Enclosing Reachable Sets for Nonlinear Control Systems using Complementarity-Based Intervals

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Abstract: Enclosing the reachable sets of nonlinear control systems is useful in state estimation and safety verification for chemical process models. We present a new approach for computing time-varying interval bounds for ordinary differential equation models based on differential inequalities. Instead of using interval arithmetic like established approaches, we instead generate bounding information for the right-hand side (RHS) function by optimizing its convex relaxations. Complementarity formulations are explored, and are found to be particularly beneficial if the RHS function is quadratic and we employ the αBB relaxations.

Keywords: reachability, bounding method, control systems, intervals, complementarity, convex relaxation, αBB relaxation

1. INTRODUCTION

The problem of interest in this paper is to compute tight bounds for the reachable set of nonlinear dynamic systems represented as system of parametric ordinary differential equations (ODEs) with uncertain inputs, parameters, and initial conditions. Such enclosures are important in many applications, including state estimation (Jaulin, 2002), parameter estimation (Singer and Barton, 2006), safety verification (Huang et al., 2002; Tomlin et al., 2003), fault detection (Lin and Stadtherr, 2008), and global dynamic optimization (Papamichail and Adjiman, 2002; Singer et al., 2006). Various strategies have been proposed to enclose this reachable set, such as solving the Hamilton-Jacobi equations (Mitchell et al., 2005), conservatively linearizing nonlinear models (Althoff et al., 2008), constructing zonotopes (Kühn, 1998; Yang and Scott, 2018) or ellipsoids (Kurzhanski and Varaiya, 2002), and computing validated solutions (Nedialkov et al., 1999; Lin and Stadtherr, 2007). This paper focuses on another category of methods that are based on differential inequalities (Walter, 1970).

Differential inequality-based methods generate time-varying interval enclosures for the original nonlinear dynamic system by constructing an auxiliary dynamic system and solving this numerically. The solutions of the auxiliary system are component-wise lower and upper bounds for the original system. Differential inequality-based methods require valid bounding information for the original system's right-hand side (RHS) function. Harrison (1977) first proposed to use natural interval extensions (NIE) (Moore et al., 2009) to calculate interval bounds of the RHS function automatically. This strategy was extended using affine relaxation techniques for tighter enclosures (Singer and Barton, 2006). Harwood et al. (2016) introduced a method to bound the RHS function with the solutions of linear programs (LPs). These LPs optimize piecewise-affine relaxations of the original RHS function that are derived with a special relaxation scheme to ensure the Lipschitz continuity. Chachuat and Villanueva (2012) presented another differential inequality-based approach that applies Taylor series expansion to the original system. Besides the various techniques for constructing an auxiliary bounding system, another direction of research in this area involves generating less conservative enclosures by exposing the "hidden constraints" of the original system, such as physical bounds and implicit conservation laws (Scott and Barton, 2013; Shen and Scott, 2017). This approach may require specialized knowledge of the system of interest to formulate effective constraints for refining the enclosures.

In this work, we propose a novel differential inequality-based method for computing enclosures for nonlinear control systems. Bounding information for the RHS function is obtained by optimizing its convex relaxations. This is distinct from the LP-based method by Harwood et al. (2016) in which the relaxations are limited to a special type of convex piecewise-affine under-estimators. Our new approach, on the other hand, is applicable to a broad range of convex relaxations. Moreover, complementarity formulations are developed in an effort to solve the optimization problems efficiently. Examples are presented for illustration.

The following notation conventions are used in this paper. Vectors are denoted with boldface lower-case letters (e.g. $\boldsymbol{x}$). Given vectors $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$, inequalities such as $\boldsymbol{x} < \boldsymbol{y}$ or $\boldsymbol{x} \leq \boldsymbol{y}$ are to be interpreted component-wise. Convexity of a vector-valued function $\boldsymbol{f}$ refers here to convexity of all components f_i. A matrix is denoted with boldface upper-case letters (e.g. $\boldsymbol{A}$), and its elements are represented by corresponding lower case letters with subscripts indicating the row and column (e.g. a_{ij}). An interval in $\mathbb{R}^n$ is a

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nonempty subset of $\mathbb{R}^n$ of the form $\{\boldsymbol{x} \in \mathbb{R}^n : \boldsymbol{a} \leq \boldsymbol{x} \leq \boldsymbol{b}\}$, which is denoted as $[\boldsymbol{a}, \boldsymbol{b}]$. $\mathbb{IR}^n$ denotes the set of all intervals in $\mathbb{R}^n$.

2. PROBLEM STATEMENT

Consider $t_0, t_f \in \mathbb{R}$ with $t_0 < t_f$, and define $I := [t_0, t_f]$. Let $U := [\boldsymbol{u}^L, \boldsymbol{u}^U] \subset \mathbb{R}^{n_u}$ be an interval, and $D \subset \mathbb{R}^{n_x}$ be open. Denote the space of all Lebesgue integrable functions $\boldsymbol{h} : I \to \mathbb{R}^n$ as $L^n(I)$. Let $\tilde{U} := \{\boldsymbol{u} \in L^{n_u}(I) : \boldsymbol{u}(t) \in U, t \in I\}$ be a set of admissible controls, and $X_0 := [\boldsymbol{x}_0^L, \boldsymbol{x}_0^U] \in D$ be a set of admissible initial conditions. Given a continuous mapping $\boldsymbol{f} : I \times U \times D \to \mathbb{R}^{n_x}$ for which $\boldsymbol{f}(t, \cdot, \cdot)$ is twice-continuously differentiable for each $t \in I$, consider an initial-value problem

$$\begin{aligned} \dot{\boldsymbol{x}}(t, \boldsymbol{u}, \boldsymbol{x}_0) &= \boldsymbol{f}(t, \boldsymbol{u}(t), \boldsymbol{x}(t, \boldsymbol{u}, \boldsymbol{x}_0)), \quad \forall t \in (t_0, t_f], \\ \boldsymbol{x}(t_0, \boldsymbol{u}, \boldsymbol{x}_0) &= \boldsymbol{x}_0, \end{aligned} \tag{1}$$

where $(\boldsymbol{u}, \boldsymbol{x}_0) \in \tilde{U} \times X_0$, and where dotted quantities indicate time-derivatives (e.g. $\dot{\boldsymbol{x}} \equiv \frac{\partial \boldsymbol{x}}{\partial t}$).

Under these conditions, the ordinary differentiable equation (ODE) (1) is guaranteed to have a unique solution by the Picard-Lindelöf Theorem, summarized as (Hartman, 2002, Theorem 1.1, Chapter II).

The objective of this work is to compute tight time-varying interval bounds for $\boldsymbol{x}(t, \boldsymbol{u}, \boldsymbol{x}_0)$ in (1). Here, we use the terminology proposed by Scott and Barton (2013) to describe such enclosures.

Definition 1 (State bounds)**.** *Functions $\boldsymbol{x}^L, \boldsymbol{x}^U : I \to \mathbb{R}^{n_x}$ are* state bounds *for the ODE* (1) *if*

$$\boldsymbol{x}^L(t) \leq \boldsymbol{x}(t, \boldsymbol{u}, \boldsymbol{x}_0) \leq \boldsymbol{x}^U(t), \quad \forall (t, \boldsymbol{u}, \boldsymbol{x}_0) \in I \times \tilde{U} \times X_0.$$

Let $X^B : I \to \mathbb{IR}^{n_x}$ denote the corresponding interval function: $X^B(t) := [\boldsymbol{x}^L(t), \boldsymbol{x}^U(t)]$ for each $t \in I$.

3. BACKGROUND

The following fundamental differential inequality theorem was presented in (Harrison, 1977).

Proposition 1. *Let $\boldsymbol{x}^L, \boldsymbol{x}^U : I \to \mathbb{R}^{n_x}$ satisfy the following conditions.*

(1) $\boldsymbol{x}_0 \in X^B(t_0)$,
(2) For a.e. $t \in I$ and each $i \in \{1, \ldots, n_x\}$,

$$\dot{x}_i^L(t) \leq \min_{\substack{\boldsymbol{z} \in X^B(t),\, z_i = x_i^L(t), \\ \boldsymbol{u} \in \tilde{U}}} f_i(t, \boldsymbol{u}, \boldsymbol{z}), \tag{2a}$$

$$\dot{x}_i^U(t) \geq \max_{\substack{\boldsymbol{z} \in X^B(t),\, z_i = x_i^U(t), \\ \boldsymbol{u} \in \tilde{U}}} f_i(t, \boldsymbol{u}, \boldsymbol{z}), \tag{2b}$$

Then $\boldsymbol{x}(t, \boldsymbol{u}, \boldsymbol{x}_0) \in X^B(t)$ for all $(t, \boldsymbol{u}) \in I \times \tilde{U}$.

Based on the above result, Harrison (1977) suggested to compute $\dot{\boldsymbol{x}}^L$ and $\dot{\boldsymbol{x}}^U$ by applying NIE to $\boldsymbol{f}$. This method generates an *inclusion function* of $\boldsymbol{f}$ that is independent of $\boldsymbol{u}$ and $\boldsymbol{z}$, satisfying the following definition.

Definition 2 (Inclusion function)**.** *Let $S \in \mathbb{IR}^n$ and $\boldsymbol{h} : S \to \mathbb{R}^m$. An interval function $H = [\boldsymbol{h}^L, \boldsymbol{h}^U] : \mathbb{IR}^n \to \mathbb{IR}^m$ is a* inclusion function *of $\boldsymbol{h}$ on S if*

$$\{\boldsymbol{h}(\boldsymbol{z}) : \boldsymbol{z} \in Z\} \subseteq H(Z), \quad \forall Z \subseteq S.$$

Harrison also noted that choosing $\dot{\boldsymbol{x}}^L$ and $\dot{\boldsymbol{x}}^U$ close to the bounds given by (2) will empirically benefit the generated state bounds. A recent comparison result for ODE solutions (Song and Khan, 2020a) also confirms this. So, we explore the possibility of providing bounding information of f_i with convex relaxation, which is typically closer to the original function compared with NIE.

Definition 3 (Convex relaxation)**.** *Let $Z \in \mathbb{IR}^n$ and $\boldsymbol{h} : Z \to \mathbb{R}^m$. Then:*

(1) $\boldsymbol{h}^{cv} : Z \to \mathbb{R}^m$ is a convex relaxation *of $\boldsymbol{h}$ on Z if $\boldsymbol{h}^{cv}(\boldsymbol{z}) \leq \boldsymbol{h}(\boldsymbol{z})$ for all $\boldsymbol{z} \in Z$ and $\boldsymbol{h}^{cv}$ is convex on Z.*
(2) $\boldsymbol{h}^{cc} : Z \to \mathbb{R}^m$ is a concave relaxation *of $\boldsymbol{h}$ on Z if $\boldsymbol{h}^{cc}(\boldsymbol{z}) \geq \boldsymbol{h}(\boldsymbol{z})$ for all $\boldsymbol{z} \in Z$ and $\boldsymbol{h}^{cc}$ is concave on Z.*
(3) The interval function $H = [\boldsymbol{h}^{cv}, \boldsymbol{h}^{cc}]$ is called a convex inclusion function *of $\boldsymbol{h}$ on Z.*

4. NEW FORMULATION

Define an interval function $F^R = [\boldsymbol{f}^{cv}, \boldsymbol{f}^{cc}] : I \times U \times \mathbb{R}^{n_x} \to \mathbb{IR}^{n_x}$, and recall the considered ODE system (1).

Assumption 1. *Suppose that the interval function $F^R = [\boldsymbol{f}^{cv}, \boldsymbol{f}^{cc}]$ has the following properties:*

(1) $\boldsymbol{f}^{cv}$ and $\boldsymbol{f}^{cc}$ are continuous,
(2) $\boldsymbol{f}^{cv}$ and $\boldsymbol{f}^{cc}$ are locally Lipschitz continuous in $\boldsymbol{x}$, uniformly in $(t, \boldsymbol{p})$,
(3) $F^R(t, \cdot, \cdot)$ is an convex inclusion function of $\boldsymbol{f}(t, \cdot, \cdot)$ on $U \times D$ for a.e. $t \in I$.

Definition 4. *Under Assumption 1, define an interval function $F^B = [\boldsymbol{f}^L, \boldsymbol{f}^U] : I \times \mathbb{IR}^{n_x} \to \mathbb{IR}^{n_x}$ such that, for each $i \in \{1, \ldots, n_x\}, t \in I$, and $\Xi = [\boldsymbol{\xi}^L, \boldsymbol{\xi}^U] \in \mathbb{IR}^{n_x}$,*

$$f_i^L(t, \Xi) = \min_{\substack{\boldsymbol{z} \in \Xi,\, z_i = \xi_i^L, \\ \boldsymbol{p} \in U}} f_i^{cv}(t, \boldsymbol{p}, \boldsymbol{z}), \tag{3a}$$

$$\text{and} \quad f_i^U(t, \Xi) = \max_{\substack{\boldsymbol{z} \in \Xi,\, z_i = \xi_i^U, \\ \boldsymbol{p} \in U}} f_i^{cc}(t, \boldsymbol{p}, \boldsymbol{z}). \tag{3b}$$

Define the following auxiliary ODE system over $t \in I$:

$$\dot{\boldsymbol{x}}^L(t) = \boldsymbol{f}^L(t, X^B(t)), \;\; \boldsymbol{x}^L(t_0) = \boldsymbol{x}_0^L, \tag{4a}$$

$$\dot{\boldsymbol{x}}^U(t) = \boldsymbol{f}^U(t, X^B(t)), \;\; \boldsymbol{x}^U(t_0) = \boldsymbol{x}_0^U. \tag{4b}$$

4.1 Existence and uniqueness

This section shows that the auxiliary ODE system (4) has exactly one solution under mild assumptions.

Theorem 1. *Under Assumption 1, the ODE* (4) *has unique solutions.*

Proof. Define $\boldsymbol{g}^{cv}, \boldsymbol{g}^{cc} : I \times \mathbb{R}^{n_x} \to \mathbb{R}^{n_x}$ such that

$$g_i^{cv}(t, \boldsymbol{z}) = \min_{\boldsymbol{p} \in U} f_i^{cv}(t, \boldsymbol{p}, \boldsymbol{z}),$$

$$g_i^{cc}(t, \boldsymbol{z}) = \max_{\boldsymbol{p} \in U} f_i^{cc}(t, \boldsymbol{p}, \boldsymbol{z}),$$

for each $i \in \{1, \ldots, n_x\}$. Then, (3) becomes

$$\begin{aligned} f_i^L(t, \Xi) &= \min_{\boldsymbol{z} \in \Xi,\, z_i = \xi_i^L} g_i^{cv}(t, \boldsymbol{z}), \\ f_i^U(t, \Xi) &= \max_{\boldsymbol{z} \in \Xi,\, z_i = \xi_i^U} g_i^{cc}(t, \boldsymbol{z}). \end{aligned} \tag{5}$$

According to Assumption 1 and Clarke (1990, Theorem 2.1), $(\boldsymbol{g}^{cv}, \boldsymbol{g}^{cc})$ are Lipschitz continuous in $\boldsymbol{z}$, uniformly in t. Moreover, because $\boldsymbol{g}^{cv}(t, \cdot)$ and $\boldsymbol{g}^{cc}(t, \cdot)$ are readily verified to be convex and concave, respectively, Proposition 2 from Song and Khan (2020b) ensures that $(\boldsymbol{f}^L, \boldsymbol{f}^U)$ in (5) are Lipschitz continuous with respect to $\boldsymbol{\xi}^L$ and $\boldsymbol{\xi}^U$, uniformly for $t \in I$. Then, the existence and uniqueness of (4) is guaranteed by the Picard-Lindelöf Theorem (Hartman, 2002, Theorem 1.1, Chapter II). $\square$

4.2 Bounding the original system

This section shows that the auxiliary ODE (4) provides valid state bounds for (1).

Theorem 2. *Under Assumption 1, let $(\boldsymbol{x}^L, \boldsymbol{x}^U)$ be solutions of the ODE (4). Then, $(\boldsymbol{x}^L, \boldsymbol{x}^U)$ are state bounds of ODE (1).*

Proof. It suffices to show that the two requirements in Proposition 1 are satisfied by $(\boldsymbol{x}^L, \boldsymbol{x}^U)$. First, $\boldsymbol{x}_0 \in X^B(t_0)$ is ensured by the construction of auxiliary ODE system (4). Second, Condition 3 in Assumption 1 guarantees that, for a.e. $t \in I$ and any $(\boldsymbol{p}, \boldsymbol{z}) \in U \times D$,

$$\boldsymbol{f}^{cv}(t, \boldsymbol{p}, \boldsymbol{z}) \leq \boldsymbol{f}(t, \boldsymbol{p}, \boldsymbol{z}).$$

So for a.e. $t \in I$, each $\Xi \in \mathbb{IR}^{n_x}$, and each $i \in \{1, \ldots, n_x\}$,

$$\begin{aligned} \dot{x}_i^L(t) = f_i^L(t, \Xi) &= \min_{\substack{\boldsymbol{z} \in \Xi,\ z_i = \xi_i^L, \\ \boldsymbol{p} \in U}} f_i^{cv}(t, \boldsymbol{p}, \boldsymbol{z}) \\ &\leq \min_{\substack{\boldsymbol{z} \in \Xi,\ z_i = \xi_i^L, \\ \boldsymbol{u} \in \tilde{U}}} f_i(t, \boldsymbol{u}, \boldsymbol{z}). \end{aligned}$$

Similarly,

$$\dot{x}_i^U(t) = f_i^U(t, \Xi) \geq \max_{\substack{\boldsymbol{z} \in \Xi,\ z_i = \xi_i^U, \\ \boldsymbol{u} \in \tilde{U}}} f_i(t, \boldsymbol{u}, \boldsymbol{z}).$$

The second condition in Proposition 1 is thus satisfied. □

5. COMPLEMENTARITY REFORMULATION

This section derives a complementarity reformulation of (3) based on Karush-Kuhn-Tucker (KKT) conditions. To simplify notation, denote $\boldsymbol{y} = (\boldsymbol{x}, \boldsymbol{p}) \in \mathbb{R}^{n_x + n_u}$ in the remainder of this paper. We also define the following operators as did Scott and Barton (2013).

Definition 5. *For each $i \in \{1, \ldots, n_x\}$, define flattening operators $\underline{B}_i, \overline{B}_i : \mathbb{IR}^{n_x} \to \mathbb{IR}^{n_x}$ such that,*

(1) $\underline{B}_i([\boldsymbol{\phi}, \boldsymbol{\psi}]) = [\boldsymbol{\phi}, \boldsymbol{\psi}']$, where $\psi_i' = \phi_i$, and $\psi_k' = \psi_k$ for all $k \in \{1, \ldots, n_x\} \backslash \{i\}$,

(2) $\overline{B}_i([\boldsymbol{\phi}, \boldsymbol{\psi}]) = [\boldsymbol{\phi}', \boldsymbol{\psi}]$, where $\phi_i' = \psi_i$, and $\phi_k' = \phi_k$ for all $k \in \{1, \ldots, n_x\} \backslash \{i\}$.

The optimization problem in (3a) can be then reformulated as follows; with $\Xi = [\boldsymbol{\xi}^L, \boldsymbol{\xi}^U]$, $[\boldsymbol{\phi}_{(i)}^L, \boldsymbol{\phi}_{(i)}^U] = \underline{B}_i([(\boldsymbol{\xi}^L, \boldsymbol{u}^L), (\boldsymbol{\xi}^U, \boldsymbol{u}^U)])$,

$$\begin{aligned} \min_{\boldsymbol{y}} \quad & f_i^{cv}(t, \boldsymbol{y}), \\ \text{s.t.} \quad & \boldsymbol{\phi}_{(i)}^L \leq \boldsymbol{y} \leq \boldsymbol{\phi}_{(i)}^U. \end{aligned} \tag{6}$$

The corresponding KKT conditions are:

$$\begin{gathered} \nabla_{\underline{\boldsymbol{y}}^*} f_i^{cv}(t, \underline{\boldsymbol{y}}^*) + \overline{\boldsymbol{\mu}} - \underline{\boldsymbol{\mu}} = \boldsymbol{0}, \\ \boldsymbol{\phi}_{(i)}^L \leq \underline{\boldsymbol{y}}^* \leq \boldsymbol{\phi}_{(i)}^U, \\ \overline{\boldsymbol{\mu}} \geq \boldsymbol{0}, \quad \underline{\boldsymbol{\mu}} \geq \boldsymbol{0}, \\ (\overline{\boldsymbol{\mu}} - \underline{\boldsymbol{\mu}})^\top \underline{\boldsymbol{y}}^* + \underline{\boldsymbol{\mu}}^\top \boldsymbol{\phi}_{(i)}^L - \overline{\boldsymbol{\mu}}^\top \boldsymbol{\phi}_{(i)}^U = 0. \end{gathered} \tag{7}$$

Under Assumption 1, (6) is a box-constrained convex optimization problem which satisfies the linearity constraint qualification. So, satisfying the condition (7) is equivalent to $\boldsymbol{y}^*$ solving (6) directly. A similar formulation can be derived for the optimization problem in (3b): with $[\boldsymbol{\psi}_{(i)}^L, \boldsymbol{\psi}_{(i)}^U] = \overline{B}_i([(\boldsymbol{\xi}^L, \boldsymbol{u}^L), (\boldsymbol{\xi}^U, \boldsymbol{u}^U)])$,

$$\begin{gathered} \nabla_{\overline{\boldsymbol{y}}^*} f_i^{cc}(t, \overline{\boldsymbol{y}}^*) - \overline{\boldsymbol{\nu}} + \underline{\boldsymbol{\nu}} = \boldsymbol{0}, \\ \boldsymbol{\psi}_{(i)}^L \leq \overline{\boldsymbol{y}}^* \leq \boldsymbol{\psi}_{(i)}^U, \\ \overline{\boldsymbol{\nu}} \geq \boldsymbol{0}, \quad \underline{\boldsymbol{\nu}} \geq \boldsymbol{0}, \\ (\overline{\boldsymbol{\nu}} - \underline{\boldsymbol{\nu}})^\top \overline{\boldsymbol{y}}^* + \underline{\boldsymbol{\nu}}^\top \boldsymbol{\psi}_{(i)}^L - \overline{\boldsymbol{\nu}}^\top \boldsymbol{\psi}_{(i)}^U = 0. \end{gathered} \tag{8}$$

So (3) can be reformulated as

$$\begin{aligned} & f_i^L(t, \Xi) = f_i^{cv}(t, \underline{\boldsymbol{y}}^*), \\ \text{and} \quad & f_i^U(t, \Xi) = f_i^{cc}(t, \overline{\boldsymbol{y}}^*), \end{aligned} \tag{9}$$

where $\underline{\boldsymbol{y}}^*$ and $\overline{\boldsymbol{y}}^*$ are the KKT points in (7) and (8), respectively.

The dynamic system (4) with its RHS defined in (9) can thus be considered as a mixed nonlinear complementarity system (NCS), for which many numerical algorithms have been developed (Schumacher, 2004). In particular, a software platform Siconos (Acary and Pérignon, 2007) has been developed to solve NCSs efficiently.

6. CONSTRUCTING CONVEX INCLUSION FUNCTIONS OF $\boldsymbol{f}$

According to Theorem 2, state bounds for (1) can be computed by constructing a convex inclusion function of $\boldsymbol{f}$, $F^R = [\boldsymbol{f}^{cv}, \boldsymbol{f}^{cc}]$, that satisfies Assumption 1. One way to construct F^R is to use convex (concave) envelopes, which are defined as the supremum (infimum) of all convex under-estimators (concave over-estimators) of $\boldsymbol{f}$. In this case, we obtain the tightest bounds that are consistent with Proposition 1. However, the convex envelope is generally cumbersome or impossible to evaluate for multivariate functions. A practical and computationally simpler method for generating such a convex inclusion function is to derive αBB relaxations (Androulakis et al., 1995) for $\boldsymbol{f}$. Other relaxation approaches, such as McCormick relaxation (Scott et al., 2011; Khan et al., 2017, 2018), are also applicable.

6.1 αBB relaxation

αBB relaxation is an established technique (Adjiman et al., 1998) for constructing convex under-estimators for general nonconvex twice differentiable functions. To construct a relaxation, a negative convex quadratic term is added to the original function, $h : \mathbb{R}^n \to \mathbb{R}^m$:

$$h^{cv}(\boldsymbol{z}) := h(\boldsymbol{z}) + \sum_{i=1}^{n} \alpha_i (z_i^L - z_i)(z_i^U - z_i),$$

where $\boldsymbol{z}^L$ and $\boldsymbol{z}^U$ are the lower and upper bounds of $\boldsymbol{z}$, and $\boldsymbol{\alpha} \in \mathbb{R}^n$ is a constant vector that is determined by h, $\boldsymbol{z}^L$, and $\boldsymbol{z}^U$. Adjiman et al. (1998) propose an approach to construct a valid $\boldsymbol{\alpha}$ that ensures the convexity of the under-estimator h^{cv}. The first step of this approach is to determine a symmetric interval matrix $[\boldsymbol{H}]$ such that

$$\nabla^2 h(\boldsymbol{z}) \in [\boldsymbol{H}], \qquad \forall \boldsymbol{z} \in [\boldsymbol{z}^L, \boldsymbol{z}^U].$$

This can be accomplished by applying NIE to the Hessian matrix of h, denoted as $\boldsymbol{H}$. Then, each component α_i, $i \in \{1, \ldots, n\}$, can be calculated as

$$\alpha_i = \max \left\{ 0, -\frac{1}{2} \left(\underline{h}_{ii} - \sum_{j \neq i} |h|_{ij} \right) \right\}, \tag{10}$$

where $|h|_{ij} = \max\{|\underline{h}_{ij}|, |\overline{h}_{ij}|\}$, and $\underline{h}_{ij}, \overline{h}_{ij}$ are the lower and upper bounds of h_{ij} in $\boldsymbol{H}$, respectively. Correspondingly, a concave over-estimator can be constructed by taking the negative of the αBB convex under-estimator of $-h(\boldsymbol{z})$.

Using αBB relaxation, a convex inclusion function F^R that satisfies Assumption 1 can be constructed as follows.

Definition 6. *Define an αBB relaxation $F^\alpha = [\boldsymbol{f}^{cv}, \boldsymbol{f}^{cc}] : I \times \mathbb{IR}^{n_y} \to \mathbb{IR}^{n_y}$ such that, for each $i \in \{1, \ldots, n_x\}$,*

$$f_i^{cv}(t, \boldsymbol{y}) = f_i(t, \boldsymbol{y}) + \sum_{j=1}^{n_y} a_{ij}^{cv}(t)(y_j^L - y_j)(y_j^U - y_j), \quad (11a)$$

$$f_i^{cc}(t, \boldsymbol{y}) = f_i(t, \boldsymbol{y}) - \sum_{j=1}^{n_y} a_{ij}^{cc}(t)(y_j^L - y_j)(y_j^U - y_j), \quad (11b)$$

where the ith rows of matrices $\boldsymbol{A}^{cv}(t)$ and $\boldsymbol{A}^{cc}(t)$ are $\boldsymbol{\alpha}$ factors for $f_i(t, \cdot)$ and $-f_i(t, \cdot)$, respectively, obtained as in (Adjiman et al., 1998).

The αBB parameters in $\boldsymbol{A}^{cv}(t)$ and $\boldsymbol{A}^{cc}(t)$ can be calculated via (10) at each $t \in I$ with $\boldsymbol{y}^L = (\boldsymbol{\xi}^L(t), \boldsymbol{u}^L)$ and $\boldsymbol{y}^U = (\boldsymbol{\xi}^U(t), \boldsymbol{u}^U)$. Alternatively, if constant bounds of $\boldsymbol{x}$ are available on $I \times U$, then these can be used to determine another valid combination of $\boldsymbol{y}^L$ and $\boldsymbol{y}^U$. Such bounds may be a rough enclosure of the reachable set, or may be computed by an established state bounding method, such as by Harrison (1977).

Since the original RHS function $\boldsymbol{f}$ is twice differentiable, it is readily verified that F^α in Definition 6 is a valid choice of F^R that satisfies Assumption 1, and may be employed in the state bounding system (4).

6.2 Specialization to quadratic functions

If the original RHS function $\boldsymbol{f}$ in (1) is quadratic, then its αBB relaxations $\boldsymbol{f}^{cv}$ and $\boldsymbol{f}^{cc}$ are also quadratic. For an arbitrary $i \in \{1, \ldots, n_x\}$, suppose that

$$f_i(t, \boldsymbol{y}) = \boldsymbol{y}^\top \boldsymbol{Q} \boldsymbol{y} + \boldsymbol{q}^\top \boldsymbol{y} + c,$$

where $\boldsymbol{Q}$ is symmetric.

Definition 7. *For matrices (or vectors) $\boldsymbol{A}, \boldsymbol{B} \in \mathbb{R}^{m \times n}$, their* Hadamard product *$\boldsymbol{A} \odot \boldsymbol{B} \in \mathbb{R}^{m \times n}$ is a matrix with elements*

$$(\boldsymbol{A} \odot \boldsymbol{B})_{ij} = a_{ij} b_{ij}.$$

Let $\boldsymbol{a}_{(i)}^{cv}$ be the transposed ith row of $\boldsymbol{A}^{cv}$. Then, (11a) provides

$$\begin{aligned} f_i^{cv}(t, \boldsymbol{y}) &= \boldsymbol{y}^\top \boldsymbol{Q} \boldsymbol{y} + \boldsymbol{q}^\top \boldsymbol{y} + c + \sum_{j=1}^{n_y} a_{ij}^{cv}(y_j^L - y_j)(y_j^U - y_j) \\ &= \boldsymbol{y}^\top \tilde{\boldsymbol{Q}} \boldsymbol{y} + \tilde{\boldsymbol{q}}^\top \boldsymbol{y} + \tilde{c}, \end{aligned}$$

where, with $\mathrm{diag}(\boldsymbol{a}_{(i)}^{cv})$ denoting the diagonal matrix with components of $\boldsymbol{a}_{(i)}^{cv}$ along its main diagonal,

$$\begin{aligned} \tilde{\boldsymbol{Q}} &:= \boldsymbol{Q} + \mathrm{diag}(\boldsymbol{a}_{(i)}^{cv}), \\ \tilde{\boldsymbol{q}} &:= \boldsymbol{q} - \boldsymbol{a}_{(i)}^{cv} \odot (\boldsymbol{y}^L + \boldsymbol{y}^U), \\ \tilde{c} &:= c + \sum_{j=1}^{n_y} a_{ij}^{cv} y_j^L y_j^U. \end{aligned}$$

Then, the optimization problem in (3a) can be expressed as a convex quadratic program (QP); with $\Xi = [\boldsymbol{\xi}^L, \boldsymbol{\xi}^U]$, $[\boldsymbol{\phi}_{(i)}^L, \boldsymbol{\phi}_{(i)}^U] = \underline{B}_i([(\boldsymbol{\xi}^L, \boldsymbol{u}^L), (\boldsymbol{\xi}^U, \boldsymbol{u}^U)])$,

$$\begin{aligned} \min_{\boldsymbol{y}} \quad & \boldsymbol{y}^\top \tilde{\boldsymbol{Q}} \boldsymbol{y} + \tilde{\boldsymbol{q}}^\top \boldsymbol{y} + \tilde{c}, \\ \text{s.t.} \quad & \boldsymbol{\phi}_{(i)}^L \leq \boldsymbol{y} \leq \boldsymbol{\phi}_{(i)}^U. \end{aligned} \quad (12)$$

The KKT conditions of (12) can be derived accordingly:

$$\begin{aligned} 2\tilde{\boldsymbol{Q}} \boldsymbol{y}^* + \tilde{\boldsymbol{q}} + \overline{\boldsymbol{\mu}} - \underline{\boldsymbol{\mu}} &= \boldsymbol{0}, \\ \boldsymbol{\phi}_{(i)}^L \leq \boldsymbol{y}^* &\leq \boldsymbol{\phi}_{(i)}^U, \\ \overline{\boldsymbol{\mu}} \geq \boldsymbol{0}, \quad \underline{\boldsymbol{\mu}} &\geq \boldsymbol{0}, \\ (\overline{\boldsymbol{\mu}} - \underline{\boldsymbol{\mu}})^\top \boldsymbol{y}^* + \underline{\boldsymbol{\mu}}^\top \boldsymbol{\phi}_{(i)}^L - \overline{\boldsymbol{\mu}}^\top \boldsymbol{\phi}_{(i)}^U &= 0. \end{aligned} \quad (13)$$

A vector $\boldsymbol{y}^*$ solves (12) if and only if there are multipliers $(\overline{\boldsymbol{\mu}}, \underline{\boldsymbol{\mu}})$ for which $(\boldsymbol{y}^*, \overline{\boldsymbol{\mu}}, \underline{\boldsymbol{\mu}})$ solves (13).

Note that the QPs described in (12) and (13) are solvable by efficient commercial solvers such as CPLEX and Gurobi. They may also be treated as multi-parametric quadratic programs (Pistikopoulos, 2009), in which the optimum of the optimization problem is considered as a function of varying parameters. The advantage of this strategy is that an analytical expression of the optimum function can in principle be obtained in advance, for quick online evaluation.

Moreover, the KKT conditions in (13) also comprise a mixed linear complementarity problem (MLCP). Comprehensive theoretical results and various numerical algorithms for LCPs and MLCPs can be found in literature; see e.g. Cottle et al. (1992).

7. NUMERICAL EXAMPLES

This section presents numerical examples in which state bounds are constructed for nonlinear dynamic system with our new method described in Sections 4 and 6. This method was implemented in Julia v1.4.2 with the auxiliary system of ODEs solved with DifferentialEquations.jl. All numerical experiments were performed on a Windows 10 machine with an AMD Ryzen 2600X CPU and 16GB memory.

The first example involves a simple ODE system with a quadratic RHS.

Example 1. *Consider the quadratic ODEs:*

$$\begin{aligned} \dot{x}_1(t, \boldsymbol{u}) &= (x_1 - u_1)^2 - (x_2 - u_1)^2, \ x_1(t_0) = 2.2, \\ \dot{x}_2(t, \boldsymbol{u}) &= (x_1 - u_2)^2 - (x_2 - u_2)^2, \ x_2(t_0) = 1.8, \end{aligned}$$

where $U \equiv [-2, 2] \times [-1, 3]$, $\boldsymbol{u} = (u_1, u_2) \in \tilde{U}$, and $I \equiv [t_0, t_f] = [0.0, 0.2]$.

Using the approach from Section 6.2, we derived quadratic αBB relaxations of $\boldsymbol{f}$, and the QPs (12) in (4) were solved with CPLEX v12.10. The resulting bounds are illustrated in Figure 1, along with Harrison's NIE-based method and trajectories of the original system. This figure shows that the time-varying bounds generated by our new method are tighter than those by Harrison's method.

Next, we consider the Van der Pol oscillator, which is a classic dynamic system that has been widely studied in electrical engineering and biological science. Relaxations of this system were obtained by Shen and Scott (2017). Here,

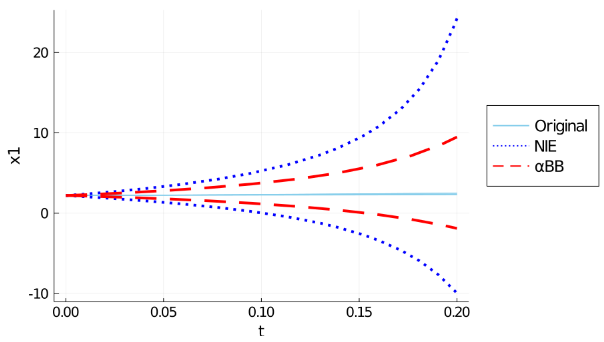

Fig. 1. State bounds of x_1 in Example 1 computed by relaxing RHS functions with NIE (dotted) and αBB relaxation in (4) (dashed). Solid (overlapping) lines are real trajectories.

we consider its two-dimensional form with uncertainty in both initial conditions and RHS functions.

Example 2. *Consider the Van der Pol oscillator:*

$$\dot{x}_1(t,\boldsymbol{u}) = x_1, \qquad x_1(t_0,\boldsymbol{u}) = u_1(t_0),$$
$$\dot{x}_2(t,\boldsymbol{u}) = u_1(1-x_1^2)x_2 - x_1, \quad x_2(t_0,\boldsymbol{u}) = u_2(t_0),$$

where $U \equiv [1.399, 1.400] \times [2.299, 2.300]$, $\boldsymbol{u} = (u_1, u_2) \in \tilde{U}$, *and* $I \equiv [t_0, t_f] = [0, 6]$.

The αBB relaxations of this ODE's RHS functions were obtained via (11) and optimized by IPOPT (Wächter and Biegler, 2006). State bounds were computed for the state variable x_1 using Harrison's method (NIE) and our new αBB-based method, and are plotted in Figure 2. In this case, the new method generates a better enclosure while Harrison's method explodes faster.

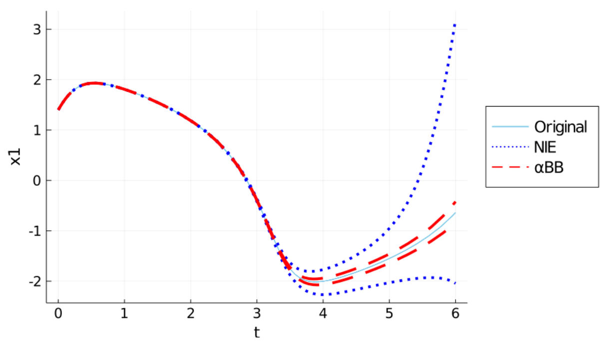

Fig. 2. State bounds of x_1 in Example 2 computed by relaxing RHS functions with NIE (dotted) and αBB relaxation in (4) (dashed). Solid (overlapping) lines are real trajectories.

The last example involves a bioreactor process (Bastin and Dochain, 1990). An enclosure of this system was obtained by Lin and Stadtherr (2006).

Example 3. *Consider a microbial growth process described by the following ODE system:*

$$\dot{X} = (\mu - \alpha D)X, \qquad X(t_0) = 0.82,$$
$$\dot{S} = D(S^i - S) - k\mu X, \quad S(t_0) = 0.8,$$

where state variables X *and* S *respectively represent the concentrations of biomass and substrate,* $I \equiv [t_0, t_f] = [0, 3]$, *and* μ *is the growth rate*

$$\mu = \frac{\mu_m S}{K_S + S + K_I S^2}.$$

The remaining quantities are parameters, whose values and uncertainties are provided in Table 1.

Table 1. Microbial growth process parameters

Parameter	Symbol	Value	Unit
Process heterogeneity	α	0.5	-
Dilution rate	D	0.36	day^{-1}
Influent concentration	S^i	5.7	g S/l
Yield coefficient	k	10.53	g S/g X
Max growth rate	μ_m	1.2	day^{-1}
Kinetic parameter	K_S	[7.0, 7.2]	g S/l
Kinetic parameter	K_I	[0.4, 0.6]	(g S/l)$^{-1}$

In this numerical experiment, we consider the two kinetic parameters K_S and K_I, to have bounded uncertainties. Corresponding state bounds were constructed with αBB relaxations in (4), and are shown in Figure 3. This figure shows that the proposed new approach produces a tighter enclosure for the biomass concentration than Harrison's method.

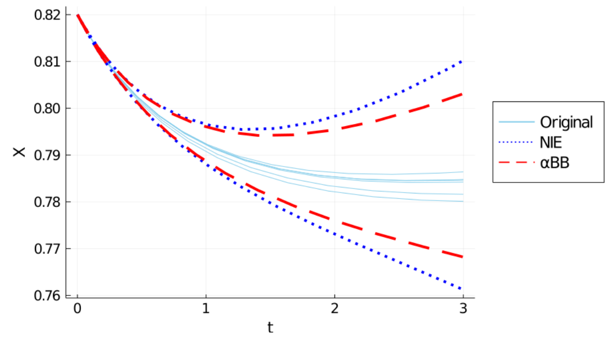

Fig. 3. State bounds of X in Example 3 computed by relaxing RHS functions with NIE (dotted) and αBB relaxation in (4) (dashed). Solid lines are real trajectories.

8. CONCLUSION

We have developed an approach for computing tight enclosures for nonlinear control systems based on differential inequalities. Bounding information for the original RHS function $\boldsymbol{f}$ is obtained by optimizing its convex relaxations. We investigated the usage of αBB relaxation in this context, and developed the corresponding complementarity reformulation as an NCS. Our numerical results illustrate the tightness of the time-varying interval bounds generated by our new method. Future work may involve exploring the usage of other established convex relaxation techniques (Scott et al., 2011; Khan et al., 2017, 2018). Our proof-of-concept implementation involves repeatedly solving optimization problems during integration, which requires a considerable amount of computing effort, especially when the system of interest is nonlinear. As suggested in Section 5, a specialized complementarity system solver would help in a more sophisticated implementation.

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