R}^{pn} \times \mathbb{R}^p$ there exists an open neighbourhood $N(\mathbf{d},\mathbf{c},\mathbf{h})$ of $(\mathbf{d},\mathbf{c},\mathbf{h})$ and $L > 0$ such that

$$|\hat{q}(\mathbf{d}_1,\mathbf{c}_1,\mathbf{h}_1) - \hat{q}(\mathbf{d}_2,\mathbf{c}_2,\mathbf{h}_2)| \leqslant L\|(\mathbf{d}_1,\mathbf{c}_1,\mathbf{h}_1) - (\mathbf{d}_2,\mathbf{c}_2,\mathbf{h}_2)\|,$$

for all $(\mathbf{d}_1,\mathbf{c}_1,\mathbf{h}_1), (\mathbf{d}_2,\mathbf{c}_2,\mathbf{h}_2) \in N(\mathbf{d},\mathbf{c},\mathbf{h}) \cap F \times \mathbb{R}^{pn} \times \mathbb{R}^p$ (for any norm $\|\cdot\|$).

In the special case that the index set $I = \{1\}$, it is clear that optimization problem (3.3) is a LP parametrized by both its cost vector and right-hand side. In this case, results from, for instance, Wets (1985) shows that the optimal objective value is locally Lipschitz continuous. In the general case, the objective function of (3.3) is a convex piecewise affine function; consequently, it can be reformulated as the LP

$$\begin{aligned} \hat{q}(\mathbf{d},\mathbf{c},\mathbf{h}) = \min_{(\mathbf{v},z)\in\mathbb{R}^{n+1}} \quad & z \\ \text{s.t.} \quad & \mathbf{A}\mathbf{v} \leqslant \mathbf{d}, \\ & \mathbf{c}_i^\top \mathbf{v} + h_i \leqslant z,\ \forall i \in I. \end{aligned}$$

However, in this form, the parameterization is now influencing the constraints of the LP, which in general is less well behaved (see for instance Wets, 1985). Thus, rather than obscure the nice parametric properties just established, the parametric optimization problems of interest in this article are left in the form (3.3), and loosely referred to as ‘linear programs.’

4. State bounding

4.1 *An auxiliary IVP*

Sufficient conditions for two functions to constitute state bounds of (2.1) are established in Scott & Barton (2013). That paper also addresses how one can leverage an *a priori* enclosure to reduce the state bound overestimation. An *a priori* enclosure $G \subset \mathbb{R}^{n_x}$ is a rough enclosure of the solutions of (2.1): $\mathbf{x}(t,\mathbf{u},\mathbf{x}_0) \in G$, $\forall (t,\mathbf{u},\mathbf{x}_0) \in T \times \mathcal{U} \times X_0$. Depending on the dynamics, physical arguments, such as conservation of mass, may inspire this. When the ODEs (2.1) are the dynamics of a chemical kinetics model, one can often determine a convex polytopal G (Scott & Barton, 2010).

For the rest of this section assume there is a convex polytope G that is a rough enclosure for the solutions of (2.1), and that U is a compact convex polytope. Let $\mathbb{K}\mathbb{R}^{n_x}_P$ denote the set of non-empty compact convex polytopes in $\mathbb{R}^{n_x}$. Let $P_i^L, P_i^U : \mathbb{KR}_P^{n_x} \to \mathbb{KR}_P^{n_x}$ be given by

$$P_i^L(\hat{P}) = \{\mathbf{z} \in \hat{P} : z_i = \min\{\zeta_i : \boldsymbol{\zeta} \in \hat{P}\}\},$$
$$P_i^U(\hat{P}) = \{\mathbf{z} \in \hat{P} : z_i = \max\{\zeta_i : \boldsymbol{\zeta} \in \hat{P}\}\}.$$

Consider the system of ODEs

$$\begin{aligned} \dot{x}_i^L(t) &= q_i^L(t, \mathbf{x}^L(t), \mathbf{x}^U(t)) = \min\{f_i^{cv}(t, \mathbf{p}, \mathbf{z}, \mathbf{x}^L(t), \mathbf{x}^U(t)) : \mathbf{p} \in U, \mathbf{z} \in P_i^L([\mathbf{x}^L(t), \mathbf{x}^U(t)] \cap G)\}, \\ \dot{x}_i^U(t) &= q_i^U(t, \mathbf{x}^L(t), \mathbf{x}^U(t)) = \max\{f_i^{cc}(t, \mathbf{p}, \mathbf{z}, \mathbf{x}^L(t), \mathbf{x}^U(t)) : \mathbf{p} \in U, \mathbf{z} \in P_i^U([\mathbf{x}^L(t), \mathbf{x}^U(t)] \cap G)\}, \end{aligned} \tag{4.1}$$

for $i \in \{1, \ldots, n_x\}$, with initial conditions that satisfy $X_0 \subset [\mathbf{x}^L(t_0), \mathbf{x}^U(t_0)]$, where for each i, $f_i^{cv}(t, \cdot, \cdot, \mathbf{v}, \mathbf{w})$ is a convex piecewise affine under-estimator of $f_i(t, \cdot, \cdot)$ on $U \times P_i^L([\mathbf{v}, \mathbf{w}] \cap G)$ and $f_i^{cc}(t, \cdot, \cdot, \mathbf{v}, \mathbf{w})$ is a concave piecewise affine over-estimator of $f_i(t, \cdot, \cdot)$ on $U \times P_i^U([\mathbf{v}, \mathbf{w}] \cap G)$. Specifically, there exists a positive integer n_i^L, and for $k \in \{1, \ldots, n_i^L\}$, there exist $\mathbf{c}_k^{i,L}(t, \mathbf{v}, \mathbf{w}) \in \mathbb{R}^{n_u+n_x}$ and $h_k^{i,L}(t, \mathbf{v}, \mathbf{w}) \in \mathbb{R}$ such that

$$f_i^{cv}(t, \mathbf{p}, \mathbf{z}, \mathbf{v}, \mathbf{w}) = \max\{(\mathbf{c}_k^{i,L}(t, \mathbf{v}, \mathbf{w}))^\top \mathbf{y} + h_k^{i,L}(t, \mathbf{v}, \mathbf{w}) : k \in \{1, \ldots, n_i^L\}\} \leqslant f_i(t, \mathbf{p}, \mathbf{z}),$$

for each $\mathbf{y} = (\mathbf{p}, \mathbf{z}) \in U \times P_i^L([\mathbf{v}, \mathbf{w}] \cap G)$ (and similarly for f_i^{cc}, except it is taken as the point-wise minimum of a set of affine functions). It will now be shown that the solutions (if any) of (4.1) are state bounds for the system (2.1).

The goal is to apply Theorem 2 of Scott & Barton (2013). Its statement and a required assumption are repeated below (other assumptions that include a Lipschitz continuity condition on $\mathbf{f}$ are not repeated).

ASSUMPTION 4.1 Assume $D_\Omega \subset \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$ and for $i \in \{1, \ldots, n_x\}$, $\Omega_i^L, \Omega_i^U : D_\Omega \to \mathbb{KR}^{n_x}$ satisfy the following:

1. For any $(\mathbf{v}, \mathbf{w}) \in \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$, if there exists $(t, \mathbf{u}, \mathbf{x}_0) \in T \times \mathscr{U} \times X_0$ satisfying $\mathbf{x}(t, \mathbf{u}, \mathbf{x}_0) \in [\mathbf{v}, \mathbf{w}]$ and $x_i(t, \mathbf{u}, \mathbf{x}_0) = v_i$ (respectively, $x_i(t, \mathbf{u}, \mathbf{x}_0) = w_i$), then $(\mathbf{v}, \mathbf{w}) \in D_\Omega$ and $\mathbf{x}(t, \mathbf{u}, \mathbf{x}_0) \in \Omega_i^L(\mathbf{v}, \mathbf{w})$ (respectively, $\mathbf{x}(t, \mathbf{u}, \mathbf{x}_0) \in \Omega_i^U(\mathbf{v}, \mathbf{w})$).
2. For any $(\mathbf{v}, \mathbf{w}) \in D_\Omega$, there exists an open neighbourhood $N(\mathbf{v}, \mathbf{w})$ of $(\mathbf{v}, \mathbf{w})$ and $L > 0$ such that

$$d_H(\Omega_i^L(\mathbf{v}_1, \mathbf{w}_1), \Omega_i^L(\mathbf{v}_2, \mathbf{w}_2)) \leqslant L(\|\mathbf{v}_1 - \mathbf{v}_2\|_\infty + \|\mathbf{w}_1 - \mathbf{w}_2\|_\infty)$$

   for all $(\mathbf{v}_1, \mathbf{w}_1), (\mathbf{v}_2, \mathbf{w}_2) \in N(\mathbf{v}, \mathbf{w}) \cap D_\Omega$, and a similar statement for Ω_i^U also holds.

THEOREM 4.1 (Theorem 2 in Scott & Barton, 2013) Let $\mathbf{v}$, $\mathbf{w} : I \to \mathbb{R}^{n_x}$ be absolutely continuous functions satisfying:

1. For every $t \in T$ and every index i,
   (a) $(\mathbf{v}(t), \mathbf{w}(t)) \in D_\Omega$,
   (b) $\Omega_i^L(\mathbf{v}(t), \mathbf{w}(t)) \subset D$ and $\Omega_i^U(\mathbf{v}(t), \mathbf{w}(t)) \subset D$,
2. $X_0 \subset [\mathbf{v}(t_0), \mathbf{w}(t_0)]$,

3. For a.e. $t \in T$ and each index i,

   (a) $\dot{v}_i(t) \leqslant f_i(t, \mathbf{p}, \mathbf{z})$, for all $\mathbf{z} \in \Omega_i^L(\mathbf{v}(t), \mathbf{w}(t))$ and $\mathbf{p} \in U$,

   (b) $\dot{w}_i(t) \geqslant f_i(t, \mathbf{p}, \mathbf{z})$, for all $\mathbf{z} \in \Omega_i^U(\mathbf{v}(t), \mathbf{w}(t))$ and $\mathbf{p} \in U$,

then $\mathbf{x}(t, \mathbf{u}, \mathbf{x}_0) \in [\mathbf{v}(t), \mathbf{w}(t)]$, $\forall (t, \mathbf{u}, \mathbf{x}_0) \in T \times \mathscr{U} \times X_0$.

The main challenge is defining D_Ω, Ω_i^L, Ω_i^U such that Assumption 4.1 holds. It is shown that this is the case if one lets

$$\begin{aligned} D_\Omega &= \{(\mathbf{v}, \mathbf{w}) \in \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} : [\mathbf{v}, \mathbf{w}] \cap G \neq \emptyset\}, \\ \Omega_i^L(\mathbf{v}, \mathbf{w}) &= P_i^L([\mathbf{v}, \mathbf{w}] \cap G), \\ \Omega_i^U(\mathbf{v}, \mathbf{w}) &= P_i^U([\mathbf{v}, \mathbf{w}] \cap G). \end{aligned}$$

To see this, choose any $(\mathbf{v}, \mathbf{w}) \in D_\Omega$ and let

$$\begin{aligned} z_i^m(\mathbf{v}, \mathbf{w}) &= \min\{\zeta_i : \boldsymbol{\zeta} \in [\mathbf{v}, \mathbf{w}] \cap G)\}, \\ z_i^M(\mathbf{v}, \mathbf{w}) &= \max\{\zeta_i : \boldsymbol{\zeta} \in [\mathbf{v}, \mathbf{w}] \cap G)\} \end{aligned} \tag{4.2}$$

(note that $v_i \leqslant z_i^m(\mathbf{v}, \mathbf{w}) \leqslant z_i^M(\mathbf{v}, \mathbf{w}) \leqslant w_i$). If there exists $(t, \mathbf{u}, \mathbf{x}_0) \in T \times \mathscr{U} \times X_0$ such that $\mathbf{x}(t, \mathbf{u}, \mathbf{x}_0) \in [\mathbf{v}, \mathbf{w}]$, then $\mathbf{x}(t, \mathbf{u}, \mathbf{x}_0) \in [\mathbf{v}, \mathbf{w}] \cap G$ by definition of G, so $(\mathbf{v}, \mathbf{w}) \in D_\Omega$. Further, if $\mathbf{x}(t, \mathbf{u}, \mathbf{x}_0) \in [\mathbf{v}, \mathbf{w}] \cap G$ and $x_i(t, \mathbf{u}, \mathbf{x}_0) = v_i$, then $z_i^m(\mathbf{v}, \mathbf{w}) \leqslant x_i(t, \mathbf{u}, \mathbf{x}_0) = v_i \leqslant z_i^m(\mathbf{v}, \mathbf{w})$, so it is clear that $\mathbf{x}(t, \mathbf{u}, \mathbf{x}_0) \in P_i^L([\mathbf{v}, \mathbf{w}] \cap G)$. An analogous argument gives the condition for P_i^U.

To see that the second condition holds consider the nature of the sets $P_i^L([\mathbf{v}, \mathbf{w}] \cap G)$. Since G is a convex polytope it can be expressed as $G = \{\mathbf{z} \in \mathbb{R}^{n_x} : \mathbf{A}_G\mathbf{z} \leqslant \mathbf{b}_G\}$ for some $\mathbf{A}_G \in \mathbb{R}^{m_g \times n_x}$ and $\mathbf{b}_G \in \mathbb{R}^{m_g}$. Thus $[\mathbf{v}, \mathbf{w}] \cap G = \{\mathbf{z} : \mathbf{A}\mathbf{z} \leqslant \mathbf{b}(\mathbf{v}, \mathbf{w})\}$ where

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_G \\ -\mathbf{I} \\ \mathbf{I} \end{bmatrix}, \quad \mathbf{b}(\mathbf{v}, \mathbf{w}) = \begin{bmatrix} \mathbf{b}_G \\ -\mathbf{v} \\ \mathbf{w} \end{bmatrix}. \tag{4.3}$$

By Lemmas 3.2 and 3.1, z_i^m is a Lipschitz continuous function on D_Ω with Lipschitz constant L_1. Finally, noting that

$$\Omega_i^L(\mathbf{v}, \mathbf{w}) = P_i^L([\mathbf{v}, \mathbf{w}] \cap G) = \{\mathbf{z} : \mathbf{A}\mathbf{z} \leqslant \mathbf{b}(\mathbf{v}, \mathbf{w}), z_i \leqslant z_i^m(\mathbf{v}, \mathbf{w}), z_i \geqslant z_i^m(\mathbf{v}, \mathbf{w})\},$$

by Lemma 3.2 there exists $L_2 > 0$ such that

$$\begin{aligned} d_H(\Omega_i^L(\mathbf{v}_1, \mathbf{w}_1), \Omega_i^L(\mathbf{v}_2, \mathbf{w}_2)) &\leqslant L_2(\|\mathbf{b}(\mathbf{v}_1, \mathbf{w}_1) - \mathbf{b}(\mathbf{v}_2, \mathbf{w}_2)\|_\infty + 2|z_i^m(\mathbf{v}_1, \mathbf{w}_1) - z_i^m(\mathbf{v}_2, \mathbf{w}_2)|) \\ &\leqslant L_2(\|\mathbf{v}_1 - \mathbf{v}_2\|_\infty + \|\mathbf{w}_1 - \mathbf{w}_2\|_\infty + 2L_1(\|\mathbf{v}_1 - \mathbf{v}_2\|_\infty + \|\mathbf{w}_1 - \mathbf{w}_2\|_\infty)) \\ &\leqslant L_2(1 + 2L_1)(\|\mathbf{v}_1 - \mathbf{v}_2\|_\infty + \|\mathbf{w}_1 - \mathbf{w}_2\|_\infty) \end{aligned}$$

for all $(\mathbf{v}_1, \mathbf{w}_1), (\mathbf{v}_2, \mathbf{w}_2) \in D_\Omega$. Similar reasoning shows that the required Lipschitz condition holds for each Ω_i^U as well.

The rest of the hypotheses of Theorem 4.1 are easy to verify. Solutions of (4.1) are understood in the Carathéodory sense, and thus $\mathbf{x}^L$ and $\mathbf{x}^U$ are absolutely continuous. Meanwhile, any solutions that exist must satisfy $[\mathbf{x}^L(t), \mathbf{x}^U(t)] \cap G \neq \emptyset$ (otherwise the optimization problems are not defined), which implies that $(\mathbf{x}^L(t), \mathbf{x}^U(t)) \in D_\Omega$. Further, the objective functions of the optimization problems are assumed to be affine under-estimators of $f_i(t, \cdot, \cdot)$ on $U \times P_i^L([\mathbf{x}^L(t), \mathbf{x}^U(t)] \cap G)$, implying that $P_i^L([\mathbf{x}^L(t), \mathbf{x}^U(t)] \cap G) = \Omega_i^L(\mathbf{x}^L(t), \mathbf{x}^U(t)) \subset D$ (and similarly for Ω_i^U). It is already assumed that the initial conditions satisfy Hypothesis 2 of Theorem 4.1, and clearly Hypothesis 3 is satisfied. Thus, any solutions of (4.1) are state bounds.

4.2 *Convergence*

This section considers the convergence of the state bounds constructed in Section 4.1 as the 'sizes' of the sets of admissible control values and initial conditions decrease. To begin, it is necessary to abuse notation in this section and allow the state bounds $\mathbf{x}^L$, $\mathbf{x}^U$ to have dependence on the sets of control values and initial conditions. That is to say, assume $[\mathbf{x}^L(t, U', X_0'), \mathbf{x}^U(t, U', X_0')] \ni \mathbf{x}(t, \mathbf{u}, \mathbf{x}_0)$, for any $(t, \mathbf{u}, \mathbf{x}_0) \in T \times \mathscr{U}' \times X_0'$, any solution $\mathbf{x}$ of IVP (2.1) (where $\mathscr{U}' = \{\mathbf{u} \in (L^1(T))^{n_u} : \mathbf{u}(t) \in U', \text{a.e. } t \in T\}$), and any compact convex polytope $U' \subset U$ and compact $X_0' \subset X_0$. For simplicity, write $X^B(t, U', X_0') = [\mathbf{x}^L(t, U', X_0'), \mathbf{x}^U(t, U', X_0')]$. Similarly, let the functions $\mathbf{q}^L$, $\mathbf{q}^U$ defining the dynamics in the auxiliary ODE system (4.1) have dependence on the polytopal set of control values U'.

Next, make the following definitions (taken from Chapter 3 of Schaber, 2014).

Definition 4.1 For $Y \subset \mathbb{R}^n$, denote the set of non-empty interval subsets of Y by $\mathbb{I}Y \equiv \{[\mathbf{v}, \mathbf{w}] : \mathbf{v} \leqslant \mathbf{w}, [\mathbf{v}, \mathbf{w}] \subset Y\}$. Denote the interval hull (the intersection of all interval supersets) of a set Y by $\square Y$. The width of a set Y is denoted $w(Y) \equiv \sup\{\|\mathbf{y}_1 - \mathbf{y}_2\|_\infty : \mathbf{y}_1, \mathbf{y}_2 \in Y\}$. If there exist τ, $\beta > 0$ such that

$$d_H(\square \mathbf{x}(t, \mathscr{U}', X_0'), X^B(t, U', X_0')) \leqslant \tau w(U' \times X_0')^\beta \quad \forall (t, U', X_0') \in T \times \mathbb{I}U \times \mathbb{I}X_0,$$

where $\mathscr{U}' = \{\mathbf{u} \in (L^1(T))^{n_u} : \mathbf{u}(t) \in U', \text{a.e. } t \in T\}$, then X^B is said to have Hausdorff convergence in $U \times X_0$ of order β with prefactor τ uniformly on T.

The next result establishes that the state bounds constructed in Section 4.1 have Hausdorff convergence in $U \times X_0$ of order at least 1 uniformly on T (with some prefactor). More colloquially, the state bounds are said to converge at least linearly with respect to the uncertain initial conditions and admissible control values. To simplify the discussion, the following result depends on the assumption that there exist state bounds that are known *a priori* to converge at least linearly. An example of such bounds are the 'naïve' state bounds in Definition 3.4.3 in Schaber (2014), where the functions $\tilde{\mathbf{u}}$ and $\tilde{\mathbf{o}}$ defining the dynamics of the IVP (4.4) below are the lower and upper bounds, respectively, of the natural interval extension of $\mathbf{f}$. (Although the naïve state bounds in Schaber, 2014 are for parametric ODEs instead of control systems, a modification of the proof of Theorem 3.4.9 in Schaber (2014) shows that these state bounds are also first-order convergent for control systems.) Meanwhile, Condition (4.5) is satisfied as long as interval bounds on f_i are included in the definition of the piecewise affine estimators f_i^{cv}, f_i^{cc}. Since the affine relaxation method described in Section 5.2 requires simultaneous evaluation of interval bounds, this is easily satisfied.

Proposition 4.1 Let $\tilde{\mathbf{u}}, \tilde{\mathbf{o}} : T \times \mathbb{I}D \times \mathbb{I}U \to \mathbb{R}^{n_x}$ be locally Lipschitz continuous and monotonic in the sense that

$$\tilde{\mathbf{u}}(t, [\mathbf{v}, \mathbf{w}], U') \leqslant \tilde{\mathbf{u}}(t, [\mathbf{v}', \mathbf{w}'], U'), \text{ and } \tilde{\mathbf{o}}(t, [\mathbf{v}', \mathbf{w}'], U') \leqslant \tilde{\mathbf{o}}(t, [\mathbf{v}, \mathbf{w}], U'),$$
$$\text{a.e. } t \in T \quad \forall ([\mathbf{v}, \mathbf{w}], [\mathbf{v}', \mathbf{w}'], U') \in \mathbb{I}D \times \mathbb{I}D \times \mathbb{I}U : [\mathbf{v}', \mathbf{w}'] \subset [\mathbf{v}, \mathbf{w}].$$

Suppose that for all $(U', X_0') \in \mathbb{I}U \times \mathbb{I}X_0$, $\tilde{\mathbf{v}}, \tilde{\mathbf{w}} : T \times \mathbb{I}U \times \mathbb{I}X_0 \to \mathbb{R}^{n_x}$ are solutions of

$$\begin{aligned}\dot{\tilde{\mathbf{v}}}(t, U', X_0') &= \tilde{\mathbf{u}}(t, [\tilde{\mathbf{v}}(t, U', X_0'), \tilde{\mathbf{w}}(t, U', X_0')], U'),\\ \dot{\tilde{\mathbf{w}}}(t, U', X_0') &= \tilde{\mathbf{o}}(t, [\tilde{\mathbf{v}}(t, U', X_0'), \tilde{\mathbf{w}}(t, U', X_0')], U'),\end{aligned} \tag{4.4}$$

with initial conditions that satisfy $[\tilde{\mathbf{v}}(t_0, U', X_0'), \tilde{\mathbf{w}}(t_0, U', X_0')] \supset [\mathbf{x}^L(t_0, U', X_0'), \mathbf{x}^U(t_0, U', X_0')]$. Assume that $\tilde{\mathbf{v}}(\cdot, U', X_0')$, $\tilde{\mathbf{w}}(\cdot, U', X_0')$ are state bounds for the solutions of (2.1) and that $\tilde{\mathbf{v}}$ and $\tilde{\mathbf{w}}$ have Hausdorff convergence in $U \times X_0$ of order 1 uniformly in T:

$$d_H\left(\Box\mathbf{x}(t, \mathscr{U}', X_0'), [\tilde{\mathbf{v}}(t, U', X_0'), \tilde{\mathbf{w}}(t, U', X_0')]\right) \leqslant \tau w(U' \times X_0') \quad \forall (t, U', X_0') \in T \times \mathbb{I}U \times \mathbb{I}X_0.$$

Assume that

$$\begin{aligned}&[\mathbf{q}^L(t, \mathbf{v}, \mathbf{w}, U'), \mathbf{q}^U(t, \mathbf{v}, \mathbf{w}, U')] \subset [\tilde{\mathbf{u}}(t, [\mathbf{v}, \mathbf{w}], U'), \tilde{\mathbf{o}}(t, [\mathbf{v}, \mathbf{w}], U')],\\ &\text{a.e. } t \in T \quad \forall ([\mathbf{v}, \mathbf{w}], U') \in \mathbb{I}D \times \mathbb{I}U.\end{aligned} \tag{4.5}$$

Then the state bounds $\mathbf{x}^L$, $\mathbf{x}^U$ constructed in Section 4.1 (the solutions, if any, of the IVP (4.1)), have Hausdorff convergence in $U \times X_0$ of order 1 uniformly in T.

Proof. By Theorem 3.4.6 of Schaber (2014), we have

$$[\tilde{\mathbf{v}}(t, U', X_0'), \tilde{\mathbf{w}}(t, U', X_0')] \supset [\mathbf{x}^L(t, U', X_0'), \mathbf{x}^U(t, U', X_0')]$$

for all $(t, U', X_0') \in T \times \mathbb{I}U \times \mathbb{I}X_0$. Since both are state bounds,

$$d_H(\Box\mathbf{x}(t, \mathscr{U}', X_0'), [\mathbf{x}^L(t, U', X_0'), \mathbf{x}^U(t, U', X_0')]) \leqslant d_H(\Box\mathbf{x}(t, \mathscr{U}', X_0'), [\tilde{\mathbf{v}}(t, U', X_0'), \tilde{\mathbf{w}}(t, U', X_0')]),$$

and so by the assumption on the convergence of $\tilde{\mathbf{v}}$ and $\tilde{\mathbf{w}}$, we also have that $\mathbf{x}^L$ and $\mathbf{x}^U$ have Hausdorff convergence in $U \times X_0$ of order 1 uniformly in T. □

5. ODEs with LPs embedded

This section will analyse the IVP (4.1) that must be solved to obtain state bounds. Specifically, it will consider how to construct the convex and concave piecewise affine under and over-estimators of the dynamics as well as the numerical solution.

The system (4.1) is indeed an IVP in ODEs, where the dynamics are given by parametric optimization problems. Consider the equations defining $\dot{x}_i^L(t)$ for example. As discussed as the end of Section 3, since the objective function $f_i^{cv}(t, \cdot, \cdot, \mathbf{x}^L(t), \mathbf{x}^U(t))$ is a convex piecewise affine function, and the feasible set $U \times P_i^L([\mathbf{x}^L(t), \mathbf{x}^U(t)] \cap G)$ is a polytope, this is equivalent to a parametric linear optimization problem. Further, because the parameterization of this LP depends on the dynamic states $(\mathbf{x}^L(t), \mathbf{x}^U(t))$, these LPs must be solved along with the dynamic states during the integration routine. This is the essence of 'ODEs with LPs embedded.'

This formulation is similar to others that have appeared in the literature; see for instance, the work on complementarity systems (Schumacher, 2004) and differential variational inequalities (Pang & Stewart, 2008). However, much of the work on these problems is slightly more general than necessary to understand and efficiently solve the IVP (4.1). Instead, the approach taken here will be to establish that, under mild assumptions, standard numerical integration routines and LP solvers can be used to solve the IVP of interest.

5.1 *Lipschitz continuity of dynamics*

First, it will be established that the dynamics of the IVP (4.1) satisfy a Lipschitz continuity condition. The purpose is to establish that the IVP (4.1) is amenable to solution by many different classes of numerical integration methods, including implicit and explicit Runge–Kutta and linear multistep methods; see for example, Lambert (1991).

To achieve this, define the following parametric optimization problems which define the dynamics in Equation (4.1):

$$q_i^L(t,\mathbf{v},\mathbf{w}) = \min\{f_i^{cv}(t,\mathbf{p},\mathbf{z},\mathbf{v},\mathbf{w}) : \mathbf{p} \in U, \mathbf{z} \in P_i^L([\mathbf{v},\mathbf{w}] \cap G)\}, \tag{5.1}$$

$$q_i^U(t,\mathbf{v},\mathbf{w}) = \max\{f_i^{cc}(t,\mathbf{p},\mathbf{z},\mathbf{v},\mathbf{w}) : \mathbf{p} \in U, \mathbf{z} \in P_i^U([\mathbf{v},\mathbf{w}] \cap G)\}. \tag{5.2}$$

Analyse the LP (5.1) (the analysis for LP (5.2) is similar). Since U is a polytope, there exist a matrix $\mathbf{A}_U \in \mathbb{R}^{m_u \times n_u}$ and vector $\mathbf{b}_U \in \mathbb{R}^{m_u}$ such that the feasible set of (5.1) can be rewritten as

$$U \times P_i^L([\mathbf{v},\mathbf{w}] \cap G) = \{(\mathbf{p},\mathbf{z}) \in \mathbb{R}^{n_u} \times \mathbb{R}^{n_x} : \mathbf{A}_U\mathbf{p} \leqslant \mathbf{b}_U, \mathbf{A}\mathbf{z} \leqslant \mathbf{b}(\mathbf{v},\mathbf{w}), z_i \leqslant z_i^m(\mathbf{v},\mathbf{w}), z_i \geqslant z_i^m(\mathbf{v},\mathbf{w})\},$$

where $\mathbf{A}$ and $\mathbf{b}$ are given by Equation (4.3) and z_i^m is given by Equation (4.2). For brevity, write this as

$$U \times P_i^L([\mathbf{v},\mathbf{w}] \cap G) = \{\mathbf{y} \in \mathbb{R}^{n_u+n_x} : \mathbf{A}_i^L\mathbf{y} \leqslant \mathbf{b}_i^L(\mathbf{v},\mathbf{w})\}.$$

By the discussion in Section 4, z_i^m is a Lipschitz continuous function on D_Ω. Thus, it is clear that $\mathbf{b}_i^L$ is as well.

Next, by definition, for some integer n_i^L, there are functions $\mathbf{c}^{i,L} : T \times D_\Omega \to \mathbb{R}^{n_i^L(n_u+n_x)}$ and $\mathbf{h}^{i,L} : T \times D_\Omega \to \mathbb{R}^{n_i^L}$ such that

$$f_i^{cv}(t,\mathbf{p},\mathbf{z},\mathbf{v},\mathbf{w}) = \max\{(\mathbf{c}_k^{i,L}(t,\mathbf{v},\mathbf{w}))^\top\mathbf{y} + h_k^{i,L}(t,\mathbf{v},\mathbf{w}) : k \in \{1,\ldots,n_i^L\}\},$$

where $\mathbf{y} = (\mathbf{p},\mathbf{z})$ and $\mathbf{c}^{i,L} = (\mathbf{c}_1^{i,L},\ldots,\mathbf{c}_{n_i^L}^{i,L})$. Furthermore, assume that these functions are locally Lipschitz continuous in the specific sense that for all $(\mathbf{v},\mathbf{w}) \in D_\Omega$ there exists a neighbourhood $N_c^i(\mathbf{v},\mathbf{w})$ and $L_c^i > 0$ such that

$$\|\mathbf{c}^{i,L}(t,\mathbf{v}_1,\mathbf{w}_1) - \mathbf{c}^{i,L}(t,\mathbf{v}_2,\mathbf{w}_2)\| \leqslant L_c^i\|(\mathbf{v}_1,\mathbf{w}_1) - (\mathbf{v}_2,\mathbf{w}_2)\|, \tag{5.3}$$

for all $(\mathbf{v}_1,\mathbf{w}_1)$, $(\mathbf{v}_2,\mathbf{w}_2) \in N_c^i(\mathbf{v},\mathbf{w}) \cap D_\Omega$ and all $t \in T$. As well, assume that the image of $T \times N_c^i(\mathbf{v},\mathbf{w}) \cap D_\Omega$ under $\mathbf{c}^{i,L}$ is bounded. Assume that similar conditions hold for $\mathbf{h}^{i,L}$. Section 5.2 will discuss how to construct piecewise affine relaxations to ensure that this holds.

If

$$\tilde{q}_i^L(\tilde{\mathbf{b}},\tilde{\mathbf{c}},\tilde{\mathbf{h}}) = \min\{\max\{(\tilde{\mathbf{c}}_k^\top\mathbf{y} + \tilde{h}_k : k \in \{1,\ldots,n_i^L\}\} : \mathbf{y} \in \mathbb{R}^{n_u+n_x}, \mathbf{A}_i^L\mathbf{y} \leqslant \tilde{\mathbf{b}}\}, \tag{5.4}$$

then $q_i^L(t,\mathbf{v},\mathbf{w}) = \tilde{q}_i^L(\mathbf{b}_i^L(\mathbf{v},\mathbf{w}),\mathbf{c}^{i,L}(t,\mathbf{v},\mathbf{w}),\mathbf{h}^{i,L}(t,\mathbf{v},\mathbf{w}))$. Let F_i^L be the set of $\tilde{\mathbf{b}}$ such that the feasible set of optimization problem (5.4) is non-empty. It is easy to see that F_i^L is a closed set; see Section 4.7 of Bertsimas & Tsitsiklis (1997). Then for all $\tilde{\mathbf{b}} \in F_i^L$, (5.4) is an optimization problem with a convex piecewise affine objective over a non-empty, bounded polytopal set. Consequently, one can apply Proposition 3.1 to see that $\tilde{q}_i^L$ is locally Lipschitz continuous on $F_i^L \times \mathbb{R}^{n_i^L(n_u+n_x)} \times \mathbb{R}^{n_i^L}$. This implies that $\tilde{q}_i^L$ is Lipschitz continuous on any compact subset of $F_i^L \times \mathbb{R}^{n_i^L(n_u+n_x)} \times \mathbb{R}^{n_i^L}$. Then, choose $(\mathbf{v},\mathbf{w}) \in D_\Omega$. Let $N(\mathbf{v},\mathbf{w})$ be a neighbourhood so that the Lipschitz conditions such as Inequality (5.3) hold for $\mathbf{c}^{i,L}$ and $\mathbf{h}^{i,L}$. Let K_i^L be the closure of $\mathbf{b}_i^L(N(\mathbf{v},\mathbf{w}) \cap D_\Omega) \times \mathbf{c}^{i,L}(T \times N(\mathbf{v},\mathbf{w}) \cap D_\Omega) \times \mathbf{h}^{i,L}(T \times N(\mathbf{v},\mathbf{w}) \cap D_\Omega)$. Note that K_i^L is a bounded subset of $F_i^L \times \mathbb{R}^{n_i^L(n_u+n_x)} \times \mathbb{R}^{n_i^L}$, using the Lipschitz continuity of $\mathbf{b}_i^L$ and the boundedness property of $\mathbf{c}^{i,L}$ and $\mathbf{h}^{i,L}$. Thus, K_i^L is a compact subset of $F_i^L \times \mathbb{R}^{n_i^L(n_u+n_x)} \times \mathbb{R}^{n_i^L}$, and thus there exists a $L_q > 0$ such that

$$|q_i^L(t, \mathbf{v}_1, \mathbf{w}_1) - q_i^L(t, \mathbf{v}_2, \mathbf{w}_2)| \leqslant L_q(\|\mathbf{b}_i^L(\mathbf{v}_1, \mathbf{w}_1) - \mathbf{b}_i^L(\mathbf{v}_2, \mathbf{w}_2)\|_\infty + \|\mathbf{c}^{i,L}(t, \mathbf{v}_1, \mathbf{w}_1) - \mathbf{c}^{i,L}(t, \mathbf{v}_2, \mathbf{w}_2)\|_\infty + \|\mathbf{h}^{i,L}(t, \mathbf{v}_1, \mathbf{w}_1) - \mathbf{h}^{i,L}(t, \mathbf{v}_2, \mathbf{w}_2)\|_\infty),$$

for all $(\mathbf{v}_1, \mathbf{w}_1), (\mathbf{v}_2, \mathbf{w}_2) \in N(\mathbf{v}, \mathbf{w}) \cap D_\Omega$ and all $t \in T$. Using the Lipschitz continuity of $\mathbf{b}_i^L$ and Inequality (5.3), for instance, one sees that for each i and for all $(\mathbf{v}, \mathbf{w}) \in D_\Omega$ there exists a neighbourhood $N_i^L(\mathbf{v}, \mathbf{w})$ and $L_i^L > 0$ such that

$$|q_i^L(t, \mathbf{v}_1, \mathbf{w}_1) - q_i^L(t, \mathbf{v}_2, \mathbf{w}_2)| \leqslant L_i^L\|(\mathbf{v}_1, \mathbf{w}_1) - (\mathbf{v}_2, \mathbf{w}_2)\|,$$

for all $(\mathbf{v}_1, \mathbf{w}_1)$, $(\mathbf{v}_2, \mathbf{w}_2) \in N_i^L(\mathbf{v}, \mathbf{w}) \cap D_\Omega$ and all $t \in T$. Similar analysis establishes that q_i^U is locally Lipschitz continuous in the same way.

Consequently, one can apply many different classes of numerical integration methods to solve the IVP (4.1); as mentioned earlier this includes implicit and explicit Runge–Kutta and linear multistep methods. The benefit of this is that one can rely on the sophisticated automatic error control of implementations of these methods by adaptive time stepping. The result is that a highly accurate numerical solution of the IVP (4.1) can be obtained, although without outward rounding techniques, these solutions will not be 'validated' in the sense of Lin & Stadtherr (2007).

5.2 *Parametric affine relaxations*

It was assumed in Section 5.1 that one had appropriate convex and concave piecewise affine relaxations of the original dynamics $\mathbf{f}$. This section addresses how to construct such relaxations. It is inspired by the relaxation and subgradient propagation rules developed for McCormick relaxations described in Mitsos *et al.* (2009). It should be stressed, however, that those rules are not acceptable in the current application since the subgradients constructed are not in general continuous (since they are subgradients to potentially non-smooth functions). Similarly, the affine relaxation method in Wang & Chang (1996) cannot be used. Meanwhile, the affine relaxations developed in this section are locally Lipschitz continuous with respect to the endpoints of the interval on which they are relaxations, as required by Section 5.1.

The only assumption necessary in this section is that $\mathbf{f}$ is a 'factorable' function. As defined by Mitsos *et al.* (2009), a function is factorable if it can be written as a finite recursive composition of binary sums, binary products, and operations from a given library of univariate intrinsic functions (for a slightly more refined definition, see Chapter 2 of Scott, 2012). In effect, this definition includes almost any function that can be expressed with a standard library for computer arithmetic.

The following lemmata are useful for establishing local Lipschitz continuity of functions of the form that will be used in the construction of the affine relaxations.

LEMMA 5.1 Let $Z \subset \mathbb{R}^n$ be a non-empty set such that for each $\mathbf{z} \in Z$, there exists an open neighbourhood of $\mathbf{z}$, $C(\mathbf{z})$, such that $C(\mathbf{z}) \cap Z$ is convex. Let $\mathbf{c}_1$ and $\mathbf{c}_2$ be locally Lipschitz continuous mappings $Z \to \mathbb{R}^m$, and s be a locally Lipschitz continuous mapping $Z \to \mathbb{R}$. Define $\mathbf{c}_3 : Z \to \mathbb{R}^m$ by

$$\mathbf{c}_3(\mathbf{z}) = \begin{cases} s(\mathbf{z})\mathbf{c}_1(\mathbf{z}) & \text{if } s(\mathbf{z}) \geqslant 0, \\ s(\mathbf{z})\mathbf{c}_2(\mathbf{z}) & \text{otherwise.} \end{cases}$$

Then $\mathbf{c}_3$ is a locally Lipschitz continuous mapping on Z.

Proof. The idea of the following proof is that the product of locally Lipschitz continuous functions is locally Lipschitz continuous; although the definition of $\mathbf{c}_3$ involves an 'if' statement, the function is continuous across this transition since both branches are zero at the transition.

In detail, choose any $\mathbf{z} \in Z$. By assumption, choose $\epsilon > 0$ such that s, $\mathbf{c}_1$ and $\mathbf{c}_2$ are Lipschitz continuous with constants L_s, L_1 and L_2, respectively, on $B_\epsilon(\mathbf{z}) \cap Z$. Since it is an open ball in a normed space, $B_\epsilon(\mathbf{z})$ is an open, convex set. Again by assumption, there exists an open neighbourhood $C(\mathbf{z})$ such that $C(\mathbf{z}) \cap Z$ is convex. Let $N(\mathbf{z}) = B_\epsilon(\mathbf{z}) \cap C(\mathbf{z}) \cap Z$, which is also an open, convex neighbourhood of $\mathbf{z}$ in Z. Then using the 'reverse' triangle inequality one sees that, for instance, $\|\mathbf{c}_1(\mathbf{z}')\| \leqslant \|\mathbf{c}_1(\mathbf{z})\| + L_1\epsilon$, for all $\mathbf{z} \in N(\mathbf{z})$. Thus, for some M_1, M_2, $M_s \in \mathbb{R}$, one has

$$\begin{aligned}
\sup\{\|\mathbf{c}_1(\mathbf{z}')\| : \mathbf{z}' \in N(\mathbf{z})\} &\leqslant M_1, \quad \text{and similarly} \\
\sup\{\|\mathbf{c}_2(\mathbf{z}')\| : \mathbf{z}' \in N(\mathbf{z})\} &\leqslant M_2, \quad \text{and} \\
\sup\{|s(\mathbf{z}')| : \mathbf{z}' \in N(\mathbf{z})\} &\leqslant M_s.
\end{aligned}$$

Then for any $\mathbf{z}_1$, $\mathbf{z}_2 \in N(\mathbf{z})$ such that $s(\mathbf{z}_1)$ and $s(\mathbf{z}_2)$ are both non-negative,

$$\begin{aligned}
\|\mathbf{c}_3(\mathbf{z}_1) - \mathbf{c}_3(\mathbf{z}_2)\| &= \|s(\mathbf{z}_1)\mathbf{c}_1(\mathbf{z}_1) - s(\mathbf{z}_2)\mathbf{c}_1(\mathbf{z}_2)\| \\
&\leqslant \|s(\mathbf{z}_1)\mathbf{c}_1(\mathbf{z}_1) - s(\mathbf{z}_1)\mathbf{c}_1(\mathbf{z}_2)\| + \|s(\mathbf{z}_1)\mathbf{c}_1(\mathbf{z}_2) - s(\mathbf{z}_2)\mathbf{c}_1(\mathbf{z}_2)\| \\
&\leqslant M_s\|\mathbf{c}_1(\mathbf{z}_1) - \mathbf{c}_1(\mathbf{z}_2)\| + M_1|s(\mathbf{z}_1) - s(\mathbf{z}_2)| \\
&\leqslant (M_sL_1 + M_1L_s)\|\mathbf{z}_1 - \mathbf{z}_2\|.
\end{aligned}$$

Similarly, if $s(\mathbf{z}_1)$ and $s(\mathbf{z}_2)$ are both non-positive,

$$\|\mathbf{c}_3(\mathbf{z}_1) - \mathbf{c}_3(\mathbf{z}_2)\| \leqslant (M_sL_2 + M_2L_s)\|\mathbf{z}_1 - \mathbf{z}_2\|.$$

Consider the case that $s(\mathbf{z}_1)$ and $s(\mathbf{z}_2)$ have different signs. Consider $\tilde{s} : [0, 1] \ni \lambda \mapsto s(\lambda\mathbf{z}_1 + (1 - \lambda)\mathbf{z}_2)$. Clearly $\tilde{s}$ is a continuous function which changes sign, thus there exists a $\lambda' \in [0, 1]$ at which $\tilde{s}(\lambda') = 0$. Since $N(\mathbf{z})$ is convex, the point $\mathbf{z}' = (\lambda')\mathbf{z}_1 + (1 - \lambda')\mathbf{z}_2$ is in $N(\mathbf{z})$. Also, $\mathbf{c}_3(\mathbf{z}') = \mathbf{0}$, and for $i = 1, 2$, $\|\mathbf{z}_i - \mathbf{z}'\| \leqslant \|\mathbf{z}_1 - \mathbf{z}_2\|$. Consequently,

$$\begin{aligned}
\|\mathbf{c}_3(\mathbf{z}_1) - \mathbf{c}_3(\mathbf{z}_2)\| &\leqslant \|\mathbf{c}_3(\mathbf{z}_1) - \mathbf{0}\| + \|\mathbf{0} - \mathbf{c}_3(\mathbf{z}_2)\| \\
&\leqslant \|\mathbf{c}_3(\mathbf{z}_1) - \mathbf{c}_3(\mathbf{z}')\| + \|\mathbf{c}_3(\mathbf{z}') - \mathbf{c}_3(\mathbf{z}_2)\| \\
&\leqslant (M_sL_1 + M_1L_s)\|\mathbf{z}_1 - \mathbf{z}'\| + (M_sL_2 + M_2L_s)\|\mathbf{z}_2 - \mathbf{z}'\| \\
&\leqslant (M_sL_1 + M_1L_s + M_sL_2 + M_2L_s)\|\mathbf{z}_1 - \mathbf{z}_2\|.
\end{aligned}$$

Clearly this Lipschitz constant holds for all $\mathbf{z}_1$, $\mathbf{z}_2 \in N(\mathbf{z})$, no matter what the signs of $s(\mathbf{z}_1)$ and $s(\mathbf{z}_2)$ are, and so $\mathbf{c}_3$ is locally Lipschitz continuous. □

LEMMA 5.2 Let $Z \subset \mathbb{R}^n$ be a non-empty open set. Let $H = \{(\mathbf{v}, \mathbf{w}) \in \mathbb{R}^n \times \mathbb{R}^n : \mathbf{v} \leqslant \mathbf{w}\}$. Let $Z^{\mathbb{I}} = \{(\mathbf{v}, \mathbf{w}) \in H : [\mathbf{v}, \mathbf{w}] \subset Z\}$. Then for all $(\mathbf{v}, \mathbf{w}) \in Z^{\mathbb{I}}$, there exists an open neighbourhood of $(\mathbf{v}, \mathbf{w})$, $C(\mathbf{v}, \mathbf{w})$, such that $C(\mathbf{v}, \mathbf{w}) \cap Z^{\mathbb{I}}$ is convex.

Proof. Choose $(\mathbf{v}, \mathbf{w}) \in Z^{\mathbb{I}}$. Since Z is open, for each $\mathbf{z} \in [\mathbf{v}, \mathbf{w}]$, there exists an open ball $B_{\epsilon'}(\mathbf{z})$ around $\mathbf{z}$ (with radius ϵ' which may depend on $\mathbf{z}$) which is a subset of Z. The set of all such open balls is an open cover of $[\mathbf{v}, \mathbf{w}]$; since $[\mathbf{v}, \mathbf{w}]$ is compact, there is a finite subcover. Thus, there exists an $\epsilon > 0$ such that for each $\mathbf{z} \in [\mathbf{v}, \mathbf{w}]$, $B_\epsilon(\mathbf{z})$ is a subset of Z. Consequently, if $\mathbf{v}' \in B_\epsilon(\mathbf{v})$, $\mathbf{w}' \in B_\epsilon(\mathbf{w})$ and $\mathbf{v}' \leqslant \mathbf{w}'$, it follows that for each $\mathbf{z}' \in [\mathbf{v}', \mathbf{w}']$, there exists a $\mathbf{z} \in [\mathbf{v}, \mathbf{w}]$ such that $\mathbf{z}' \in B_\epsilon(\mathbf{z})$, and so $[\mathbf{v}', \mathbf{w}'] \subset Z$. Thus $(B_\epsilon(\mathbf{v}) \times B_\epsilon(\mathbf{w})) \cap H$ is a subset of $Z^{\mathbb{I}}$. Let $\delta > 0$ be such that $B_\delta(\mathbf{v}, \mathbf{w}) \subset B_\epsilon(\mathbf{v}) \times B_\epsilon(\mathbf{w})$. Finally, since H is a halfspace in $\mathbb{R}^{n+n}$, and $B_\delta(\mathbf{v}, \mathbf{w})$ is an open ball in a normed space, both are convex, and thus so is their intersection. Therefore, let $C(\mathbf{v}, \mathbf{w}) = B_\delta(\mathbf{v}, \mathbf{w})$, and note that $B_\delta(\mathbf{v}, \mathbf{w}) \cap Z^{\mathbb{I}} = B_\delta(\mathbf{v}, \mathbf{w}) \cap H$, since $Z^{\mathbb{I}} \subset H$ by definition and $B_\delta(\mathbf{v}, \mathbf{w}) \cap H \subset (B_\epsilon(\mathbf{v}) \times B_\epsilon(\mathbf{w})) \cap H \subset Z^{\mathbb{I}}$. □

Next, a multivariate composition result is proved. The usual operations of addition, multiplication, and univariate composition can be seen as instances of multivariate composition. Furthermore, this approach allows more flexibility to define tight affine relaxations. This result requires locally Lipschitz continuous bounds (e.g., g_i^L and g_i^U), however, these are readily available for factorable functions via interval analysis; see for instance Section 2.5 of Scott (2012) for discussion of the regularity of interval extensions.

Proposition 5.1 Let $Z \subset \mathbb{R}^n$ be a non-empty open set and let $Y \subset \mathbb{R}^m$. Let $\mathbf{g} : Z \to \mathbb{R}^m$ and $s : Y \to \mathbb{R}$. Define $Z^{\mathbb{I}} = \{(\mathbf{v}, \mathbf{w}) \in \mathbb{R}^n \times \mathbb{R}^n : \mathbf{v} \leqslant \mathbf{w}, [\mathbf{v}, \mathbf{w}] \subset Z\}$, 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 $Z^{\mathbb{I}} \to \mathbb{R}^n$ and g_i^{bl}, g_i^{bu}, g_i^L, g_i^U be locally Lipschitz continuous mappings $Z^{\mathbb{I}} \to \mathbb{R}$ which satisfy

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

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

$$
\mathbf{s}^{al}(\mathbf{v}', \mathbf{w}')^\top \mathbf{y} + s^{bl}(\mathbf{v}', \mathbf{w}') \leqslant s(\mathbf{y}) \leqslant \mathbf{s}^{au}(\mathbf{v}', \mathbf{w}')^\top \mathbf{y} + s^{bu}(\mathbf{v}', \mathbf{w}') \quad \forall \mathbf{y} \in [\mathbf{v}', \mathbf{w}'],
$$

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

Let $f : Z \to \mathbb{R}$ be defined by $f(\mathbf{z}) = s(\mathbf{g}(\mathbf{z}))$. Then for $i \in \{1, \dots, m\}$, let

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

Let $\mathbf{c}^L, \mathbf{c}^U : Z^{\mathbb{I}} \to \mathbb{R}^n$ and $h^L, h^U : Z^{\mathbb{I}} \to \mathbb{R}$ be defined by

$$\mathbf{c}^L(\mathbf{v},\mathbf{w}) = \sum_i \mathbf{f}_i^{al}(\mathbf{v},\mathbf{w}), \quad h^L(\mathbf{v},\mathbf{w}) = s^{bl}(\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w})) + \sum_i f_i^{bl}(\mathbf{v},\mathbf{w}),$$
$$\mathbf{c}^U(\mathbf{v},\mathbf{w}) = \sum_i \mathbf{f}_i^{au}(\mathbf{v},\mathbf{w}), \quad h^U(\mathbf{v},\mathbf{w}) = s^{bu}(\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w})) + \sum_i f_i^{bu}(\mathbf{v},\mathbf{w}).$$

Then $\mathbf{c}^L$, $\mathbf{c}^U$, h^L, h^U are locally Lipschitz continuous mappings on $Z^{\mathbb{I}}$ which satisfy

$$\mathbf{c}^L(\mathbf{v},\mathbf{w})^\top \mathbf{z} + h^L(\mathbf{v},\mathbf{w}) \leqslant f(\mathbf{z}) \leqslant \mathbf{c}^U(\mathbf{v},\mathbf{w})^\top \mathbf{z} + h^U(\mathbf{v},\mathbf{w}) \quad \forall \mathbf{z} \in [\mathbf{v},\mathbf{w}],$$

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

Proof. Local Lipschitz continuity is established first. By assumption, $\mathbf{g}^L(\mathbf{v},\mathbf{w}) \leqslant \mathbf{g}^U(\mathbf{v},\mathbf{w})$ and

$$[\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w})] \subset Y,$$

thus $(\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w})) \in Y^{\mathbb{I}}$ for each $(\mathbf{v},\mathbf{w}) \in Z^{\mathbb{I}}$. By the local Lipschitz continuity of the composition of locally Lipschitz continuous functions (see for instance Theorem 2.5.6 in Scott, 2012), $s_i^{al}(\mathbf{g}^L(\cdot,\cdot),\mathbf{g}^U(\cdot,\cdot))$ and $s_i^{au}(\mathbf{g}^L(\cdot,\cdot),\mathbf{g}^U(\cdot,\cdot))$ are locally Lipschitz continuous functions on $Z^{\mathbb{I}}$, for each i. Similarly, $s^{bl}(\mathbf{g}^L(\cdot,\cdot),\mathbf{g}^U(\cdot,\cdot))$ and $s^{bu}(\mathbf{g}^L(\cdot,\cdot),\mathbf{g}^U(\cdot,\cdot))$ are locally Lipschitz continuous on $Z^{\mathbb{I}}$. Then by Lemmata 5.1 and 5.2, $\mathbf{f}_i^{al}$, $\mathbf{f}_i^{au}$, f_i^{bl}, and f_i^{bu} are locally Lipschitz continuous for each i. Finally, noting that the sum of locally Lipschitz continuous functions is locally Lipschitz continuous, we have that $\mathbf{c}^L$, $\mathbf{c}^U$, h^L and h^U are locally Lipschitz continuous on $Z^{\mathbb{I}}$.

Next, the lower and upper estimation properties are established. Choose any $(\mathbf{v},\mathbf{w}) \in Z^{\mathbb{I}}$. By assumption, $(\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w})) \in Y^{\mathbb{I}}$, and since $\mathbf{g}(\mathbf{z}) \in [\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w})]$ for any $\mathbf{z} \in [\mathbf{v},\mathbf{w}]$, we have

$$\begin{aligned} \mathbf{s}^{al}(\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w}))^\top \mathbf{g}(\mathbf{z}) + s^{bl}(\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w})) &\leqslant s(\mathbf{g}(\mathbf{z})), \\ \mathbf{s}^{au}(\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w}))^\top \mathbf{g}(\mathbf{z}) + s^{bu}(\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w})) &\geqslant s(\mathbf{g}(\mathbf{z})), \end{aligned} \tag{5.5}$$

for any $\mathbf{z} \in [\mathbf{v},\mathbf{w}]$. Consider each term in the inner products. If, for instance, $s_i^{al}(\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w})) \geqslant 0$, then we have

$$s_i^{al}(\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w}))(\mathbf{g}_i^{al}(\mathbf{v},\mathbf{w})^\top \mathbf{z} + g_i^{bl}(\mathbf{v},\mathbf{w})) \leqslant s_i^{al}(\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w}))g_i(\mathbf{z}),$$

and otherwise

$$s_i^{al}(\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w}))(\mathbf{g}_i^{au}(\mathbf{v},\mathbf{w})^\top \mathbf{z} + g_i^{bu}(\mathbf{v},\mathbf{w})) \leqslant s_i^{al}(\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w}))g_i(\mathbf{z}).$$

Applying the definitions of $\mathbf{f}_i^{al}$ and f_i^{bl}, we have

$$\begin{aligned} &\left(\sum_i \mathbf{f}_i^{al}(\mathbf{v},\mathbf{w})\right)^\top \mathbf{z} + \sum_i (f_i^{bl}(\mathbf{v},\mathbf{w})) + s^{bl}(\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w})) \\ &\leqslant \mathbf{s}^{al}(\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w}))^\top \mathbf{g}(\mathbf{z}) + s^{bl}(\mathbf{g}^L(\mathbf{v},\mathbf{w}),\mathbf{g}^U(\mathbf{v},\mathbf{w})), \end{aligned}$$

TABLE 1 *Some arithmetic operations s and their parameterized affine relaxations on $[\mathbf{y}^L, \mathbf{y}^U]$. These relaxations satisfy the local Lipschitz continuity assumptions of Proposition 5.1*

s	$\mathbf{s}^{al}(\mathbf{y}^L, \mathbf{y}^U)$	$s^{bl}(\mathbf{y}^L, \mathbf{y}^U)$	$\mathbf{s}^{au}(\mathbf{y}^L, \mathbf{y}^U)$	$s^{bu}(\mathbf{y}^L, \mathbf{y}^U)$
$c \in \mathbb{R}, y \mapsto cy$	c	0	c	0
$c \in \mathbb{R}, y \mapsto y + c$	1	c	1	c
$(y_1, y_2) \mapsto y_1 + y_2$	$(1, 1)$	0	$(1, 1)$	0
$(y_1, y_2) \mapsto y_1 - y_2$	$(1, -1)$	0	$(1, -1)$	0
$(y_1, y_2) \mapsto y_1 y_2$	(y_2^L, y_1^L)	$-y_1^L y_2^L$	(y_2^L, y_1^U)	$-y_1^U y_2^L$
$(y_1, y_2) \mapsto y_1 y_2$	(y_2^L, y_1^L)	$-y_1^L y_2^L$	(y_2^U, y_1^L)	$-y_1^L y_2^U$
$(y_1, y_2) \mapsto y_1 y_2$	(y_2^U, y_1^U)	$-y_1^U y_2^U$	(y_2^L, y_1^U)	$-y_1^U y_2^L$
$(y_1, y_2) \mapsto y_1 y_2$	(y_2^U, y_1^U)	$-y_1^U y_2^U$	(y_2^U, y_1^L)	$-y_1^L y_2^U$
$y \mapsto \exp(y)$	$\exp(y^L)$	$-\exp(y^L) y^L + \exp(y^L)$	$\dfrac{\exp(y^U) - \exp(y^L)}{y^U - y^L}$	$-\dfrac{\exp(y^U) - \exp(y^L)}{y^U - y^L} y^L + \exp(y^L)$
$y > 0, y \mapsto 1/y$	$-(y^U)^{-2}$	$2/y^U$	$\dfrac{1/y^U - 1/y^L}{y^U - y^L}$	$-\dfrac{1/y^U - 1/y^L}{y^U - y^L} y^L + 1/y^L$

which, combined with Inequality (5.5), and using the definitions of $\mathbf{c}^L$ and h^L establishes

$$\mathbf{c}^L(\mathbf{v}, \mathbf{w})^\top \mathbf{z} + h^L(\mathbf{v}, \mathbf{w}) \leqslant s(\mathbf{g}(\mathbf{z})) = f(\mathbf{z}),$$

for each $\mathbf{z} \in [\mathbf{v}, \mathbf{w}]$. Similar reasoning establishes the case for the affine over-estimator $(\mathbf{c}^U(\mathbf{v}, \mathbf{w}), h^U(\mathbf{v}, \mathbf{w}))$. $\square$

Table 1 defines $\mathbf{s}^{al}$, $\mathbf{s}^{au}$, s^{bl} and s^{bl} for some bivariate and univariate operations so that the local Lipschitz continuity assumptions of Proposition 5.1 hold. That these functions are locally Lipschitz continuous is fairly clear from inspection. That these are relaxations is also clear for such operations as scalar multiplication, scalar addition, and bivariate addition. In the case of smooth convex univariate functions such as $\exp(\cdot)$ and $1/(\cdot)$, one notes that any tangent supports the function from below. When the function is non-decreasing (such as the exponential), intuitively the 'best' under-estimator is obtained when the tangent is evaluated at the lower bound, and similarly when the function is non-increasing (such as the reciprocal), the best under-estimator is obtained when the tangent is evaluated at the upper bound. For convex functions the affine over-estimator is obtained from a secant. In the case of multiplication, two affine under-estimators and two affine over-estimators can be defined. These are obtained from the convex and concave hulls of the bilinear term, which are defined as the point-wise maximum of two affine functions and point-wise minimum of two affine functions, respectively. See for instance the relaxation of binary products in Mitsos *et al.* (2009).

Consider the construction of affine relaxations of a component f_i of the factorable function $\mathbf{f}$ on some interval $[t, t] \times [\mathbf{v}_u, \mathbf{w}_u] \times [\mathbf{v}, \mathbf{w}] \subset T \times D_u \times D$. The 'seed' factors $\{g_i : i = 1, \dots, 1 + n_u + n_x\}$ have affine under and over-estimators given by $(\mathbf{g}_i^{al}, g_i^{bl}) = (\mathbf{g}_i^{au}, g_i^{bu}) = (\mathbf{e}_i, 0)$, where $\mathbf{e}_i$ is the ith unit vector in $\mathbb{R}^{1+n_u+n_x}$. Then, by recursively applying the rule for multivariate composition defined in

Proposition 5.1 and the definitions in Table 1, affine under and over-estimators can be constructed for f_i. For the examples considered in Section 6 the operations listed in Table 1 suffice. Including dependence on t suffices to establish the local Lipschitz continuity condition in Inequality (5.3). Further, the relaxations will then be continuous functions of $(t, \mathbf{v}, \mathbf{w})$, which will serve to satisfy the additional boundedness condition. An interval enclosure $[\mathbf{v}_u, \mathbf{w}_u]$ of U can be obtained by the procedure in Definition 4 in Scott & Barton (2013). Since relaxations of $f_i(t, \cdot, \cdot)$ on $U \times P_i^{L/U}([\mathbf{v}, \mathbf{w}] \cap G)$ are sought, the same procedure can be used to obtain a 'tightened' interval enclosure of $P_i^{L/U}([\mathbf{v}, \mathbf{w}] \cap G)$, on which relaxations can be constructed.

However, for every binary product that appears in the factorable representation of f_i, as already noted, Table 1 indicates that *four* valid combinations of affine under- and over-estimators can be defined. Thus, by repeating the evaluation of the affine relaxations, but using a different choice for the affine relaxation for each binary product allows one to construct multiple valid affine relaxations of f_i. Taking the point-wise maximum of the under-estimators yields a convex piecewise affine under-estimator of f_i, while similarly taking the point-wise minimum of the over-estimators yields a concave piecewise affine over-estimator.

5.3 *Numerical solution*

Recall that the hypotheses of Theorem 4.1 include the requirement that any solutions of the IVP (4.1) must satisfy $\{(\mathbf{x}^L(t), \mathbf{x}^U(t)) : t \in T\} \subset D_\Omega$. The complication is that D_Ω may not be an open set, and most numerical methods for the integration of a system of ODEs assume that the domain of the dynamics is an open set, much like in the theoretical results for existence such as Carathéodory's. Results from viability theory could be used; see for instance Aubin (1991). Unfortunately, the numerical methods based on this theory require a more explicit characterization of the set D_Ω than is available here. However, in the authors' experience, there is little complication when using 'standard' integration methods, such as the ones mentioned in Section 5.1 The main concern is how to most efficiently evaluate the functions $(\mathbf{q}^L, \mathbf{q}^U)$ defined in Equations (5.1) and (5.2), since this involves the repeated solution of LPs.

To address this concern, consider the reformulation of the LPs (5.1) and (5.2) as standard form LPs. Let $\mathbf{z} = (t, \mathbf{v}, \mathbf{w}) \in T \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$ denote the vector parameterizing these problems. These programs share the same following formulation when put in standard form via elementary techniques (see, for instance, Chapter 1 of Bertsimas & Tsitsiklis, 1997):

$$q(\mathbf{z}) = \min\{\mathbf{c}^\top \mathbf{y} : \mathbf{M}(\mathbf{z})\mathbf{y} = \mathbf{d}(\mathbf{z}), \mathbf{y} \geqslant \mathbf{0}\}, \tag{5.6}$$

where, for some $m, n \in \mathbb{N}$, $\mathbf{d} : T \times D_\Omega \to \mathbb{R}^m$ and $\mathbf{M} : T \times D_\Omega \to \mathbb{R}^{m \times n}$ are continuous mappings, under the assumption that f_i^{cv} and f_i^{cc} are continuous. Note that the parameterization occurs in both the right-hand side of the constraints and the constraint matrix, and thus the so-called technology matrix case of parametric linear programming results. In general, this kind of parametric dependence can lead to a discontinuous objective value (see Wets, 1985). However, as already shown in Section 3, this cannot happen for the problems of interest, and considering the origin of the reformulation, one can show that these problems can be handled in a fairly efficient way.

First, a basis $B \subset \{1, \ldots, n\}$ is an index set which describes a vertex of the feasible set of an LP. For the LP (5.6), a basis will have m elements, and so let $\mathbf{M}_B(\mathbf{z})$ be the square submatrix formed by taking the columns of $\mathbf{M}(\mathbf{z})$ which correspond to elements of B, called a basis matrix. Similarly, given a vector $\mathbf{v} \in \mathbb{R}^n$, let $\mathbf{v}_B \in \mathbb{R}^m$ be defined by taking the components of $\mathbf{v}$ which correspond to elements of B.

Next, note that for all $\mathbf{z} \in T \times D_{\Omega}$, the LPs (5.1) and (5.2) have solutions because, in this case, the feasible sets are non-empty and bounded. Thus the equivalent problems in standard form must also have solutions. This implies that there exist bases which each describe a vertex which is optimal for the reformulated problems. These bases are called optimal bases. In terms of the standard form LP (5.6), a basis B is optimal if the corresponding basis matrix $\mathbf{M}_B(\mathbf{z})$ satisfies the algebraic conditions

$$(\mathbf{M}_B(\mathbf{z}))^{-1}\mathbf{d}(\mathbf{z}) \geqslant \mathbf{0}, \tag{5.7}$$

$$\mathbf{c}^{\top} - \mathbf{c}_B^{\top}(\mathbf{M}_B(\mathbf{z}))^{-1}\mathbf{M}(\mathbf{z}) \geqslant \mathbf{0}^{\top}, \tag{5.8}$$

referred to as primal and dual feasibility, respectively. When solving an LP with the simplex algorithm, the algorithm can be ‘warm-started’ by providing a basis which is either primal or dual feasible; the algorithm terminates much more quickly than if it was cold-started (if it had to go through Phase I first).

Thus, it is desirable to know, given an optimal basis B, whether the left-hand side of the inequality in either of (5.7) or (5.8) may be continuous on an open subset of $T \times D_{\Omega}$ containing $\mathbf{z}$. If this is the case, then a given optimal basis B that satisfies either (5.7) and/or (5.8) with strict inequality will remain primal and/or dual feasible for some finite amount of time. Consequently, in the course of numerical integration of (4.1), for many steps one can warm-start the simplex algorithm to solve the LPs. This will speed up the solution time immensely. The number of steps where a basis is unavailable to warm-start simplex may be small relative to the overall number of steps taken.

This is indeed the case: given a basis B such that $\mathbf{M}_B(\mathbf{z})$ is optimal, there is an open subset of $T \times D_{\Omega}$ containing $\mathbf{z}$ on which the left-hand side of the inequality in either of (5.7) or (5.8) is continuous. To see this, one can use Cramer’s rule; see Section 4.4 of Strang (2006). For $\mathbf{S} \in \mathbb{R}^{m \times m}$, $\mathbf{e} \in \mathbb{R}^m$, the vector $\mathbf{y} = \mathbf{S}^{-1}\mathbf{e}$ is given componentwise by

$$y_j = \frac{\det(\mathbf{T}_j)}{\det(\mathbf{S})},$$

where $\mathbf{T}_j$ is the matrix formed by replacing the jth column of $\mathbf{S}$ with $\mathbf{e}$. Since the determinant of a matrix is continuous with respect to the entries of the matrix, it is a simple application of Cramer’s rule to see that the left-hand side of the inequalities (5.7) and (5.8) are continuous on the set of those $\mathbf{z}'$ such that $\mathbf{M}_B(\mathbf{z}')$ is invertible. Further, the set of those $\mathbf{z}'$ such that $\mathbf{M}_B(\mathbf{z}')$ is invertible is an open set containing $\mathbf{z}$ noting that it is the preimage of $(-\infty, 0) \cup (0, +\infty)$, an open set, under the continuous mapping $\det(\mathbf{M}_B(\cdot))$. Consequently, the ‘direct’ method of solving the IVP (4.1) numerically by using an LP solver to evaluate the functions $(\mathbf{q}^L, \mathbf{q}^U)$ in the derivative evaluator of a numerical integration routine can be fairly efficient.

5.4 *Complexity*

This section considers the computational complexity of the proposed bounding method. As the general numerical implementation of the method involves the solution of an IVP in ODEs in which the dynamics are defined by the solution of LPs, the complexity of the method will depend on the choice of numerical integrator and LP solver. Some observations follow. For this discussion, ‘cost’ is roughly measured in terms of floating-point operations or just ‘operations.’

First, the complexity of computing a solution of an IVP in Lipschitz ODEs with a general numerical integration method is somewhat out of the scope of this article; it is a fairly open problem and has interesting ties to deeper questions in computational complexity theory. For a more theoretical discussion see Kawamura (2010), Kawamura *et al.* (2014).

A more practical observation is that, beside evaluating the dynamics, the dominant cost at each step in most implicit numerical integration methods for stiff systems is the matrix factorization required for Newton iteration (in the context of the backward differentiation formulae (BDF), see Section 5.2.2 of Brenan *et al.*, 1996). Consequently, there is, in general, an order $(2n_x)^3$ cost associated with the numerical integration of IVP (4.1). However, most implementations of the BDF, for instance, will deploy a deferred Jacobian, and avoid matrix factorization at each step; see Section 5.2.2 of Brenan *et al.* (1996) and Section 6.5 of Lambert (1991).

The focus of the rest of this section is to analyse the complexity of evaluating the right-hand sides defining the IVP (4.1). A more complete answer to this question can be found. This depends heavily on the standard-form LPs (5.6) which define the dynamics (5.1) and (5.2). First, a bound on the size of these standard-form LPs is needed. This depends on n_x, n_u, m_u (the number of halfspaces required to represent the polytopal set of control values U), m_g (the number of halfspaces required to represent the polytopal *a priori* enclosure G), and n_i^L or n_i^U (the number of affine functions that make up the piecewise affine estimators f_i^{cv} or f_i^{cc}). To define q_i^L, one can check that the number of constraints in the corresponding standard-form LP (5.6) is bounded above by $2n_x + m_g + m_u + 1 + n_i^L$, and that the number of variables is bounded above by $4n_x + 2n_p + m_g + m_u + 2 + n_i^L$ (this is obtained by a rather slavish addition of slack variables, dummy variables and splitting 'free' variables into non-negative and non-positive parts). In addition, evaluation of $\mathbf{d}$, the right-hand side of the constraints of LP (5.6), involves evaluating z_i^m (or z_i^M), which itself requires the solution of a LP.

Citing the celebrated result that there exist polynomial time algorithms for linear programming (see Chapter 8 of Bertsimas & Tsitsiklis, 1997), one can establish that one component $q_i^{L/U}$ of the dynamics defining IVP (4.1) can be evaluated with polynomial cost (with respect to n_x, n_p, m_u, m_g, n_i^L and n_i^U). However, as indicated in Section 5.3, in practice one might obtain better performance using the simplex algorithm and attempting to warm-start the method using a basis recorded from the previous function evaluation. In summary, however the LPs are solved, evaluating the dynamics requires the solution of $4n_x$ LPs since the IVP is a system in $\mathbb{R}^{2n_x}$. Compared with the interval arithmetic-based method in Scott & Barton (2013), the solution of these LPs is the most significant increase in cost.

The last step is to consider the complexity of evaluating the piecewise affine under- and over-estimators. The answer to this is closely related to the cost of evaluating interval relaxations. Consequently, the approach taken is similar to that in Section 4.4 of Griewank & Walther (2008), and a bound on the complexity of evaluating the affine estimators relative to evaluating the original function is sought. To begin, assume as in Section 5.2 that the function $\mathbf{f}$ defining the original dynamics are factorable; that is, each component can be computed as the finite recursive composition of operations from a library of multivariate intrinsic functions. Denote the sequence of intrinsic functions required for the evaluation of $\mathbf{f}$ by $\{s_1, s_2, \ldots, s_N\}$ for some finite N. As in Section 4.4 of Griewank & Walther (2008), the main assumption required for this analysis is that the cost of evaluating $\mathbf{f}$, denoted $\text{cost}(\mathbf{f})$, is equal to the sum of the cost of evaluating each intrinsic function in the sequence $\{s_k : 1 \leqslant k \leqslant N\}$; that is, $\text{cost}(\mathbf{f}) = \sum_{k=1}^{N} \text{cost}(s_k)$.

Now, analyse one step in the evaluation of the factorable function $\mathbf{f}$; that is, one evaluation of a multivariate intrinsic function $s : \mathbb{R}^m \supset Y \to \mathbb{R}$. Using the notation in Proposition 5.1, let $s^L, s^U : Y^{\mathbb{I}} \to \mathbb{R}$ be the parameterized lower and upper bounds of the interval enclosure of s (i.e. $[s^L(\mathbf{v}, \mathbf{w}), s^U(\mathbf{v}, \mathbf{w})] \ni s(\mathbf{y})$, for all $\mathbf{y} \in [\mathbf{v}, \mathbf{w}]$). Assume that the cost of evaluating s^L and s^U is no more than $\alpha\, \text{cost}(s)$, for some $\alpha > 0$, for any possible s in the library of intrinsic functions. It follows that evaluation of an interval enclosure of $\mathbf{f}$ will be no more expensive than $2\alpha\, \text{cost}(\mathbf{f})$. Thus, the cost of evaluating an interval enclosure is bounded above by a scalar multiple of the cost of evaluating the original function. This is consistent with a slightly more detailed argument in Section 4.4 of Griewank & Walther (2008).

To evaluate the affine relaxations, similar reasoning applies; again assume that evaluation of the affine relaxations $\mathbf{s}^{al}$, $\mathbf{s}^{au}$, s^{bl}, s^{bu} of any intrinsic function s is no more expensive than $\beta\,\mathrm{cost}(s)$, for some $\beta > 0$. This is reasonable based on Table 1. Let $\{\mathbf{g}_i^{al}, g_i^{bl}, \mathbf{g}_i^{au}, g_i^{bu}\}$ be the values of the affine relaxations corresponding to the previously computed factors $\mathbf{g}$. Since the affine relaxations of $\mathbf{f}$ are with respect to each of its arguments, $\mathbf{g}_i^{al}, \mathbf{g}_i^{au} \in \mathbb{R}^{1+n_x+n_u}$. Assume that the cost of scalar addition $(+)$ and multiplication $(\times)$ are bounded above by some scalar multiple of the cost of evaluating s, for any s in the library of intrinsic functions. That is, there exists $\eta > 0$ such that $\mathrm{cost}(+) \leqslant \eta\,\mathrm{cost}(s)$ and $\mathrm{cost}(\times) \leqslant \eta\,\mathrm{cost}(s)$ for all s in the library. Again, this is consistent with a slightly more detailed argument in Section 4.4 of Griewank & Walther (2008); also, this is a reasonable assumption since scalar addition and multiplication are two of the cheapest operations. Following the rules in Proposition 5.1 and keeping track of the operations required, the cost of propagating the affine relaxations for one step is bounded by $(\Psi + \Upsilon)\,\mathrm{cost}(s)$, for some $\Psi > 0$ and $\Upsilon > 0$. In this case, Ψ only depends on the library of intrinsic functions used, while Υ depends on the dimension of the system, i.e. $1 + n_x + n_u$. Thus the cost of evaluating the affine relaxations of the overall function $\mathbf{f}$ is bounded by $(\Psi + \Upsilon)\sum_{k=1}^{N}\mathrm{cost}(s_k) = (\Psi + \Upsilon)\,\mathrm{cost}(\mathbf{f})$. Adding in the cost of evaluating the interval enclosures makes this $(\Psi + \Upsilon + 2\alpha)\,\mathrm{cost}(\mathbf{f})$. Therefore, the cost of evaluating a pair of affine under- and over-estimators is no more expensive than a scalar multiple of the cost of evaluating the original function, although this multiple depends on the number of states and controls. Finally, this evaluation is repeated $\sum_{i=1}^{n_x} n_i^L + n_i^U$ times, corresponding to each piece of the piecewise affine under- and over-estimators f_i^{cv}, f_i^{cc}, $i \in \{1, \ldots, n_x\}$.

6. Examples

This section assesses the performance of a MATLAB implementation of the proposed bounding method, using an implicit linear multistep integration method (`ode113`, see Shampine & Reichelt, 1997) and CPLEX to solve the necessary LPs. MATLAB release r2011b is used on a workstation with a 3.07 GHz Intel Xeon processor.

6.1 *Polytopal control values versus interval hull*

The simple reaction network

$$\mathrm{A} + \mathrm{B} \to \mathrm{C},$$
$$\mathrm{A} + \mathrm{C} \to \mathrm{D}$$

is considered to demonstrate the ability of the system (4.1) to utilize a polytopal set U. The dynamic equations governing the evolution of the species concentrations $\mathbf{x} = (x_A, x_B, x_C, x_D)$ in a closed system are

$$\begin{aligned}
\dot{x}_A &= -u_1 x_A x_B - u_2 x_A x_C,\\
\dot{x}_B &= -u_1 x_A x_B,\\
\dot{x}_C &= u_1 x_A x_B - u_2 x_A x_C,\\
\dot{x}_D &= u_2 x_A x_C.
\end{aligned} \tag{6.1}$$

The goal to estimate the reachable set on $T = [0, 0.1]$ (s), with $X_0 = \{\mathbf{x}_0 = (1, 1, 0, 0)\}$ (M) and rate parameters $\mathbf{u} = (u_1, u_2) \in \mathscr{U}$, with

$$U = \{\mathbf{k} \in \mathbb{R}^2 : \hat{\mathbf{k}} \leqslant \mathbf{k} \leqslant 10\hat{\mathbf{k}},\ k_1 + 2.5k_2 = 550\},$$

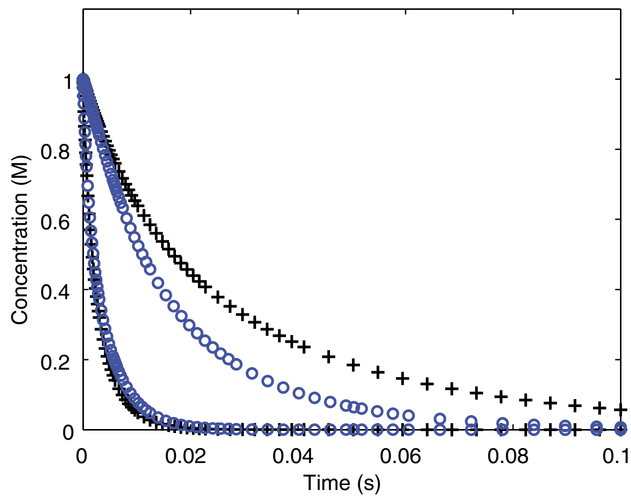

FIG. 1. State bounds for x_A (from system (6.1)) computed from the system of ODEs with LPs embedded (4.1). Bounds for polytopal U are plotted with circles, while bounds for the interval hull of U are plotted with crosses.

where $\hat{\mathbf{k}} = (50, 20)$. A polytopal enclosure G can be determined from considering the stoichiometry of the system and other physical arguments such as mass balance; see Scott & Barton (2010) for more details. For this system, one has

$$G = \{\mathbf{z} \in \mathbb{R}^4 : \mathbf{0} \leqslant \mathbf{z} \leqslant \bar{\mathbf{x}}, \mathbf{M}\mathbf{z} = \mathbf{M}\mathbf{x}_0\}, \quad \text{with}$$
$$\mathbf{M} = \begin{bmatrix} 1 & -1 & 0 & 1 \\ -1 & 2 & 1 & 0 \end{bmatrix},$$
$$\bar{\mathbf{x}} = (1, 1, 1, 0.5).$$

Bounds on the states $\mathbf{x}$ are calculated using the system of ODEs with LPs embedded (4.1), first using U as is, and again using the interval hull of U. The difference can be quite apparent; see Fig. 1. The ability to use a polytopal set of admissible control values distinguishes this method from previous work in Scott & Barton (2013) and Singer & Barton (2006a), for example. In each case, the method takes $\sim$1.3 s.

6.2 *Comparison with previous implementation*

The enzyme reaction network considered in Example 2 of Scott & Barton (2013) is used here to demonstrate the effectiveness of the system (4.1) in producing tight state bounds for an uncertain dynamic system. The reaction network is

$$\mathrm{A} + \mathrm{F} \rightleftharpoons \mathrm{F{:}A} \rightarrow \mathrm{F} + \mathrm{A}',$$
$$\mathrm{A}' + \mathrm{R} \rightleftharpoons \mathrm{R{:}A'} \rightarrow \mathrm{R} + \mathrm{A}.$$

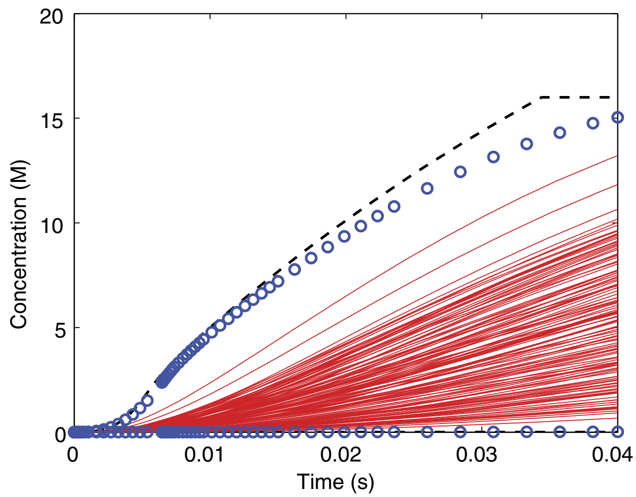

FIG. 2. State bounds for $x_{\mathrm{R:A'}}$ computed from the system of ODEs with LPs embedded (4.1) (circles) and from the implementation in Scott & Barton (2013) (dashed lines). Solutions of (6.2) for constant $\mathbf{u} \in \mathscr{U}$ are solid lines.

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

$$\begin{aligned}
\dot{x}_{\mathrm{F}} &= -u_1 x_{\mathrm{F}} x_{\mathrm{A}} + u_2 x_{\mathrm{F:A}} + u_3 x_{\mathrm{F:A}},\\
\dot{x}_{\mathrm{A}} &= -u_1 x_{\mathrm{F}} x_{\mathrm{A}} + u_2 x_{\mathrm{F:A}} + u_6 x_{\mathrm{R:A'}},\\
\dot{x}_{\mathrm{F:A}} &= u_1 x_{\mathrm{F}} x_{\mathrm{A}} - u_2 x_{\mathrm{F:A}} - u_3 x_{\mathrm{F:A}},\\
\dot{x}_{\mathrm{A'}} &= u_3 x_{\mathrm{F:A}} - u_4 x_{\mathrm{A'}} x_{\mathrm{R}} + u_5 x_{\mathrm{R:A'}},\\
\dot{x}_{\mathrm{R}} &= -u_4 x_{\mathrm{A'}} x_{\mathrm{R}} + u_5 x_{\mathrm{R:A'}} + u_6 x_{\mathrm{R:A'}},\\
\dot{x}_{\mathrm{R:A'}} &= u_4 x_{\mathrm{A'}} x_{\mathrm{R}} - u_5 x_{\mathrm{R:A'}} - u_6 x_{\mathrm{R:A'}}.
\end{aligned} \tag{6.2}$$

The goal to estimate the reachable set on $T = [0, 0.04]$ (s), with $X_0 = \{\mathbf{x}_0 = (20, 34, 0, 0, 16, 0)\}$ (M) and rate parameters $\mathbf{u} = (u_1, \ldots, u_6) \in \mathscr{U}$, with $U = \{\mathbf{k} \in \mathbb{R}^6 : \hat{\mathbf{k}} \leqslant \mathbf{k} \leqslant 10\hat{\mathbf{k}}\}$ and $\hat{\mathbf{k}} = (0.1, 0.033, 16, 5, 0.5, 0.3)$. For this system, a polytopal enclosure G is

$$\begin{aligned}
G &= \{\mathbf{z} \in \mathbb{R}^6 : \mathbf{0} \leqslant \mathbf{z} \leqslant \bar{\mathbf{x}}, \mathbf{M}\mathbf{z} = \mathbf{M}\mathbf{x}_0\}, \quad \text{with}\\
\mathbf{M} &= \begin{bmatrix} -1 & 0 & -1 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & -1 & -1\\ -1 & 1 & 0 & 1 & -1 & 0 \end{bmatrix},\\
\bar{\mathbf{x}} &= (20, 34, 20, 34, 16, 16).
\end{aligned}$$

The state bounds resulting from the solution of (4.1) and the interval arithmetic-based implementation used in Scott & Barton (2013) are similar; the bounds resulting from the solution of (4.1) are at least as tight as those in Scott & Barton (2013). See Figs 2 and 3. As demonstrated by Fig. 3, using affine relaxations can lead to a significant improvement in the bounds. The proposed method takes ~2.2 s, whereas a comparable MATLAB implementation of the method in Scott & Barton (2013) takes 0.65 s.

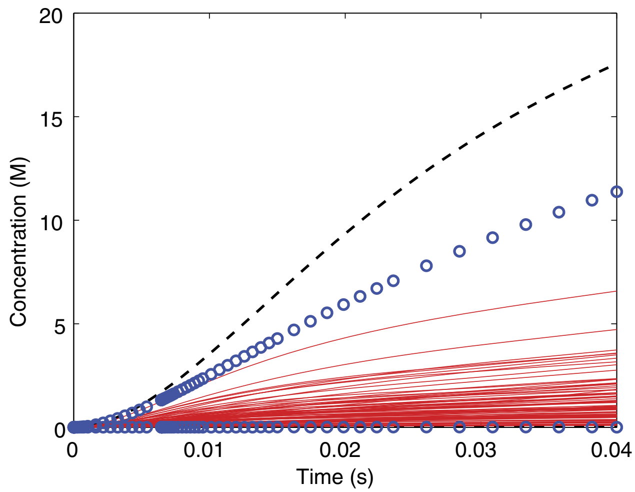

FIG. 3. State bounds for $x_{A'}$ computed from the system of ODEs with LPs embedded (4.1) (circles) and from the implementation in Scott & Barton (2013) (dashed lines). Solutions of (6.2) for constant $\mathbf{u} \in \mathscr{U}$ are solid lines.

7. Conclusions

This work has considered the problem of bounding the reachable set of a non-linear dynamic system point-wise in time. The approach taken is an implementation of the theory in Scott & Barton (2013), which in turn is based on the theory of differential inequalities. The implementation leads to a system of ODEs depending on parametric LPs. Thus, this work also analyses how numerically tractable such a system is. The new implementation yields tighter bounds than the previous one, especially when the admissible controls take values in a compact convex polytope.

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Appendix. Supporting proof

Some useful background is as follows. If f is a locally Lipschitz continuous function on metric space (X,d), then f is Lipschitz continuous on any compact subset of X, and if (X,d) is locally compact, then the converse is true. A space is locally compact if every point has a compact neighbourhood (is contained in the interior of a compact set). It follows that $\mathbb{R}^n$ is locally compact. Further, any closed or open subset of a locally compact space is locally compact as well; see Munkres (1975).

The following lemma will be useful.

LEMMA A.1 Let (X,d) be a metric space. Let $\mathscr{K}$ be a compact subset of $\mathbb{K}X$ (with the Hausdorff metric). Then $\hat{K} = \bigcup_{Z\in\mathscr{K}} Z$ is compact.

Proof. Choose a sequence $\{x_i\} \subset \hat{K}$. We will show that a subsequence of it converges to an element of $\hat{K}$. By the definition of $\hat{K}$, we can construct a corresponding sequence $\{Z_i\} \subset \mathscr{K}$ such that $Z_i \ni x_i$ for each i. Since $\mathscr{K}$ is compact, there exists a subsequence $\{Z_{i_j}\}$ which converges (with respect to the Hausdorff metric) to some $Z^* \in \mathscr{K}$. Using the definition of the Hausdorff metric and the fact that Z_i and Z^* are compact, we have

$$\forall \epsilon > 0, \quad \exists J > 0 : \forall j > J, \quad \exists z_j \in Z^* : d(x_{i_j}, z_j) \leqslant \epsilon.$$

It follows that we can construct a subsequence of $\{x_{i_j}\}$, which we will denote $\{x_\ell\}$, and $\{z_\ell\} \subset Z^*$ such that $\forall \epsilon > 0$, $\exists L > 0 : \forall \ell > L$, $d(x_\ell, z_\ell) \leqslant \epsilon$. But since Z^* is compact, a subsequence $\{z_{\ell_m}\}$ converges to some $z \in Z^*$. Using the triangle inequality, we have $\forall \epsilon > 0$, $\exists M > 0 : \forall m > M$, $d(x_{\ell_m}, z) \leqslant d(x_{\ell_m}, z_{\ell_m}) + d(z_{\ell_m}, z) < \epsilon$. Thus, $\{x_{\ell_m}\}$ converges to $z \in \hat{K}$, and so $\hat{K}$ is compact. □

A.1 *Proof of Proposition* 3.1

An important fact is that F is closed, see Section 4.7 of Bertsimas & Tsitsiklis (1997). It follows that $F \times \mathbb{R}^{pn} \times \mathbb{R}^p$ is locally compact, and so it suffices to show that $\hat{q}$ is Lipschitz continuous on any compact subset. So, choose compact $K \subset F \times \mathbb{R}^{pn} \times \mathbb{R}^p$. Then there exist compact $K_d \subset F$, $K_c \subset \mathbb{R}^{pn}$ and $K_h \subset \mathbb{R}^p$ such that $K \subset K_d \times K_c \times K_h$.

To apply Lemma 3.1, we need to extend the domain of P so that we consider it a function of $\mathbf{c} \in K_c$ and $\mathbf{h} \in K_h$ as well. In an abuse of notation, denote this function $P : K_d \times K_c \times K_h \rightrightarrows \mathbb{R}^n$. By Lemma 3.2, P is Lipschitz continuous on $K_d \times K_c \times K_h$, so the image of $K_d \times K_c \times K_h$ under P, denoted $\mathscr{K}$, is compact in $\mathbb{K}\mathbb{R}^n$. By Lemma A.1, $K_v \equiv \cup_{Z\in\mathscr{K}} Z$ is compact. Since f given by $f(\mathbf{v},\mathbf{d},\mathbf{c},\mathbf{h}) = \max_{i\in I}\{\mathbf{c}_i^\top \mathbf{v} + h_i\}$ is locally Lipschitz continuous on all of $\mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^{pn} \times \mathbb{R}^p$, it is Lipschitz continuous on $K_v \times K_d \times K_c \times K_h$.

By assumption, $P(\mathbf{d},\mathbf{c},\mathbf{h})$ is closed, bounded, non-empty, and a subset of K_v for all $(\mathbf{d},\mathbf{c},\mathbf{h}) \in K_d \times K_c \times K_h$, and by Lemma 3.2 is Lipschitz continuous in the sense required by Lemma 3.1. Thus, $f(\cdot,\mathbf{d},\mathbf{c},\mathbf{h})$ achieves its minimum on $P(\mathbf{d},\mathbf{c},\mathbf{h})$ for each $(\mathbf{d},\mathbf{c},\mathbf{h}) \in K_d \times K_c \times K_h$. So, we can apply Lemma 3.1 and obtain that $\hat{q}$ is Lipschitz continuous on $K_d \times K_c \times K_h$, and thus on K.