Set-Theoretic Approaches in Analysis, Estimation and Control of Nonlinear Systems

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Abstract: This paper gives an overview of recent developments in set-theoretic methods for nonlinear systems, with a particular focus on the activities in our own research group. Central to these approaches is the ability to compute tight enclosures of the range of multivariate systems, e.g. using ellipsoidal calculus or higher-order inclusion techniques based on multivariate polynomials, as well as the ability to propagate these enclosures to enclose the trajectories of parametric or uncertain differential equations. We illustrate these developments with a range of applications, including the reachability analysis of nonlinear dynamic systems; the determination of all equilibrium points and bifurcations in a given state-space domain; and the solution of set-membership parameter estimation problems. We close the paper with a discussion about on-going research in tube-based methods for robust model predictive control.

Keywords: affine-set parameterization; differential equations; reachable set; bifurcation analysis; set-membership estimation

1. INTRODUCTION

Many engineering design and control problems can be formulated, analyzed or solved in a set-theoretic framework. By set-theoretic we refer here to any method which exploits properties of suitably chosen sets or constructed sets in the state space (Blanchini and Miani, 2008). In designing a control system for instance, the constraints, uncertainties and design specifications all together are described naturally in terms of sets; and in measuring the effect of a disturbance on a system's response or in bounding the error of an estimation algorithm likewise, sets play a central role. A number of key set-theoretic concepts have been proposed in the early 1970s, but their systematic applications were not possible until enough computational capability became widely available.

Today, many such methods and tools are available for the estimation and control of linear systems – Witness for instance the popularity of Matlab's Multi-Parametric Toolbox (Herceg et al., 2013). To name but a few features, they support the construction and a variety of operations on convex sets, the synthesis and implementation of explicit model predictive control (MPC) for linear time invariant or piecewise affine systems, the construction of maximal invariant sets or Lyapunov functions for piecewise affine systems, *etc* (see, e.g., Kurzhanski and Valyi, 1997; Blanchini and Miani, 2008).

The focus in this paper is on set-theoretic methods for nonlinear systems which can offer computational guarantees or certificates, with a strong emphasis on recent developments in our own research group. As such, the paper may not be considered a review or survey paper, although effort is made to point the reader to relevant, alternative approaches or related work throughout. Despite enormous progress in recent years, set-theoretic methods and tools for nonlinear systems are not as developed as their linear counterparts, and they still constitute a widely open field of research when it comes to computational efficiency; see, e.g., Streif et al. (2013) for a recent survey (with applications to biochemical networks).

A key enabler for set-theoretic methods is the ability to enclose the range of nonlinear multivariate systems, and the class of factorable functions—namely, those functions which can be represented by means of a finite computational graph—has attracted much attention. Since the invention of interval analysis by Moore more than 50 years ago, many computational techniques have been developed to construct tight enclosures for the range of factorable functions. The focus in the first part of the paper (Sect. 2) is on so-called affine set-parameterizations, which encompass both convex and nonconvex set parameterizations. Among the alternatives to enclose the range of functions or sets defined by equalities and/or inequalities, mention should be made of the sum-of-squares (SOS) approaches which provide nested sequences outer-approximations as hierarchies of linear matrix inequality (LMI) relaxations (Lasserre, 2009); see also Parrilo (2003).

Questions of reachability and invariance have been studied extensively in the dynamics and control literature due to their wide range of applications. Direct characterization of reachability concepts is one of the topics addressed by viability theory (Aubin, 1991), and the development of computational tools supported by these theories is an ongoing effort. In Sect. 3, we describe a number of direct approaches that rely on the discrete- or continuous-time propagation of affine set-parameterizations. Similar to the factorable case above, alternative approaches recently developed involve constructing outer-approximations of the reachable set of (possible controlled and constrained) dynamic systems as hierarchies of linear matrix inequality (LMI) relaxations (Henrion and Korda, 2014). Moreover, so-called indirect approaches have also been developed, which formulate reachability questions as optimal control (or game theory) problems and determine reachable-set outer-approximations by Hamilton-Jacobi projections (Mitchell and Tomlin, 2003; Lygeros, 2004). Related to reachability analysis, the problems of computing the region of attraction of a target set or the maximum invariant set are also essential and long-standing challenges in dynamic system and control theory (Henrion and Korda, 2014; Korda et al., 2014).

A great variety of algorithms, including complete search methods for problems in global optimization, constraint satisfaction or robust estimation, hinge on the ability to enclose the range of functions or the reachable set of dynamic systems. Our focus in the second part of the paper (Sect. 4) is more specifically on two selected problems: (i) the determination of all equilibrium points and bifurcations of a nonlinear dynamic system (Mönnigmann and Marquardt, 2002; Waldherr and Allgöwer, 2011); and (ii) the solution of set-membership parameter estimation problems in dynamic systems (Walter and Piet-Lahanier, 1990). Finally, we conclude the paper with a discussion about the application of set-theoretic methods in tube-based methods for robust model predictive control (Sect. 5).

1.1 Case Study Problem Definition

The modeling of bioprocesses often gives rise to challenging dynamic systems, whereby differential equations describing species mass balances in the system are coupled with algebraic equations describing charge balance or other fast phenomena that are assumed to be at equilibrium (or quasi steady-state). Throughout this paper, we consider a two-reaction model of anaerobic digestion inspired from (Bernard et al., 2001)—All the parameter values are reported in Table A.1 (Appendix) for the sake of reproducibility.

The model involves an acetogenesis step, where organic compounds (S_1) are converted into VFA (S_2), followed by a methanogenic step; these steps are associated with the bacterial populations X_1 and X_2, respectively:

- Acetogenesis: $k_1\, S_1 \overset{\mu_1(\cdot)X_1}{\longrightarrow} X_1 + k_2\, S_2 + k_4\, \mathrm{CO_2}$
- Methanogenesis: $k_3\, S_2 \overset{\mu_2(\cdot)X_2}{\longrightarrow} X_2 + k_5\, \mathrm{CO_2} + k_6\, \mathrm{CH_4}$

The biological kinetics for the reactions are:

$$\mu_1(S_1) = \bar{\mu}_1 \frac{S_1}{S_1 + K_{S1}}, \quad \mu_2(S_2) = \bar{\mu}_2 \frac{S_2}{S_2 + K_{S2} + \frac{S_2^2}{K_{I2}}}.$$

Under the assumptions that the liquid phase is perfectly mixed and that only a fraction α of the biomass is not attached onto a support inside the digester, the species balance equations for the state variables S_1, X_1, S_2, X_2, inorganic carbon (C) and alkalinity Z are given by:

$$\dot{S}_1 = D(S_1^{\rm in} - S_1) - k_1\mu_1(S_1)X_1 \quad (1)$$

$$\dot{X}_1 = (\mu_1(S_1) - \alpha D)X_1 \quad (2)$$

$$\dot{S}_2 = D(S_2^{\rm in} - S_2) + k_2\mu_1(S_1)X_1 - k_3\mu_2(S_2)X_2 \quad (3)$$

$$\dot{X}_2 = (\mu_2(S_2) - \alpha D)X_2 \quad (4)$$

$$\dot{Z} = D(Z^{\rm in} - Z) \quad (5)$$

$$\dot{C} = D(C^{\rm in} - C) - q_{\rm CO_2} + k_4\mu_1(S_1)X_1 + k_5\mu_2(S_2)X_2\,, \quad (6)$$

with D, the dilution rate; and $S_1^{\rm in}$, $S_2^{\rm in}$, $C^{\rm in}$ and $Z^{\rm in}$, the inlet concentrations. Note that these balances neglect gaseous emissions other than $\mathrm{CO_2}$ and methane. Under the assumption that the pH range is between 6-8 (normal operation), a charge-balance equation gives:

$$\mathrm{CO_{2aq}} = C + S_2 - Z\,.$$

Finally, assuming that the partial pressures of $\mathrm{CO_2}$ ($P_{\rm CO_2}$) and methane ($P_{\rm CH_4}$) quickly reach equilibrium and that the gas phase behaves ideally, we have:

$$\frac{P_{\rm tot} - P_{\rm CO_2}}{q_{\rm CH_4}} = \frac{P_{\rm CO_2}}{q_{\rm CO_2}}\,, \quad (7)$$

where the liquid-gas transfer rate of $\mathrm{CO_2}$ and methane are given by:

$$q_{\rm CH_4} = \alpha_{11}\mu_2(S_2)X_2$$

$$q_{\rm CO_2} = k_{\rm L}a\left(\mathrm{CO_{2aq}} - K_{\rm H}P_{\rm CO_2}\right)$$

with $K_{\rm H}$, Henry's constant for $\mathrm{CO_2}$; and $k_{\rm L}a$, the liquid-gas transfer coefficient.

Notice that (7) leads to a quadratic equation in $P_{\rm CO_2}$, and therefore the model (1)-(7) comes in the form of a (semi-explicit index-1) DAE system. Nonetheless, (7) has a unique nonnegative root in the form:

$$P_{\rm CO_2} = \frac{\phi_{\rm CO_2} - \sqrt{\phi_{\rm CO_2}^2 - 4K_{\rm H}P_{\rm t}\mathrm{CO_{2aq}}}}{2K_{\rm H}}$$

$$\text{with: } \phi_{\rm CO_2} := \mathrm{CO_{2aq}} + K_{\rm H}P_{\rm t} + \frac{k_6}{k_{\rm L}a}\mu_2(S_2)X_2,$$

which can be used to formulate an equivalent ODE system.

Overall, this anaerobic digestion model is challenging as it features complex dynamics due to pH self-regulation and liquid-gas transfer. Moreover, the processes span multiple time scales, with fast dynamics acting on a time-scale of minutes/hours, and slow dynamics acting on a time-scale of days.

1.2 Notation

The set of compact subsets of $\mathbb{R}^n$ is denoted by $\mathbb{K}^n$, and the subset of compact convex subsets of $\mathbb{K}^n$, by $\mathbb{K}^n_{\rm C}$. The diameter $\text{diam}\,(Z)$ of a set $Z \in \mathbb{K}^n$ is defined as

$$\text{diam}\,(Z) := \max_{z,z' \in Z} \|z - z'\| \,,$$

for any given norm on $\mathbb{R}^n$, and the support function $V[Z] : \mathbb{R}^n \to \mathbb{R}$ of Z as

$$\forall c \in \mathbb{R}^n \,, \quad V[Z](c) := \max_z \; \left\{ c^{\mathrm{T}} z \mid z \in Z \right\} \,. \qquad (8)$$

The Minkowski sum $W \oplus Z$, the Minkowski difference $W \ominus Z$ and the Haussdorf distance $d_{\mathrm{H}}(W, Z)$ between two compact sets $W, Z \in \mathbb{K}^n$ are given by

$$\begin{aligned} W \oplus Z &:= \{ w + z \mid w \in W, z \in Z \} \,, \\ W \ominus Z &:= \{ w - z \mid w \in W, z \in Z \} \,, \\ d_{\mathrm{H}}(W, Z) &:= \max \left\{ \max_{w \in W} \min_{z \in Z} \|w - z\| \,, \max_{z \in Z} \min_{w \in W} \|w - z\| \right\} . \end{aligned}$$

In particular, if $W \subseteq Z$ we have

$$d_{\mathrm{H}}(W, Z) = \max_{z \in Z} \min_{w \in W} \|w - z\| \,.$$

The set of n-dimensional interval vectors is denoted by $\mathbb{IR}^n$. The midpoint and radius of an interval vector $P := \left[p^{\mathrm{L}}, p^{\mathrm{U}}\right] \in \mathbb{IR}^n$ are defined as $\text{mid}(P) := \frac{1}{2}(p^{\mathrm{U}} + p^{\mathrm{L}})$ and $\text{rad}(P) := \frac{1}{2}(p^{\mathrm{U}} - p^{\mathrm{L}})$, respectively. The n-by-n matrix $\text{diag rad}\,(P) \in \mathbb{R}^{n \times n}$ is a diagonal matrix whose elements are the components of $\text{rad}(P)$.

The set of n-dimensional positive semi-definite symmetric matrices is denoted by $\mathbb{S}^n_+$. An ellipsoid with shape matrix $S \in \mathbb{S}^n_+$ and centered at the origin is denoted by

$$\mathcal{E}(S) := \left\{ S^{\frac{1}{2}} v \;\mid\; v \in \mathbb{R}^n, v^{\mathrm{T}} v \leq 1 \right\} .$$

2. THE BUILDING BLOCKS

Central to set-theoretic approaches described in this paper is the selection of parameterizations that can describe/approximate compact subset in $\mathbb{R}^n$. To keep our considerations general, we consider *affine set-parameterizations* (Houska et al., 2014), a particular class of computer-representable sets in the form $(\mathbb{E}_m, \mathbb{D}_{n,m})$ such that:

$$\forall Q \in \mathbb{D}_{n,m}, \quad \text{Im}_{\mathbb{E}_m}(Q) \;:=\; \left\{ Q \, [\, b \; 1\,]^{\mathsf{T}} \mid b \in \mathbb{E}_m \right\} ,$$

with $\mathbb{E}_m \subseteq \mathbb{R}^m$, $m \geq 1$, the so-called basis set; and $\mathbb{D}_{n,m} \subseteq \mathbb{R}^{n \times (m+1)}$, $n \geq 1$, associated domain set.

Usual convex sets such as intervals, ellipsoids or polytopes can be characterized using affine set-parameterizations with convex basis sets—see top row of Fig. 1. In particular, the parameterization $(\mathbb{E}^{\text{ball}}_m, \mathbb{R}^{n \times (m+1)})$ with $\mathbb{E}^{\text{ball}}_m := \{ \xi \in \mathbb{R}^m \mid \|\xi\|_2 \leq 1 \}$ describes ellipsoids in $\mathbb{R}^n$.

Nonconvex sets too can be represented in terms of affine set-parameterizations. For instance, the affine set-parameterization $(\mathbb{E}^{\text{pol}(q)}_m, \mathbb{R}^{n \times \alpha^{(q)}_m})$ with nonconvex basis set $\mathbb{E}^{\text{pol}(q)}_m := \{ P^{(q)}_m(\xi) \mid \xi \in [-1, 1]^m \}$, where $P^{(q)}_m(\xi) \in \mathbb{R}^{\alpha^{(q)}_m}$ is the vector containing the first $\alpha^{(q)}_m$ monomials in ξ in lexicographic order,

$$P^{(q)}_m(\xi) := \{ 1, \xi_1, \ldots, \xi_m, \xi_1^2, \xi_1 \xi_2, \ldots, \xi_m^2, \xi_1^3, \ldots, \xi_m^q \} \,,$$

describes the image set of qth-order polynomials in m variables. Naturally, alternative polynomial parameterizations are possible with different polynomial bases, such as the Chebyshev polynomials of the first kind defined by the recurrence relation

$$\begin{aligned} T_0(\xi) &= 1, \quad T_1(\xi) = \xi \\ T_{k+1}(\xi) &= 2\xi T_k(\xi) - T_{k-1}(\xi), \quad k \geq 1 \,, \end{aligned}$$

which leads to:

$$\begin{aligned} P^{(q)}_m(\xi) := \{ & 1, T_1(\xi_1), \ldots, T_1(\xi_m), T_2(\xi_1), T_1(\xi_1) T_1(\xi_2), \ldots, \\ & T_2(\xi_m), T_3(\xi_1), \ldots, T_q(\xi_m) \} \,. \end{aligned}$$

More involved representations of nonconvex sets can be constructed by combining convex and nonconvex basis sets in turn. Polynomial image sets combined with intervals or ellipsoids, for instance, are illustrated in the bottom row of Fig. 1. These are commonly referred to as Taylor or Chebyshev models in the literature—see Sect. 2.2.

An important property of affine set-parameterizations is invariance under affine transformation, that is, the property of a parameterized set's image under any affine transformation to be *exactly* representable on the same basis set. Among the foregoing examples, the classes of ellipsoids, polytopes and polynomial image sets are all invariant under affine transformation, and so is any finite combination of these parameterizations. In contrast, the class of interval boxes is not invariant under affine transformation given that the rotation of an interval box may yield another interval box whose edges are no longer aligned with the original axes—this is one of the main sources of the wrapping effect in interval analysis. It should also be clear that any affine set-parameterization obtained from the combination with interval boxes will fail to be invariant under affine transformation, including Taylor/Chebyshev models with interval remainder terms.

2.1 Affine Set-Parameterization Extensions

Factorable functions cover an extremely inclusive class of functions which can be represented finitely on a computer by means of a code list or a computational graph involving atom operations. These are typically unary and binary operations within a library of atom operators, which can be based for example on the C-code library `math.h`. Natural interval extensions and their variants (Moore et al., 2009) were among the first techniques developed for bounding the range of factorable functions. The concept of interval extension in interval analysis extends readily to affine set-parameterizations.

Given a function $g : \mathbb{R}^n \to \mathbb{R}^p$ and two affine set-parameterizations $(\mathbb{E}_m, \mathbb{D}_{n,m})$ and $(\mathbb{E}_m, \mathbb{D}_{p,m})$, we call the function $g^{\mathbb{E}_m} : \mathbb{D}_{n,m} \to \mathbb{D}_{p,m}$ an $\mathbb{E}_m$-extension of g if

$$\forall Q \in \mathbb{D}_{n,m}, \; \text{Im}_{\mathbb{E}_m}\left(g^{\mathbb{E}_m}(Q) \right) \;\supseteq\; g(\text{Im}_{\mathbb{E}_m}(Q)) \,,$$

with $g(\text{Im}_{\mathbb{E}_m}(Q)) := \{ g(z) \mid z \in \text{Im}_{\mathbb{E}_m}(Q) \}$. A key property of an affine set-parameterization extension is how much overestimation it carries with respect to the image set of the original function (Fig. 2). In particular, the extension $g^{\mathbb{E}_m}$ is said to have Hausdorff convergence order $\beta \geq 1$, if

$$\begin{aligned} \forall Q \in \mathbb{D}_{n,m}, \quad & d_{\mathrm{H}}\left(\text{Im}_{\mathbb{E}_m}\left(g^{\mathbb{E}_m}(Q) \right), g(\text{Im}_{\mathbb{E}_m}(Q)) \right) \\ & \in O(\text{diam}(\text{Im}_{\mathbb{E}_m}(Q))^{\beta}) \,. \quad (9) \end{aligned}$$

In general, extensions that have Hausdorff convergence order two (or higher) may not exist when the underlying affine set-parameterizations is not invariant under affine transformation.

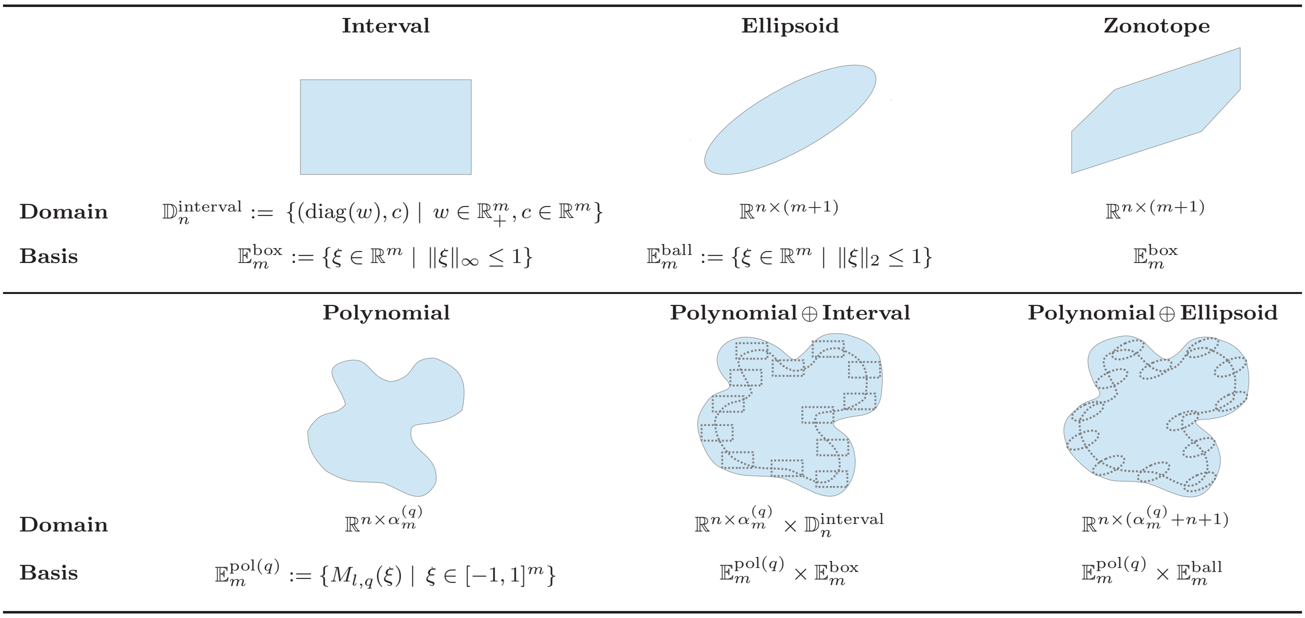

Fig. 1. Illustration of affine set parameterizations with convex (top row) and nonconvex (bottom row) basis sets.

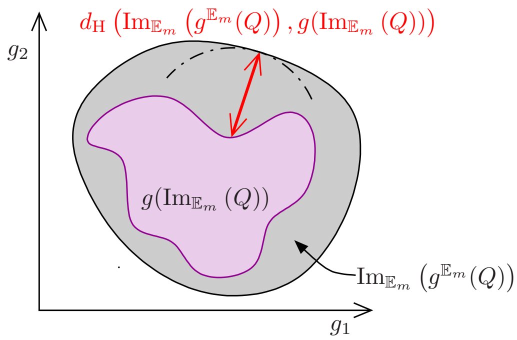

Fig. 2. Illustration of an extension and the corresponding overestimation in terms of the Hausdorff distance.

2.2 Practical Construction of High-Order Inclusions

The construction of extensions can be automated for factorable functions using a variety of arithmetics, which can be conveniently implemented in computer programs. Unlike interval arithmetic, Taylor and Chebyshev model arithmetics can be used to construct extension functions that enjoy higher-order Hausdorff convergence (see Fig. 3). The idea is to propagate the polynomial part (expressed either in monomial or Chebyshev basis) by symbolic calculations wherever possible, and processing the interval remainder term as well as the higher-order terms according to the rules of interval arithmetic.

Given a $(q+1)$-times continuously-differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ on the set $P \in \mathbb{IR}^n$, a qth-order Taylor model of f on P at a point $\hat{p} \in P$ is the pair $(\mathcal{P}_{f,P}^q, \mathcal{R}_{f,P}^q)$ of a qth-order multivariate polynomial $\mathcal{P}_{f,P}^q : \mathbb{R}^n \to \mathbb{R}$ with an interval remainder $\mathcal{R}_{f,P}^q \in \mathbb{IR}$ satisfying [1]

[1] Multi-index notation: A multi-index γ is a vector in $\mathbb{N}^n$, $n > 0$. The order of γ is $|\gamma| := \sum_{i=1}^n \gamma_i$. Given a point $p \in \mathbb{R}^n$, p^γ is a shorthand notation for the expression $\prod_{i=1}^n p_i^{\gamma_i}$, and $T_\gamma(p)$ for $\prod_{i=1}^n T_{\gamma_i}(p_i)$. Moreover, $\partial^\gamma f$ is a shorthand notation for the partial derivative $\frac{\partial^{|\gamma|} f}{\partial p_1^{\gamma_1} \cdots \partial p_n^{\gamma_n}}$.

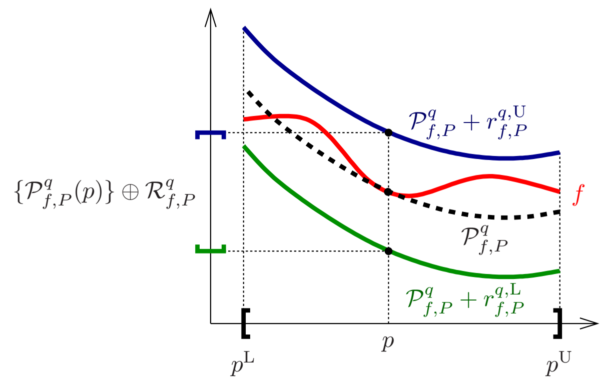

Fig. 3. Illustration of Taylor/Chebyshev models.

$$\forall p \in P\,, \quad f(p) - \mathcal{P}_{f,P}^q(p) \in \mathcal{R}_{f,P}^q \quad \text{and}$$
$$\mathcal{P}_{f,P}^q(p) = \sum_{\gamma\in\mathbb{N}^n, |\gamma|\leq q} \frac{\partial^\gamma f(\hat{p})}{\gamma!}\,(p-\hat{p})^\gamma\,.$$

Likewise, $(\mathcal{P}_{f,P}^q, \mathcal{R}_{f,P}^q)$ is called a qth-order Chebyshev model of f on P if

$$\forall p \in P\,, \quad f(p) - \mathcal{P}_{f,P}^q(p) \in \mathcal{R}_{f,P}^q \quad \text{and}$$
$$\mathcal{P}_{f,P}^q(p) = \sum_{\gamma\in\mathbb{N}^n, |\gamma|\leq q} a_\gamma(P)\, T_\gamma(p^{\text{s}})\,,$$

with $a_\gamma(P) \in O(\text{diam}\,(P)^{|\gamma|})$ and $p_i^{\text{s}} := \frac{p - \text{mid}(P_i)}{\text{rad}(P_i)}$.

Rules for binary sum, binary product and univariate composition between Taylor models or Chebyshev models have been described and analyzed, e.g., in Makino and Berz (2003); Bompadre et al. (2013); Dzetkulič (2014); Rajyaguru et al. (2014). As well as enabling the computation of Taylor and Chebyshev models for factorable functions, these rules guarantee high-order convergence of the remainder term to zero with the diameter of the parameter host set P as

$$\mathcal{R}_{f,P}^q \in O(\text{diam}\,(P)^{q+1})\,. \tag{10}$$

Naturally, the same approach applies to vector-valued functions $f : \mathbb{R}^n \to \mathbb{R}^p$ by treating each function component separately, also retaining the high-order convergence property (10).

In connection to the affine set-parameterization formalism introduced in Sect. 2.1, Taylor and Chebyshev model arithmetics support the constructions of extensions for a vector-valued function $f:\mathbb{R}^n\to\mathbb{R}^p$ in the form $f^{\mathbb{E}_m^{\mathrm{pol}(q)}\times\mathbb{E}_m^{\mathrm{box}}}:\mathbb{R}^{n\times\alpha_m^{(q)}}\times\mathbb{D}_n^{\mathrm{interval}}\to\mathbb{R}^{p\times\alpha_m^{(q)}}\times\mathbb{D}_p^{\mathrm{interval}}$. In the sense of (9) nonetheless, such extensions may only have Hausdorff convergence order $\beta=1$ regardless of the polynomial order q, since the underlying affine set-parameterization is not invariant under affine transformation. Note that this result is not in contradiction with (10), which only guarantees $(q+1)^{\mathrm{th}}$-order convergence for extensions from $(\mathbb{E}_m^{\mathrm{pol}(q)},\mathbb{R}^{n\times\alpha_m^{(q)}})$ into $(\mathbb{E}_m^{\mathrm{pol}(q)}\times\mathbb{E}_m^{\mathrm{ball}},\mathbb{R}^{p\times\alpha_m^{(q)}}\times\mathbb{D}_p^{\mathrm{interval}})$.

A procedure that makes use of Taylor/Chebyshev model arithmetic for the construction of extensions that are quadratically convergent was proposed by Houska et al. (2013); see also Houska et al. (2014). This construction is based on Taylor/Chebyshev models with ellipsoidal remainder terms as the pair $(\mathcal{P}_{f,P}^q,S_{f,P}^q)$, with $S_{f,P}^q$ the shape matrix of the ellipsoidal remainder $\mathcal{E}(S_{f,P}^q)$, thus yielding extensions in the form $f^{\mathbb{E}_m^{\mathrm{pol}(q)}\times\mathbb{E}_m^{\mathrm{ball}}}:\mathbb{R}^{n\times(\alpha_m^{(q)}+n+1)}\to\mathbb{R}^{p\times(\alpha_m^{(q)}+p+1)}$.

Finally, because the image set of a multivariate polynomial of order 2 or higher is nonconvex in general, applications of Taylor/Chebyshev models often call for constant/affine bounds or convex/polyhedral enclosures of such sets.

- Tight interval bounds can be obtained using LMI methods (Lasserre, 2009). Other ways of deriving rigorous interval bounds involve exact bounding of the polynomial's first- and second-order terms (Makino and Berz, 2003; Lin and Stadtherr, 2007b) or expressing the polynomial in Bernstein bases (Lin and Rokne, 1995).
- Affine bounds can be obtained likewise by retaining the first-order term, while bounding all of the other terms using one of the foregoing approaches.
- Polyhedral enclosures can be obtained on application of the reformulation-linearization technique (RLT) by Sherali and Fraticelli (2002); Sherali et al. (2012). Other approaches to convex/polyhedral enclosures include the decomposition/relaxation/outer-approximation technique (Smith and Pantelides, 1999; Tawarmalani and Sahinidis, 2004) as well as McCormick's relaxation technique (McCormick, 1976; Mitsos et al., 2009).

Both the Taylor and Chebyshev model arithmetics, along with the aforementioned bounding and relaxation approaches to enclose the range of these estimators, are implemented in MC++, our in-house library that is freely available from `https://bitbucket.org/omega-icl/mcpp`. The following example illustrates some of these features in connection to the anaerobic digestion model in Sect. 1.1.

Case Study 1. We consider the nonlinear relationship between the concentration S_2 and the partial pressure P_{CO_2} in the anaerobic digestion model in Sect. 1.1. After substitution of the various subexpressions, we obtain:

$$f(P_{\mathrm{CO}_2},S_2)=K_{\mathrm{H}}P_{\mathrm{CO}_2}^2+P_{\mathrm{t}}(C+S_2-Z)+\left(C+S_2-Z+K_{\mathrm{H}}P_{\mathrm{t}}+\frac{k_6}{k_{\mathrm{L}}a}\frac{\bar{\mu}_2S_2X_2}{S_2+K_{S2}+\frac{S_2^2}{K_{I2}}}\right)P_{\mathrm{CO}_2}$$

The parameter values are those given in Table A.1 and the other states are taken as $C=30$ [mmol L^{-1}], $Z=50$ [mmol L^{-1}] and $X_2=4$ [g(cell) L^{-1}]. Moreover, all the computations are carried out with MC++.

The set of points $(P_{\mathrm{CO}_2},S_2)\in Y:=[0.1,1]\times[0,15]$ satisfying $f(P_{\mathrm{CO}_2},S_2)=0$ is represented in solid black line on the plots of Fig. 4. We investigate several parameterizations of this (nonconvex) set in the form of Chebyshev models of orders $q=2,\ldots,4$. The blue, green and purple lines on the left plot of Fig. 4 enclose the set of points (P_{CO_2},S_2) such that:

$$\mathcal{P}_{f,Y}^q(P_{\mathrm{CO}_2},S_2)+r=0\,,\quad\text{for some } r\in\mathcal{R}_{f,Y}^q\,,$$

with $(\mathcal{P}_{f,Y}^q,\mathcal{R}_{f,Y}^q)$ a qth-order Chebyshev model of f on Y. These parameterizations provide tighter and tighter approximations as the order q increases. For comparison, convex and concave relaxations obtained from the McCormick relaxation of f on Y are shown in dashed lines on the figure. It is clear that, for this example, Chebyshev models of order 3 or higher provide tighter enclosures than McCormick relaxations, mainly due to their ability to capture nonconvexity.

The middle and right plots of Fig. 4 show polyhedral enclosures $f(P_{\mathrm{CO}_2},S_2)=0$, as constructed by constructing convex/concave bounds of the multivariate polynomial using McCormick's approach (middle plot) or by extracting the first-order term of the Chebyshev models and bounding the remaining terms (right plot). These simple bounds appear to be better than, or at least comparable to, those computed directly from McCormick relaxations. Moreover, the Chebyshev-derived bounds are found to progressively outperform the latter as the parameter range is reduced (results not shown). Note that tighter polyhedral enclosures could also be obtained by accounting for the dependencies in higher-order terms of the Chebyshev models. $\diamond$

3. REACHABILITY ANALYSIS OF NONLINEAR DYNAMIC SYSTEMS

The problem addressed in this section is the computation of time-varying enclosures $\overline{X}(t,P)\supseteq X(t,P)$, where $X(t,P):=\{x(t,p)\mid p\in P\}$ stands for the reachable set of parametric dynamic systems in the form

$$\begin{aligned}\forall t\in[0,T]\,,\quad &\dot{x}(t,p)=f(x(t,p),p)\\ \text{with}\quad &x(0,p)=x_0(p)\,.\end{aligned}\tag{11}$$

In this formulation, the state $x:[0,T]\times P\to\mathbb{R}^{n_x}$ is regarded as a function of the uncertain parameter vector $p\in P\subseteq\mathbb{R}^{n_p}$ along the time horizon $[0,T]$. A major complication in computing the enclosures $\overline{X}(t,P)$ is that these functions do not have a factorable representation in general, and therefore the bounding/relaxation techniques introduced in Sect. 2 may not be applied directly. Nonetheless, algorithms for bounding the solution set of such parametric dynamic systems can take advantage of the fact that the right-hand side function f and the initial value function x_0 are usually factorable.

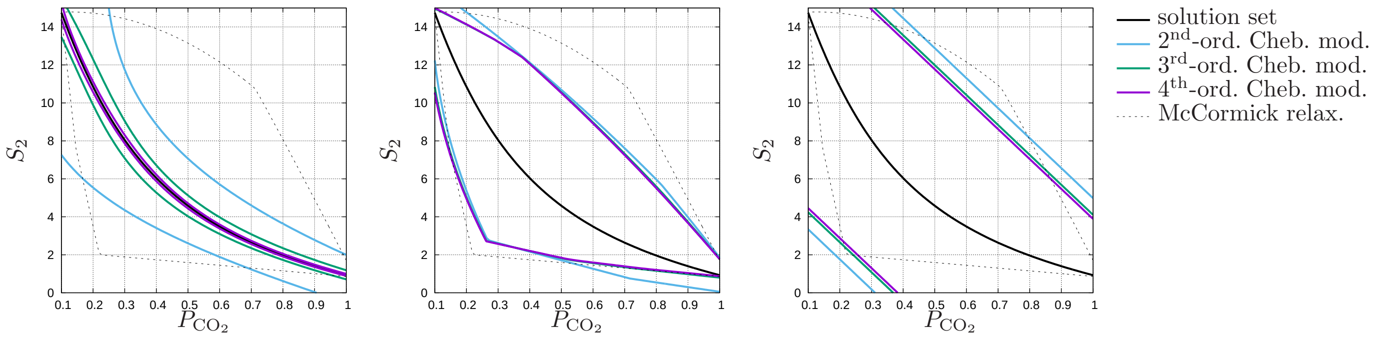

Fig. 4. Result of various parameterizations in enclosing the nonlinear relationship between S_2 and P_{CO_2} in the two-step anaerobic digestion model. *Left plot*: full Chebyshev model; *Middle plot*: Chebyshev-based convex/concave bounds; *Right plot*: Chebyshev-based affine bounds.

Existing methods for set-valued ODE integration can be broadly classified as discrete-time and continuous-time. Discrete-time methods proceed by first discretizing the integration horizon into finite steps, and then propagating a reachable set enclosure through each step. Many such integrators go back to the original work by Moore (1979), who presented a simple test for checking the existence and uniqueness of ODE solutions over a finite time step using interval analysis. This test was later incorporated into an algorithm that implements a two-phase approach (Lohner et al., 1992; Nedialkov et al., 1999): (i) determine a step-size and an a priori enclosure of the ODE solutions over the current step; then, (ii) propagate a tightened enclosure until the end of that step. Both phases typically rely on a high-order Taylor expansion of the ODE solutions in time, and the enclosures are propagated by a variety of affine set-parameterization extensions (Berz and Makino, 2006; Lin and Stadtherr, 2007b; Neher et al., 2007). Recently, Houska et al. (2013) have proposed a reversed, two-phase algorithm that starts by constructing a predictor of the reachable set and then determines a step-size for which this predictor yields a valid enclosure.

In contrast, continuous-time methods involve constructing an auxiliary system of ODEs whose solution is guaranteed to enclose the reachable set of the original ODEs. These methods are inspired from the theory of differential inequalities (Walter, 1970; Scott et al., 2012), viability theory (Aubin, 1991), or other set-theoretic methods such as ellipsoidal calculus (Kurzhanski and Valyi, 1997; Houska et al., 2012). Recently, Villanueva et al. (2014) have developed a unifying framework based on a generalized differential inequality for continuous-time propagation of convex and non-convex enclosures of the reachable set of uncertain ODEs. Other recent developments of continuous-time methods are concerned with enclosing the reachable set of implicit differential equations (Scott and Barton, 2013; Rajyaguru et al., 2015).

The following subsections further detail both approaches and their properties, with a focus on the authors' own contributions and using the set-theoretic concepts and tools in Sect. 2. Specifically, given a parameterization Q_p of the parameter set P on the affine set $(\mathbb{E}_m, \mathbb{D}_{n_p,m})$, we describe techniques for constructing a matrix valued function $Q_x : [0,T] \to \mathbb{D}_{n_x,m}$ such that

$$\forall t \in [0,T], \quad \mathrm{Im}_{\mathbb{E}_m}\left(Q_x(t)\right) \supseteq X(t,P)\,. \tag{12}$$

An application is presented for the two-step anaerobic digestion model at the end of the section.

3.1 Discrete-Time Set Propagation

Many discrete-time methods consider a Taylor expansion in time of the ODE solutions. Assuming that $x(\cdot,p)$ is the solution of (11) up to time $t \in [0,T)$ for a given parameter p, and provided that this solution can be extended until $t+h$ with $h \in (0, T-t]$, the application of Taylor's theorem for an s-th order expansion gives

$$x(t+h,p) = \sum_{i=0}^{s} h^i \phi_i(x(t,p),p) + h^{s+1}\phi_{s+1}(x(\tau,p),p)$$

for some $\tau \in [t, t+h]$; and with $\phi_0, \phi_1, \ldots, \phi_{s+1}$ the Taylor coefficient functions of the solution, defined recursively as

$$\phi_0(x,p) := x \quad \text{and} \quad \phi_i(x,p) := \frac{1}{i}\frac{\partial \phi_{i-1}}{\partial x}(x,p)\, f(x,p).$$

In reversing the two phases of the traditional discrete-time approach, the algorithm by Houska et al. (2013) removes the need for an a priori enclosure of the solution and also provides a natural mechanism for step-size selection. The propagation starts from a parameterization $Q_x(0) := x_0^{\mathbb{E}_m}(Q_p)$, with $x_0^{\mathbb{E}_m}$ an extension of the initial-value function x_0, so that $\mathrm{Im}_{\mathbb{E}_m}(Q_x(0)) \supseteq X(0,P)$. Then, the following two steps are applied repeatedly:

(1) Given a parameterization $Q_x(t)$ at some $t \in [0,T)$ such that $\mathrm{Im}_{\mathbb{E}_m}(Q_x(t)) \supseteq X(t,P)$, compute a predictor $Q_x(t+h)$ of the solution for all $h \in (0, T-t]$ as:
$$Q_x(t+h) := \biguplus_{i=0}^{s} h^i \phi_i^{\mathbb{E}_m}(Q_x(t),Q_p) \uplus h\,\mathrm{TOL}\,Q_{\mathrm{unit}}$$
for a pre-specified tolerance $\mathrm{TOL} > 0$ and $Q_{\mathrm{unit}} \in \mathbb{D}_{n_x,m}$; and where $\phi_i^{\mathbb{E}_m}$ are extensions of the Taylor coefficient functions ϕ_i for each $i = 0, \ldots, s$ and $\uplus$ stands for the extension of the addition operator.

(2) Determine a step-size $\bar{h}$ such that the predictor $Q_x(t+h)$ is guaranteed to yield a valid enclosure of the reachable set, $\mathrm{Im}_{\mathbb{E}_m}(Q_x(t+h)) \supseteq X(t+h,P)$, for all $h \in [0,\bar{h}]$; that is,
$$\forall \tau \in [t,t+h], \quad \mathrm{Im}_{\mathbb{E}_m}\Big((\tau - t)^s\, \phi_{s+1}^{\mathbb{E}_m}(Q_x(\tau),Q_p) \Big) \subseteq \mathrm{TOL}\ \mathrm{Im}_{\mathbb{E}_m}(Q_{\mathrm{unit}})\,,$$
with $\phi_{s+1}^{\mathbb{E}_m}$ an extension of the Taylor coefficient function ϕ_{s+1}.

A practical way of finding a valid step-size $\bar{h}$ is given in Houska et al. (2013, 2014).

Especially appealing within this approach is the inherent flexibility of the algorithm, which can be used with any affine set-parameterization, including the propagation of convex sets (e.g., interval boxes, ellipsoids) and nonconvex sets (e.g., polynomial image sets derived from Taylor/Chebyshev models).

3.2 Continuous-Time Set Propagation

This approach involves constructing auxiliary ODEs that describe the coefficient Q_x of a parameterization of the state variables; that is,

$$\forall t \in [0,T], \quad \dot{Q}_x(t) = F(Q_x(t), Q_p), \tag{13}$$

with initial parameterization $Q_x(0) := x_0^{\mathbb{E}_m}(Q_p)$. Clearly, a possible choice for the right-hand-side function F in (13) is the extension $f^{\mathbb{E}_m}$ of the original right-hand side f in (11). However, it is useful in practice to account for certain facet constraints that mitigate the growth of the reachable set enclosure; this includes the method of standard differential inequalities as well as ellipsoidal set propagation techniques. Recently, Villanueva et al. (2014) have formulated a generalized differential inequality (GDI) that contains the usual facet constraint methods as special cases. This GDI describes sufficient conditions on the support function $V[\overline{X}(t,P)]$ of a convex enclosure $\overline{X}(t,P)$ of the reachable set as follows:

$$\text{a.e. } t \in [0,T], \quad \forall c \in \mathbb{R}^{n_x},$$
$$\dot{V}[\overline{X}(t,P)](c) \geq \max_{\xi,\rho} \left\{ c^{\mathrm{T}} f(\xi,\rho) \;\middle|\; \begin{array}{l} \xi \in \overline{X}(t,P) \\ c^{\mathrm{T}}\xi = V[\overline{X}(t,P)](c) \\ \rho \in P \end{array} \right\}$$

with $V[\overline{X}(0,P)](c) \geq \max_\rho \left\{ c^{\mathrm{T}} x_0(\rho) \,\middle|\, \rho \in P \right\}$.

Interestingly, the GDI also supports the construction of nonconvex enclosures, e.g., in the form of Taylor or Chebyshev models with convex remainder bounds $(\mathcal{P}^q_{x,P}(t,\cdot), \mathcal{R}^q_{x,P}(t))$ for each $t \in [0,T]$, so that:

$$\overline{X}(t) := \{\mathcal{P}^q_{x,P}(t,p) \,|\, p \in P\} \oplus \mathcal{R}^q_{x,P}(t) \;\supseteq\; X(t,P). \tag{14}$$

The polynomial part $\mathcal{P}^q_x$ can be directly obtained via the solution of the auxiliary ODEs (13) in the desired polynomial image basis $\mathbb{E}_m^{\mathrm{pol}(q)}$ and with $F := f^{\mathbb{E}_m^{\mathrm{pol}(q)}}$. In the case of Taylor models, for instance, these ODEs correspond to the sensitivities of (11) up to order q.

Besides the polynomial part, ways of propagating convex remainder enclosures in the form of interval bounds or ellipsoids are also described in Villanueva et al. (2014). An interval remainder $\mathcal{R}^q_x(t) := \left[r^{\mathrm{L}}_x(t), r^{\mathrm{U}}_x(t)\right]$ can be propagated by integrating the following $2 \times n_x$ system of auxiliary ODEs, for all $i = 1, \ldots, n_x$:

$$\dot{r}^{\mathrm{L}}_i(t) = \min_{\xi,\rho} \left\{ \begin{array}{l} f_i(\mathcal{P}^q_x(t,\rho)+\xi,\rho) \\ -\,\dot{\mathcal{P}}^q_{x_i}(t,\rho) \end{array} \;\middle|\; \begin{array}{l} \xi_i = r^{\mathrm{L}}_{x_i}(t) \\ \xi \in [r^{\mathrm{L}}_x(t), r^{\mathrm{U}}_x(t)] \\ \rho \in P \end{array} \right\}$$
$$\dot{r}^{\mathrm{U}}_i(t) = \max_{\xi,\rho} \left\{ \begin{array}{l} f_i(\mathcal{P}^q_x(t,\rho)+\xi,\rho) \\ -\,\dot{\mathcal{P}}^q_{x_i}(t,\rho) \end{array} \;\middle|\; \begin{array}{l} \xi_i = r^{\mathrm{U}}_{x_i}(t) \\ \xi \in [r^{\mathrm{L}}_x(t), r^{\mathrm{U}}_x(t)] \\ \rho \in P \end{array} \right\}.$$

Likewise, an ellipsoidal enclosure $\mathcal{E}(S^q_x(t))$ can be propagated by integrating the following $n_x \times n_x$ system of auxiliary ODEs:

$$\dot{S}^q_x(t) = A(t)S^q_x(t) + S^q_x(t)A(t)^{\mathrm{T}} + \sum_{i=1}^{n_x} \kappa_i(t)\, S^q_x(t) + \mathrm{diag}(\kappa(t))^{-1}\, \mathrm{diag}\ \mathrm{rad}(\Omega^q_f[S^q_x(t)])^2,$$

with $A(t) = \left(\frac{\partial f}{\partial x}(\mathcal{P}^q_x(t,\hat{p}),\hat{p})\right)$. Here, the nonlinearity bounder $\Omega^q_f[S] \in \mathbb{IR}^{n_x}$ must satisfy

$$f(\mathcal{P}^q_x(t,\rho)+r,\rho) - \dot{\mathcal{P}}^q_x(t,\rho) - \frac{\partial f}{\partial x}(\mathcal{P}^q_x(t,\rho),\rho)\, r \in \Omega^q_f[S],$$

for all $(r,\rho) \in \mathcal{E}(S) \times P$, and its construction can be automated using interval analysis for instance. Moreover, the scaling function $\kappa : [0,T] \to \mathbb{R}^{n_x}_{++}$ can be chosen in such a way as to minimize $\mathrm{tr}(S^q_x(t))$.

Continuous-time methods based on differential inequalities are appealing in that the auxiliary ODEs can be solved using off-the-shelf ODE solvers. However, because of the need for applying a numerical discretization and since the right-hand side function defining the auxiliary ODE is typically non-differentiable, it is hard to give any guarantee on the discretization error. This non-differentiability can also impair the step-size control mechanism of the numerical integration algorithm, and in principle it should be addressed in the framework of hybrid discrete-continuous systems (see, e.g., Singer, 2004).

3.3 Properties

A common feature of discrete- and continuous-time set propagation methods is their ability to propagate sets described by a variety of affine-set parameterizations, including both convex and nonconvex sets. Despite the fact that these methods rely on rather different ideas, they share several important properties regarding their convergence order and stability.

We have already stressed the importance of high-order inclusions in Sect. 2. As far as the convergence of reachable set enclosures is concerned, the computed enclosures $\mathrm{Im}_{\mathbb{E}_m}(Q_x(t))$ can, under certain conditions and at each time $t \in [0,T]$, inherit the convergence order of function extensions in the chosen affine set-parameterization $\mathbb{E}_m$. In the particular case of qth-order Taylor/Chebyshev models with convex remainder bounds, $(\mathcal{P}^q_{x,P}(t,\cdot), \mathcal{R}^q_{x,P}(t))$, computer implementations can be devised such that (Villanueva et al., 2014):

- for continuous-time set propagation,
$$\forall t \in [0,T], \quad \mathcal{R}^q_{x,P}(t) \in O(\mathrm{diam}\,(P)^{q+1});$$
- for discrete-time set propagation,
$$\forall t \in [0,T], \quad \mathcal{R}^q_{x,P}(t) \in O(\mathrm{diam}\,(P)^{q+1}) + O(\mathrm{TOL}).$$

Notwithstanding these high-order convergence properties, both continuous and discretized set-valued integration methods are subject to the wrapping effect, which typically results in the diameter of the reachable set enclosure diverging to infinity, even on finite time horizons—the so-called 'bound explosion' phenomenon. For stable ODE systems in particular, a rather natural requirement would appear to be that the computed enclosures are themselves stable, at least for small enough initial value or uncertain parameter sets.

Recently, Houska et al. (2014) have derived sufficient conditions for the discrete-time method outlined in Sect. 3.1 to be locally asymptotically stable, in the sense that the computed enclosures are guaranteed to remain stable on infinite time horizons when applied to a dynamic system in the neighborhood of a locally asymptotically stable periodic orbit (or equilibrium point). The key requirement here is quadratic Hausdorff convergence of function extensions in the chosen affine set-parameterization, since the enclosures may not contract fast enough to neutralize the wrapping effect otherwise. Note that this result also applies to continuous-time set propagation. This stability analysis sheds light on the fundamental reason why those currently available set-valued ODE integrators relying on interval arithmetics in one way or another fail to be locally asymptotically stable, regardless of the size of the uncertainty set; and even state-of-the-art integrators based on Taylor models with interval remainders, such as VSPODE (Lin and Stadtherr, 2007b) or COSY Infinity (Makino and Berz, 2005), may not stabilize the reachable set enclosures of asymptotically stable dynamic systems, despite the fact that they implement advanced heuristics for rotating the basis of the interval remainder.

One way to promote asymptotic stability involves propagating Taylor/Chebyshev models with ellipsoidal remainder bounds, for which extensions with quadratic Hausdorff convergence can be constructed (see Sect. 2.2). Both discrete- and continuous-time set-valued ODE integrators implementing this approach based on MC++ are made freely available at `https://bitbucket.org/omega-icl/eqbnd`. The following example illustrates these stability considerations.

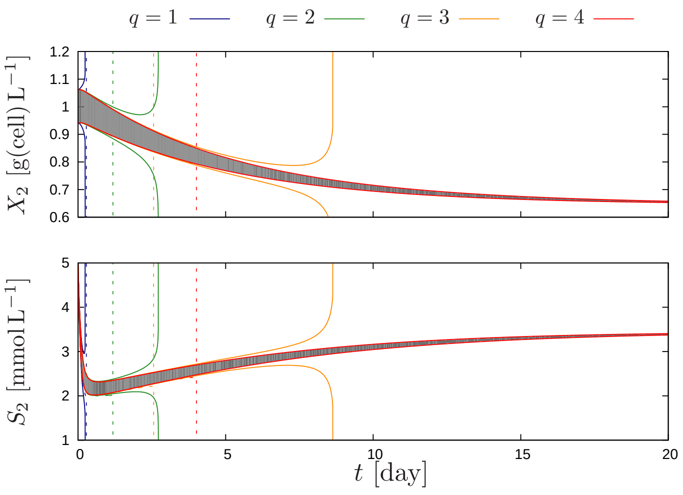

Fig. 5. Projections onto X_2 (top plot) and S_2 (bottom plot) of the reachable set $X(t, P)$ (shaded area) and of the enclosures $\overline{X}(t, P)$ computed with Taylor models of order $q = 1, \ldots, 4$ with interval remainders (dashed lines) and ellipsoidal remainders (solid lines) in the two-step anaerobic digestion model.

Case Study 2. We consider the nonlinear ODE model (1)-(6) of anaerobic digestion, with uncertain initial conditions as $X_1(0) \in 0.5 \pm 4\%$ [g(cell) L^{-1}], $X_2(0) \pm 4\%$ [g(cell) L^{-1}] and $C(0) \in 40 \pm 4\%$ [mmol L^{-1}]. The rest of the initial conditions are given by $S_1(0) = 1$ [g(COD) L^{-1}], $S_2(0) = 5$ [mmol L^{-1}] and $Z(0) = 50$ [mmol L^{-1}], in addition to the parameter values in Table A.1.

Projections onto the variables X_2 and S_2 of the actual reachable set and of the bounds derived from Taylor models of order $q = 1, \ldots, 4$ with either interval or ellipsoidal remainders are shown in Fig. 5. We note that it only takes a few seconds to generate the bounds in all of the cases for this problem; see Villanueva et al. (2014) for a detailed numerical comparison.

For Taylor models with interval remainders, increasing the order q delays the blow up time significantly, up to about $t \approx 4$ [day] with 4th-order Taylor models. In comparison, bounds derived from the propagation of Taylor models with ellipsoidal remainders are found to be superior for $q \geq 2$ here. In particular, Taylor models with ellipsoidal remainders of order $q \geq 4$ are found to stabilize the reachable set enclosure for this level of uncertainty; that is, the bounds converge to the actual steady-state values as $t \to \infty$. Stabilizing the enclosures with lower-order Taylor models would require reducing the level of uncertainty. $\diamond$

4. APPLICATIONS OF SET-THEORETIC APPROACHES FOR COMPLETE SEARCH

A great variety of algorithms, including complete search methods for problems in global optimization, constraint satisfaction or robust estimation, hinge on the ability to construct tight enclosures for the range of (nonlinear and non-necessarily factorable) functions, such as the methods described in Sect. 2 and Sect. 3. Our focus in this section is on set-inversion techniques (Moore, 1992; Jaulin and Walter, 1993), which enable approximation of sets defined in implicit form, such as

$$P_e := \{p \in P_0 \mid g(p) \in \Gamma\}\,, \tag{15}$$

using subpavings (sets of non-overlapping boxes). Obviously, these techniques bear many similarities with branch-and-bound search in global optimization (Neumaier, 2004; Tawarmalani and Sahinidis, 2004). They are similar in flavor to set-oriented numerical methods, as developed, e.g., by Dellnitz et al. (2001).

Given a compact set $P_0 \subset \mathbb{R}^{n_p}$, a set $\Gamma \subset \mathbb{R}^{n_g}$, and a continuous function $g : \mathbb{R}^{n_p} \to \mathbb{R}^{n_g}$, set-inversion algorithms compute partitions $\mathbb{P}_{\rm in}$ and $\mathbb{P}_{\rm bnd}$ such that

$$\bigcup_{P \in \mathbb{P}_{\rm in}} P \subseteq P_e \subseteq \bigcup_{P \in \mathbb{P}_{\rm in} \cup \mathbb{P}_{\rm bnd}} P\,, \tag{16}$$

with $\mathbb{P}_{\rm bnd}$ sufficiently small. A prototypical algorithm is given below.

Algorithm 1. Set-inversion algorithm.

Input: Termination tolerances $\epsilon_{\rm box} \geq 0$ and $\epsilon_{\rm bnd} \geq 0$
Initialization: Set partitions $\mathbb{P}_{\rm bnd} = \{P_0\}$ and $\mathbb{P}_{\rm in} = \emptyset$; Set iteration counter $k = 0$
Main Loop:
(1) Select a parameter box P in the partition $\mathbb{P}_{\rm bnd}$ and remove it from $\mathbb{P}_{\rm bnd}$
(2) Compute an enclosure $\overline{g}(P) \supseteq \{g(p) \mid p \in P\}$
(3) Exclusion Tests:
  (a) **If** $\overline{g}(P) \subset \Gamma$, insert P into $\mathbb{P}_{\rm in}$
  (b) **Else if** $\overline{g}(P) \cap \Gamma = \emptyset$, fathom P
  (c) **Else** bisect P and insert subsets back into $\mathbb{P}_{\rm bnd}$
(4) **If** width$(P) \leq \epsilon_{\rm box}$ for all $P \in \mathbb{P}_{\rm bnd}$ **or** $V_{\rm bnd} := \sum_{P\in\mathbb{P}_{\rm bnd}} \text{volume}(P) \leq \epsilon_{\rm bnd}$, **stop**
(5) Increment counter k+=1; **Return** to step 1
Output: Partitions $\mathbb{P}_{\rm in}$ and $\mathbb{P}_{\rm bnd}$; Iteration count k

Clearly, Step 2 of Algorithm 1 calls for a procedure capable of computing an enclosure of the image set $\{g(p) \mid p \in P\}$ for a given parameter subpartition P. Should the function g be factorable, such enclosures can be obtained by considering an extension $g^{\mathbb{E}_m}$ on a suitable affine set-parameterization basis $\mathbb{E}_m$, as explained in Sect. 2. If g is defined implicitly via the solution of differential equations, the set-propagation techniques described in Sect. 3 can be used instead. Both cases are considered subsequently, with applications to bifurcation analysis (Sect. 4.1) and set-membership parameter estimation (Sect. 4.2).

The use of Taylor/Chebyshev models to construct enclosures $\overline{g}$ is appealing in that it can capture the parametric dependencies in the actual solution set $P_{\rm e}$ (besides enjoying higher-order convergence properties). Given a parameter box $P := [p^{\rm L}, p^{\rm U}]$ and a qth-order Taylor/Chebyshev model enclosure $\overline{g}(P) := \{\mathcal{P}^q_{g,P}(p) \,|\, p \in P\} \oplus \mathcal{R}^q_{g,P}$, the lower and upper parameter bounds $p_j^{\rm L}$ and $p_j^{\rm U}$ for each $j = 1, \ldots, n_p$ can be tightened by solving optimization problems of the form Paulen et al. (2015):

$$p_j^{\rm L/U} = \min/\max_p \, p_j \text{ s.t. } \mathcal{P}^q_{g,P}(p) \in \Gamma \ominus \mathcal{R}^q_{g,P}\} \,. \quad (17)$$

This way, a reduced box P is obtained after solving $2 \times n_p$ optimization problems—one problem for the lower bound and one for the upper bound of each parameter. As written, the bound-reduction problems (17) are in general nonconvex for $q \geq 2$. Instead of attempting to solve these problems directly, one can construct polyhedral relaxations in the form of linear programs (LPs), similar to the approach used for bound contraction in branch-and-bound search (see, e.g., Neumaier, 2004; Tawarmalani and Sahinidis, 2004). In a related approach, Lin and Stadtherr (2007a) and Kletting et al. (2011) use constraint propagation in the domain reduction procedure.

In effect, the domain-reduction procedure can be performed as an extra step in Algorithm 1, between Steps 2 and 3. In the case that the reduction of a parameter box P is larger than a given threshold, it can be repeated multiple times. It is important to bear in mind that repeating the reduction several times involves recomputing the enclosures $\overline{g}(P)$ of the model outputs on the reduced box P though. This defines a clear trade-off between the extra computational burden and the reduction in the size of the partition $\mathbb{P}_{\rm bnd}$, which is of course problem-dependent. Paulen et al. (2015) have also presented a simple approach to avoid recomputing the enclosures $\overline{g}(P)$ as soon as the remainder term in the Taylor/Chebyshev model is within a given threshold.

4.1 Bifurcation Analysis

Locating the equilibrium and bifurcation points of a nonlinear dynamic system occurring within a given state-space domain is an important problem in control. The set-inversion algorithm described above provides a means for addressing this problem rigorously. Not only is this a powerful alternative to the classical continuation methods (Allgower and Georg, 1990), but it also enables bifurcation analysis with respect to multiple parameters simultaneously; see, e.g., Hasenauer et al. (2009); Waldherr and Allgöwer (2011); Smith et al. (2014) for recent related studies.

The equilibrium manifold of a dynamic system given in the form of parametric ODEs (11) is defined as the pair of points $(p, x) \in \mathbb{R}^{n_p+n_x}$ such that $f(x, p) = 0$. The problem of approximating this manifold as close as possible can be therefore cast as the set-inversion problem (15) by considering the extended parameter-state space $\mathbb{R}^{n_x+n_p}$ as

$$P_{\rm e} \times X_{\rm e} := \{(p, x) \in P_0 \times X_0 \;\mid\; f(x, p) = 0\} \,. \quad (18)$$

Once a subpaving of $P_{\rm e} \times X_{\rm e}$ has been constructed using Algorithm 1, so that (16) is satisfied with $\mathbb{P}_{\rm bnd}$ sufficiently small, one can then infer the stability of the equilibrium points contained in each subpartition of $\mathbb{P}_{\rm bnd}$ and isolate those subpartitions which may contain a bifurcation point.

Recall that a dynamic system is stable if and only if the determinant of its n_x-by-n_x Hurwitz matrix,

$$H(x, p) := \begin{pmatrix} c_1(x,p) & c_3(x,p) & c_5(x,p) & \cdots & 0 \\ c_0(x,p) & c_2(x,p) & c_4(x,p) & \cdots & 0 \\ 0 & c_1(x,p) & c_3(x,p) & \cdots & 0 \\ 0 & c_0(x,p) & c_2(x,p) & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & c_{n_x}(x,p) \end{pmatrix},$$

and all its leading principal minors are positive, where $c_i(x, p)$ are the coefficients of the characteristic polynomial of the Jacobian matrix $J_f := \frac{\partial f}{\partial x}$,

$$\det(J_f(x, p) - \lambda I) =: \lambda^{n_x} + \sum_{i=1}^{n_x} c_i(x, p)\lambda^{n_x - i} \,.$$

In practice, symbolic expressions for the coefficients c_i can be obtained using the Faddeev-Leverrier algorithm (Helmberg et al., 1993). Moreover, the Hurwitz matrix can be reduced to an upper triangular form, say U, using a modified Neville elimination algorithm in $O(n_x^2)$ operations (Gasca and Peña, 1992). The following stability tests can be performed sequentially on a subpartition $P \times X$ by evaluating the elements c_i and U_{ii} in a given arithmetic, such as interval arithmetic or Taylor/Chebyshev model arithmetic (see Sect. 2):

(1) If none of the coefficients c_i or diagonal elements U_{ii} are nonnegative, then all the equilibrium points in the considered subpartition are stable;
(2) If at least one element c_i or U_{ii} is negative, then all the equilibrium points in the subpartition are unstable;

(3) Otherwise (that is, if any one of the elements c_i or U_{ii} have zero in range), the subpartition may contain a bifurcation point.

The types of bifurcation points that can be detected this way include:

- Steady-state bifurcation points, whereby the Jacobian matrix J_f has a zero eigenvalue; their occurrence can be tested by checking if any element c_i or U_{ii} vanishes.
- Hopf bifurcation points, which occur in the presence of a limit cycle when J_f has one conjugate pair of eigenvalues with zero real part and the other eigenvalues all have negative real parts; their occurrence can be tested by checking that
$$c_{n_x} > 0,\ \Delta_{n_x-1} = 0,\ \Delta_{n_x-2} > 0,\ \ldots, \Delta_1 > 0,$$
with Δ_i the ith principal minor of H (El Kahoui and Weber, 2000).

Note that enclosures of the bifurcation points can also be directly computed on appending the foregoing bifurcation characterization constraints to the equilibrium constraints in (18). This removes the need for computing the full equilibrium manifold.

Case Study 3. We consider the problem of determining the equilibrium points of the two-step anaerobic digestion model (1)-(7), along with characterizing their stability. The focus is on varying the dilution rate D as the bifurcation parameter in the range $P_0 := [10^{-3}, 1.5]$, and the state-space domain for $[X_1\ X_2\ S_1\ S_2\ Z\ C\ P_{CO_2}]$ is $X_0 := [0, 0.6]\times[0, 0.8]\times[0, 5.]\times[0, 80]\times[0, 80]\times[0, 80]\times[0, 1]$. As previously, the model parameter values are those listed in Table A.1.

The results produced by the set-inversion algorithm are shown in Fig. 6, with an indication of the stable and unstable parts of the equilibrium manifold. In order to compute the enclosures in Step 2 of Algorithm 1, we use affine relaxations derived from 2nd-order Chebyshev models of the equilibrium constraints, similar to the approach described in Case Study 1 above. Moreover, we perform domain reduction at each node via the solution of auxiliary LPs in order to refine the equilibrium set approximation. The set-inversion algorithm is interrupted after 40,000 iterations, with a corresponding runtime of a few minutes only.

Note that only steady-state bifurcations occur in this problem, which correspond to a change in stability of the equilibrium manifold. One such bifurcation occurs here around $D = 1$ [day], where both a stable branch and an unstable branch merge into a single stable branch. Another bifurcation is seen to occur around $D = 1.07$ [day] with a change in stability along a single branch. ⋄

4.2 Set-Membership Parameter Estimation

Among the available techniques to account for uncertainty in parameter estimation, set-membership estimation, also known as guaranteed parameter estimation, aims to determine all the parameter values of a model that are consistent with a set of measurements under given uncertainty scenarios. Initially developed for algebraic models in the early 1990s (Moore, 1992; Jaulin and Walter, 1993), these techniques were later extended to dynamic models using ODE bounding techniques (e.g., Jaulin, 2002; Raissi et al., 2004). Our focus in this subsection shall be on the latter and we consider the case where the uncertainty enters the estimation problem in the form of bounded measurement errors.

Given a nonlinear dynamic system in the form of parametric ODEs (11), consider a set of output functions
$$y(t, p) = g(x(t, p), p) \in \mathbb{R}^{n_y}\,. \tag{19}$$
Now, for a set of output measurements $y_{\rm m}(t_i)$ at N time points $t_1, \ldots, t_i, \ldots, t_N \leq T$, *classical* parameter estimation seeks to determine *one* particular instance $p^\star$ of the parameter values for which the (possibly weighted) normed difference between these measurements and the corresponding model outputs y is minimal. We note by the way that such optimization problems are typically nonconvex and call for global optimization, for which one can use branch-and-bound search in combination with the ODE bounding techniques described earlier in Sect. 3 (Esposito and Floudas, 2000; Singer and Barton, 2006).

In contrast, *guaranteed* (bounded-error) parameter estimation accounts for the fact that the actual process outputs, $y_{\rm p}$, are only known within some bounded measurement error $e \in E := [e^L, e^U]$, so that
$$y_{\rm p}(t_i)\ \in\ y_{\rm m}(t_i) + [e^L, e^U]\ =:\ Y_{\rm p}(t_i)\,.$$
The main objective then is to estimate the set $P_{\rm e}$ of *all* possible parameter values p such that $y(t_i, p) \in Y_{\rm p}(t_i)$ for every $i = 1, \ldots, N$. Clearly, this problem can be cast as the following set inversion:
$$P_{\rm e} := \left\{ p \in P_0 \,\middle|\, \begin{array}{l} \forall i = 1, \ldots, N, \\ y_{\rm m}(t_i) + e^{\rm L} \leq y(t_i, p) \leq y_{\rm m}(t_i) + e^{\rm U} \end{array} \right\}. \tag{20}$$
Depicted in red on the top plot of Fig. 7 is the set of all output trajectories satisfying $y(t_i, p) \in Y_{\rm p}(t_i)$ with $i = 1, \ldots, N$, and on the bottom plot the corresponding set $P_{\rm e}$ projected onto the (p_1, p_2) space.

A practical limitation for the guaranteed parameter estimation problem as given in (20) is the need for consistent measurement data and bounds throughout the entire time series; otherwise, there may not be any model response matching the output measurements within the specified error bounds, and the parameter set $P_{\rm e}$ is empty. In most applications based on real data, this calls for data preprocessing, for instance using data reconciliation techniques, in order to get rid of the outliers. For instance, these outliers could be due to over-optimistic noise bounds or to sensor failures at given time instants. To handle this situation, it is possible to 'protect' the estimator against a prespecified number of outliers, by allowing for a number of output variables to be outside of their prior feasible intervals (see, e.g., Jaulin et al., 2001; Kieffer and Walter, 2005). Another situation whereby the parameter set $P_{\rm e}$ may be empty is in the presence of significant model mismatch, which calls for the development of further robustification strategies or alternative guaranteed parameter estimation paradigms (Csáji et al., 2012; Kieffer and Walter, 2014).

In a related work, Rumschinski et al. (2010) apply a set-inversion approach in order to discriminate between com-

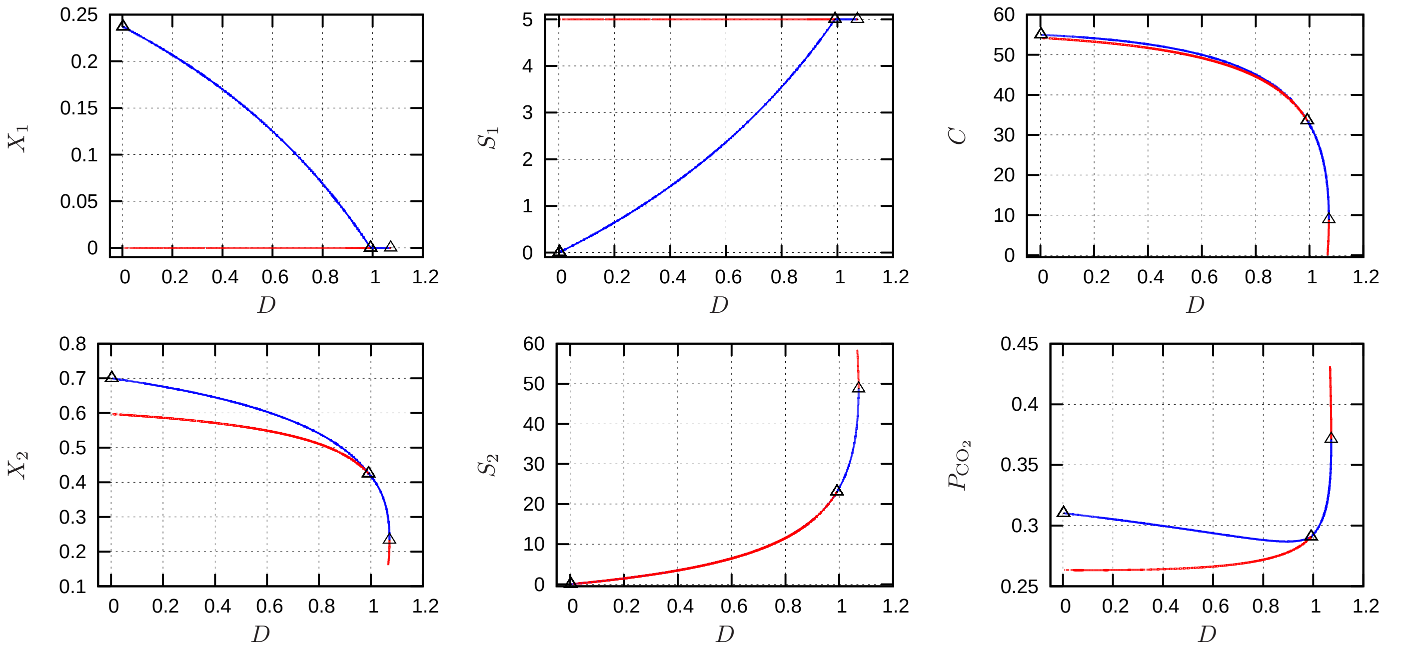

Fig. 6. Set of stable (blue) and unstable (red) equilibrium points of the two-step anaerobic digestion model with respect to the dilution rate D.

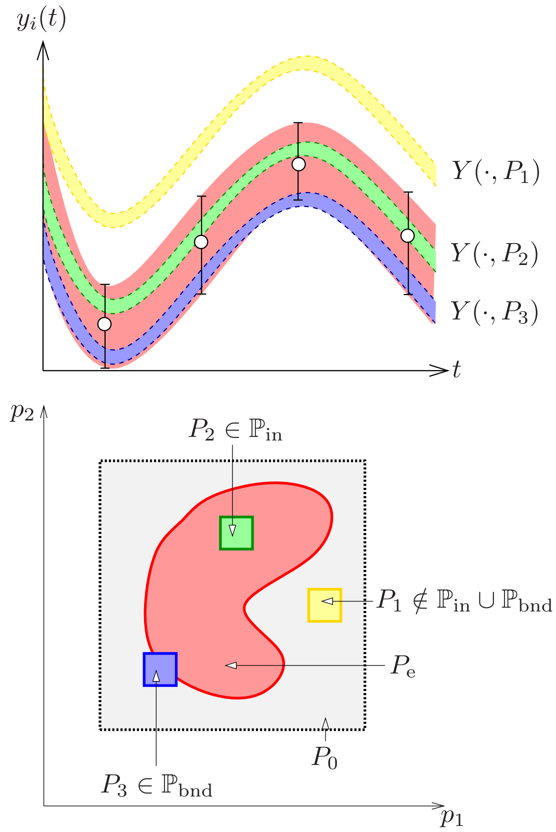

Fig. 7. Illustration of guaranteed parameter estimation concepts in the space of output trajectories (top plot) and in the parameter space (bottom plot).

peting model hypotheses and to provide guaranteed outer estimates on the model parameters that are consistent with the experimental measurements. They consider nonlinear dynamic systems with polynomial/rational right-hand sides, and construct SDP relaxations in order to

Table 1. Dilution rate and inlet concentration profiles in guaranteed estimation problem.

Input	Day 1	Day 2	Day 3	Day 4
D [/day]	0.25	1.00	1.00	0.25
S_1^{in} [g(COD)/L]	2.38	2.38	4.76	2.38
S_2^{in} [mmol/L]	80.0	80.0	160.0	80.0
Z^{in} [mmol/L]	50.0	50.0	100.0	50.0
C^{in} [mmol/L]	5.0	5.0	10.0	5.0

carry out the exclusion tests after discretizing the differential equations. In a follow up work, Streif et al. (2012) have developed the Matlab toolbox ADMIT automating the analysis.

Case Study 4. We consider the problem of computing guaranteed parameter sets for the nonlinear ODE model (1)-(6). Three outputs are considered to carry out the estimation, namely S_1, S_2, and C, with measurements every 4 hours over a 4-day period. Pseudo-experimental data are generated by simulating a nominal model with parameter values from Table A.1 and using the dilution rate and influent concentrations in Table 1. Moreover, the effect of measurement noise is simulated by rounding the nominal outputs up or down to the nearest values by retaining, respectively, 2, 1 and 1 significant digits; then, measurement error ranges of, respectively, ± 0.01, ± 0.1 and ± 0.1 are added to these values. Regarding the parameters, the focus is on estimating the kinetic parameters describing biomass growth, namely $\bar{\mu}_1 \in [1.15, 1.25]$, $K_{S_1} \in [6.7, 7.3]$, $\bar{\mu}_2 \in [0.735, 0.75]$, $K_{S_2} \in [9.2, 9.5]$, and $K_{I_2} \in [235, 265]$.

The results produced by the set-inversion algorithm are shown in Fig. 8. The shape of the guaranteed parameter set is indeed characteristic of the large correlations between the parameters $\bar{\mu}_1$ and K_{S_1}, which indicates that $\mu_1(S_1) \approx \frac{\bar{\mu}_1}{K_{S_1}} X_1$ in this case. Likewise, a large correlation is observed between $\bar{\mu}_2$, K_{S_2} and K_{I_2}. We also note that the nominal parameter values (red cross on Fig. 8) lie inside the approximation of the set P_e.

In order to compute the reachable set enclosures we use 4th-order Taylor models with ellipsoidal remainders, in agreement with the results of the reachability analysis conducted in Case Study 2. Moreover, we perform domain reduction at each node via the solution of auxiliary LPs constructed from the polyhedral relaxations of the Taylor models of the predicted outputs at each measurement time, and we apply up to 10 passes as long as the range reduction for any parameter exceeds 20%. Finally, we do not recompute the reachable sets on children nodes when all the Taylor model remainders at their parent nodes have converged to within 10^{-4}. With these settings, the set-inversion algorithm reaches a tolerance of $\epsilon_{\text{bnd}} = 5 \cdot 10^{-5}$ after 3,130 iterations and a runtime of about 35 minutes. See Paulen et al. (2015) for further numerical comparisons, including the solution of a related guaranteed parameter estimation problem in 7 parameters. ◇

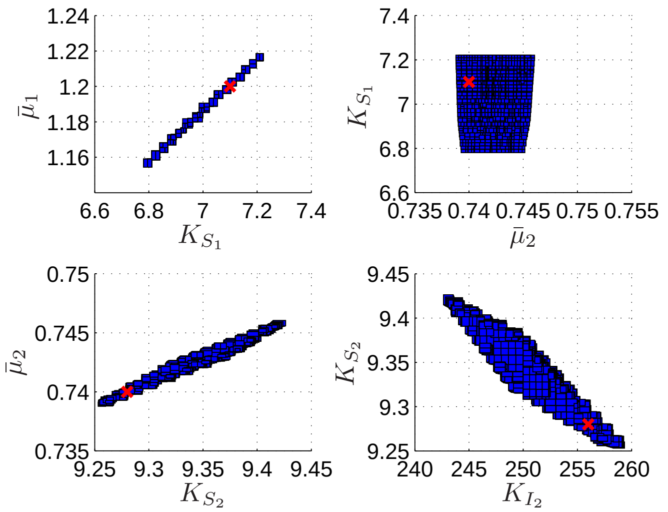

Fig. 8. Projections onto the subspaces $(K_{S_1},\bar{\mu}_1)$, $(\bar{\mu}_2,K_{S_1})$, $(K_{S_2},\bar{\mu}_2)$ and (K_{I_2},K_{S_2}) of the guaranteed parameter sets for the two-step anaerobic digestion model.

5. SUMMARY AND FUTURE DIRECTIONS

This paper has presented an overview of some of the set-theoretic methods developed in our research group for the analysis of uncertain/parametric nonlinear dynamic systems. These methods are heavily dependent on our ability to compute tight bounds on the range of factorable functions and on the reachable set of dynamic systems. In particular, we have presented a formalism based on so called affine-set arithmetics and set propagation, and we have applied this formalism so as to cast problems in bifurcation analysis and set-membership parameter estimation as set-inversion problems. This way, these problems can be addressed both rigorously and efficiently using complete search methods.

Besides complete search applications, it is important to reemphasize that set-theoretic methods also hold many promises in other areas of mathematics and engineering, such as fault diagnosis (Scott et al., 2014) or model predictive control (MPC). To reinforce this latter point, we provide in this following subsection a formulation for robust MPC, which makes use (and extends) the generalized differential inequality presented in Sect. 3.

5.1 Tube-Based Methods for Robust MPC

Model predictive controllers are a class of feed-back controllers, which proceed by solving an optimal control problem to predict the future behavior of a dynamic system on a finite time-horizon. The computed optimal input is then applied to the real process until the next measurement arrives and the process is then repeated, following a receding horizon approach. In this procedure, the future behavior of the system is optimized without accounting for external disturbances or model-plant mismatch, although these uncertainties are the only reason why feedback is needed at all.

For applications with hard constraints, MPC implementations can lead to constraint violations, and it is for those applications that robust MPC can be used to correct the optimistic predictions of MPC. Of the possible approaches for implementing robust MPC (see, e.g., Bertsekas, 2007; Dadhe and Engell, 2008; Goulart and Kerrigan, 2006), our focus here is on tube-based MPC (Langson et al., 2004), whereby the predicted trajectories used in traditional MPC are replaced by robust forward invariant tubes; that is, tubes enclosing all the response trajectories for a chosen control law regardless of the particular realization of the uncertainty.

Consider a controlled dynamic system with time-varying uncertainties in the form

$$\forall t \in [0,T], \quad \dot{x}(t) = f(x(t), u(t), w(t)),$$

where $u(t) \in U \subseteq \mathbb{K}^{n_u}$ and $w(t) \in W \subseteq \mathbb{K}^{n_w}$ denote the control and disturbances, respectively. By letting $\mathcal{Y}$ denote the set of all robust forward invariant tubes, we can formulate the tube-based MPC problem as:

$$\min_{Y\in\mathcal{Y}} \int_t^{t+T} \ell(Y(\tau))\mathrm{d}\tau \quad \text{s.t.} \quad \begin{cases} Y(\tau) \subseteq F_x, \\ Y(t) = \{\hat{x}_t\}, \end{cases}$$

where the feasibility constraints $F_x := \{x \in \mathbb{R}^{n_x} | g(x) \leq 0\}$ are enforced for all $\tau \in [t, t+T]$; the set-valued function $\ell : \Pi(\mathbb{R}^{n_x}) \to \mathbb{R}$ is the objective function in the MPC controller; and $\hat{x}_t$ denotes the current state measurement at time t.

This formulation shows deep connections between forward invariant tubes and the reachable-set enclosure $\overline{X}(\cdot, P)$, e.g., computed via the generalized differential inequality presented in Sect. 3. In particular, we envision extensions of the work by Villanueva et al. (2014) towards the following min-max differential inequality:

a.e. $t \in [0,T]$, $\forall c \in \mathbb{R}^{n_x}$,

$$\dot{V}[\overline{X}(t)](c) \geq \min_{\nu} \max_{\xi,\omega} \left\{ c^{\mathrm{T}} f(\xi,\nu,\omega) \;\middle|\; \begin{array}{l} \xi \in \overline{X}(t) \\ c^{\mathrm{T}}\xi = V[\overline{X}(t)](c) \\ \nu \in U \\ \omega \in W \end{array} \right\},$$

which defines a sufficient condition for the set-valued function $\overline{X} : [0,T] \to \Pi(\mathbb{R}^{n_x})$ to be a robust forward invariant tube.

Our on-going investigations aim at developing efficient and tractable numerical procedures for constructing such robust forward invariance tubes, as well as tractable algorithms for the on-line solution of the corresponding tube-based MPC problems.

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Appendix A. CASE STUDY MODEL PARAMETERS

The parameter values used in the two-step anaerobic digestion model in Sect. 1.1 can be found in Table A.1.

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Table A.1. Parameter values in two-step anaerobic digestion model Bernard et al. (2001).

Parameter	Value		Parameter	Value	
$\bar{\mu}_1$	1.2	day^{-1}	k_1	42.14	$\mathrm{g(COD)\,g(cell)^{-1}}$
K_{S_1}	7.1	$\mathrm{g(COD)\,L^{-1}}$	k_2	116.5	$\mathrm{mmol\,g(cell)^{-1}}$
$\bar{\mu}_2$	0.74	day^{-1}	k_3	268.0	$\mathrm{mmol\,g(cell)^{-1}}$
K_{S_2}	9.28	$\mathrm{mmol\,L^{-1}}$	k_4	50.6	$\mathrm{mmol\,g(cell)^{-1}}$
K_{I_2}	256	$\mathrm{mmol\,L^{-1}}$	k_5	343.6	$\mathrm{mmol\,g(cell)^{-1}}$
$k_{\mathrm{L}}a$	19.8	day^{-1}	k_6	453.0	$\mathrm{mmol\,g(cell)^{-1}}$
K_{H}	16	$\mathrm{mmol\,L^{-1}\,atm^{-1}}$	S_1^{in}	5	$\mathrm{g(COD)\,L^{-1}}$
P_{t}	1	atm	S_2^{in}	80	$\mathrm{mmol\,L^{-1}}$
α	0.5	–	Z^{in}	50	$\mathrm{mmol\,L^{-1}}$
D	0.4	day^{-1}	C^{in}	0	$\mathrm{mmol\,L^{-1}}$

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