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On the Stability of Set-Valued Integration for Parametric Nonlinear ODEs

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Abstract

This paper is concerned with bounding the reachable set of parametric nonlinear ordinary differential equations using set-valued integration methods. The focus is on discrete-time set-propagation algorithms that proceed by first constructing a predictor of the reachable set and then determine a step-size for which this predictor yields a valid enclosure. For asymptotically stable systems, we give general conditions under which the computed bounds are stable, at least for small enough parametric variations. We also propose a strategy accounting for possible invariants of the dynamic system in order to further enhance stability. These novel developments are illustrated by means of numerical examples.

Keywords: ordinary differential equations, set-valued integration, stability, invariants

1. Introduction

Enclosing the reachable set of uncertain dynamic systems, also known as set-valued integration, finds applications in many research fields, including reachability analysis for control systems, robust optimal control, and global optimization of dynamic systems [e.g., 2–4]. This paper considers parametric nonlinear ordinary differential equations (ODEs) of the form:

$$\forall t \in [0,T], \quad \dot{x}(t,p) = f(x(t,p),p) \quad \text{with} \quad x(0,p) = x_0(p)\,, \tag{1}$$

where the state $x : [0,T] \times P \to \mathbb{R}^{n_x}$ is regarded as a function of the parameter vector $p \in P \subseteq \mathbb{R}^{n_p}$ along $[0,T]$; f and x_0 are sufficiently often continuously differentiable.

The focus is on algorithms that compute a time-varying enclosure $Y(t)$ of the actual reachable set $X(t) := \{x(t,p) \mid p \in P\}$ of (1). Existing approaches for set-valued integration can be broadly classified into either continuous-time or discrete-time set-propagation methods. The emphasis here is on the latter methods, which discretize the integration horizon into finite steps and typically proceed in two phases [8]: (i) obtain 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 the step. In particular, the second phase relies on a high-order Taylor expansion of the ODE solutions in time, for instance evaluated using interval arithmetic or Taylor model arithmetic with interval remainder bounds [7, 9]. Even though care is taken to minimize the over-estimation of the enclosures and to mitigate the wrapping effect, bounds computed with these approach typically explode after a finite time, even when the solution of the original system does not.

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In fact, a natural requirement for a consistent set-valued integrator would appear to be that, for a stable ODE system, the computed enclosures should themselves be stable, at least for small enough parametric variations. Recently, we 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 [6]. Moreover, we introduced a new type of bounder for vector-valued functions, namely Taylor model with ellipsoidal remainder. The main objective of this paper is to present general conditions under which this algorithm generates stable enclosures. A second principal contribution concerns the development of strategies accounting for possible invariants of the ODEs in order to further improve the enclosure stability.

The paper is organized as follows. In Sect. 2 we recall the set-valued integration algorithm. The main contributions of the paper, namely providing stability conditions and incorporating invariants, are presented in Sects. 3 and 4, respectively, and these developments are illustrated with numerical examples. Finally, Sect. 5 concludes the paper.

2. Set-Valued Integrator

Notations and concepts are introduced first in order to present the set-valued integration from [6]. To keep our considerations general, we consider affine set-parameterizations, a particular class of computer-representable sets in the form

$$\forall Q \in \mathbb{D}_{n,\ell}, \quad \mathrm{Im}_{\mathbb{E}_\ell}(Q) \;:=\; \{\, Q\,[\,b\;1\,]^{\mathrm{T}} \;\mid\; b \in \mathbb{E}_\ell \,\}\,,$$

where $\mathbb{E}_\ell \subseteq \mathbb{R}^\ell$, $\ell \geq 1$, is the so-called basis set; and $\mathbb{D}_{n,\ell} \subseteq \mathbb{R}^{n\times(\ell+1)}$, $n \geq 1$, the associated domain set. Usual convex sets such as intervals, ellipsoids or zonotopes can all be characterized using affine set-parameterizations on convex basis sets. For instance, choosing $\mathbb{E}_\ell^{\mathrm{ball}} := \{\, \xi \in \mathbb{R}^\ell \;\mid\; \|\xi\|_2 \leq 1 \,\}$ and the associated domain $\mathbb{R}^{\ell\times(n+1)}$ allows representation of ellipsoids in $\mathbb{R}^n$. Nonconvex sets too can be represented in terms of affine set-parameterizations. For instance, qth-order polynomial models with ellipsoidal remainder terms can be constructed using the basis set $\mathbb{E}_\ell^{\mathrm{pol}(q)} \times \mathbb{E}_\ell^{\mathrm{ball}}$, where $\mathbb{E}_\ell^{\mathrm{pol}(q)} := \{M_{\ell,q}(\xi) \mid \xi \in [-1,1]^\ell\}$ and $M_\ell^{(q)}(\xi) \in \mathbb{R}^{\alpha_\ell^{(q)}}$ is the vector containing the first $\alpha_\ell^{(q)}$ monomials in ξ in lexicographic order.

Now, given a function $g : \mathbb{R}^n \to \mathbb{R}^m$ as well as an affine set-parameterization on the basis set $\mathbb{E}_\ell$ with associated domains $\mathbb{D}_{n,\ell}$ and $\mathbb{D}_{m,\ell}$, we call the function $g^{\mathbb{E}_\ell} : \mathbb{D}_{n,\ell} \to \mathbb{D}_{m,\ell}$ an $\mathbb{E}_\ell$-extension of g if

$$\forall Q \in \mathbb{D}_{n,\ell}, \quad \mathrm{Im}_{\mathbb{E}_\ell}\left(g^{\mathbb{E}_\ell}(Q)\right) \;\supseteq\; \{\, g(z) \;\mid\; z \in \mathrm{Im}_{\mathbb{E}_\ell}(Q) \,\}\,.$$

Moreover, we say that the extension $g^{\mathbb{E}_\ell}$ has Hausdorff convergence order $q \geq 1$, if

$$\forall Q \in \mathbb{D}_{n,\ell}, \;\; d_{\mathrm{H}}\left(\mathrm{Im}_{\mathbb{E}_\ell}\left(g^{\mathbb{E}_\ell}(Q)\right), \{\, g(z) \;\mid\; z \in \mathrm{Im}_{\mathbb{E}_\ell}(Q) \,\}\right) \leq \mathcal{O}(\mathrm{diam}(\mathrm{Im}_{\mathbb{E}_\ell}(Q))^q)\,,$$

where d_{H} denotes the usual Hausdorff distance. The construction of extensions on the set of intervals or Taylor models with interval remainders can be automated for tree-decomposable (factorable) functions using interval analysis and Taylor model arithmetic, respectively, yet such extensions enjoy linear Hausdorff convergence only. On the other hand, a procedure for constructing extensions on the set of Taylor models with ellipsoidal remainders that enjoys quadratic Hausdorff convergence is detailed in [6].

Discrete-time approaches for set-valued integration typically consider a Taylor expansion in time of the solutions as

$$\exists \tau \in [t, t+h]: \quad x(t_j + h_j, p) = \sum_{i=0}^{s} h_j^i \phi_i(x(t,p),p) + h_j^{s+1}\phi_{s+1}(x(\tau,p),p)\,, \tag{2}$$

with s the expansion order; and $\phi_0, \ldots, \phi_{s+1}$, the Taylor coefficients of the ODE solution. Given parameterizations Q_p of the parameter set and $Q_x(t_j)$ of the reachable set at t_j, so that $\mathrm{Im}_{\mathbb{E}_{n_p}}\left(Q_p\right) \supseteq P$ and $\mathrm{Im}_{\mathbb{E}_{n_p}}\left(Q_x(t_j)\right) \supseteq X(t_j)$, a predictor of the reachable set is given by:

$$\forall h \in (0, T - t_j], \quad Q_x(t_j + h) := \bigoplus_{i=0}^{s} h^i \phi_i^{\mathbb{E}_{n_p}}(Q_x(t_j), Q_p) \,\oplus\, h\,\mathrm{TOL}\,Q_{\mathrm{unit}}\,, \tag{3}$$

where $\oplus$ denotes the extension of the addition operator; $\mathrm{TOL} > 0$ is a user-defined tolerance; $Q_{\mathrm{unit}} \in \mathbb{D}_{n_x,n_p}$; and $\phi_i^{\mathbb{E}_{n_p}}$ are extensions of the Taylor coefficients ϕ_i. In turn, a step-size $\bar{h} > 0$ can be computed such that the parameterization $Q_x(t_j + h)$ yields an enclosure of the reachable set, $\mathrm{Im}_{\mathbb{E}_{n_p}}\left(Q_x(t_j+h)\right) \supseteq X(t_j + h)$, for all $\bar{h} \in [0, h]$.

An algorithmic procedure applying these two phases repeatedly in order to compute a matrix-valued enclosure function $Q_x : [0, T] \to \mathbb{D}_{n_x,n_p}$ is summarized next:

Input: ODE with factorable right-hand side and initial value functions f, x_0; tolerance $\mathrm{TOL} > 0$; affine parameterization Q_p of the parameter set P on the basis $\mathbb{E}_{n_p}$; maximum and minimum step-sizes $h_{\max} \geq h_{\min} > 0$; step-size reduction parameter $0 < \varrho < 1$

Initialization:

1. Set $j = 0$, $t_0 = 0$, and $Q_x(0) = x_0^{\mathbb{E}_{n_p}}(Q_p)$

Repeat:

2. Construct predictor $Q_x(t_j + h)$ for all $h \in [t_j, T - t_j]$ as in (2) with extensions $\phi_0^{\mathbb{E}_{n_p}}, \ldots, \phi_s^{\mathbb{E}_{n_p}}$
3. Set step-size guess $\bar{h} = \min\left\{ \varrho\left(\frac{\mathrm{TOL}}{\|\Phi(0)\|}\right)^{\frac{1}{s}}, h_{\max} \right\}$
   While $\bar{h}^s\,\Phi(\bar{h}) \not\subseteq \mathrm{TOL}\,\mathbb{I}(Q_{\mathrm{unit}})$, **Repeat** $\bar{h} \leftarrow \varrho\bar{h}$, where $\Phi(h) := \phi_{s+1}^{\mathbb{I}}(\mathbb{I}(Q(t_j + h)), \mathbb{I}(Q_p))$
4. **If** $\bar{h} < h_{\min}$, **Return** with an error message
5. **If** $t_j + \bar{h} \geq T$, **Return** with an indication of success; Otherwise, set $t_{j+1} \leftarrow t_j + \bar{h}$, increment $j \leftarrow j + 1$, and **Return** to Step 2

Output: Enclosure function $Q_x : [0, t_j] \to \mathbb{D}_{n_x,n_p}$ such that $\mathrm{Im}_{\mathbb{E}_{n_p}}\left(Q_x(t)\right) \supseteq X(t)$ for all $t \in [0, t_j]$

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3. Stability of the Set-Valued Integrator

Conditions under which the set-valued integration algorithm outlined previously inherits the stability properties of the underlying dynamic system are now discussed. Due to space limitations, these conditions are given without a proof; see, e.g., [5].

The focus is on those asymptotically stable systems that have a unique (stable) equilibrium point $\bar{x}(p)$ for every initial value $x(0,p)$ in the set $\{x_0(p) \mid p \in P\}$ and for all $p \in P$. In particular, let us denote by $\bar{X}(P) := \{\,\bar{x}(p) \mid p \in P\}$ the set of all equilibrium points and by $Y(t,P) := \{\,\mathrm{Im}_{\mathbb{E}_{n_p}}\left(Q_x(t)\right) \mid p \in P\}$ the parameterized reachable set enclosures for $t \geq 0$. We say that a set-valued integrator itself is locally asymptotically stable if the following conditions are satisfied for all sufficiently small tolerances $\mathrm{TOL} > 0$ and all sufficiently small maximum step size $h_{\max} > 0$:

$$\exists M < \infty \text{ such that: } \quad \forall t \geq 0, \;\; d_{\mathrm{H}}(Y(t,P), \bar{X}(P)) \; < \; M + \mathcal{O}(\mathrm{TOL}) + \mathcal{O}(h_{\max}^s)\;,$$

for all parameter set P with sufficiently small diameter, and

$$\forall p \in P, \quad \limsup_{t\to\infty} \; d_{\mathrm{H}}(Y(t,\{p\}), \bar{x}(p)) \; < \; \mathcal{O}(\mathrm{TOL}) + \mathcal{O}(h_{\max}^s)\;.$$

It can be shown that the local asymptotic stability of the proposed set-valued integrator depends essentially on the way the enclosures are constructed; that is, on the underlying set arithmetic used to construct the extensions of the Taylor coefficients $\phi_0,\ldots,\phi_s$ and of the initial value function x_0. More specifically, the key requirement is that these extensions must exhibit at least quadratic Hausdorff convergence in order for the set-valued integrator to be locally asymptotically stable. This is the case for instance when Taylor models with ellipsoidal remainders are used, as illustrated in the following example.

Case Study: Anaerobic Digestion Consider the two-reaction model of an anaerobic digester with self-regulated pH, as developed in [1]:

$$\begin{aligned}
\dot{X}_1 &= (\mu_1(\xi) - \alpha D)X_1\\
\dot{X}_2 &= (\mu_2(\xi) - \alpha D)X_2\\
\dot{S}_1 &= D(S_1^{\mathrm{in}} - S_1) - k_1\mu_1(S_1)X_1\\
\dot{S}_2 &= D(S_2^{\mathrm{in}} - S_2) + k_2\mu_1(S_1)X_1 - k_3\mu_2(S_2)x_2\\
\dot{Z} &= D(Z^{\mathrm{in}} - Z)\\
\dot{C} &= D(C^{\mathrm{in}} - C) - q_{\mathrm{C}} + k_4\mu_1(S_1)x_1 + k_5\mu_2(S_2)x_2
\end{aligned}$$

with:

$$\begin{aligned}
\mu_1(S_1) &:= \frac{\bar{\mu}_1 S_1}{S_1 + K_{S_1}}\\
\mu_2(S_2) &:= \frac{\bar{\mu}_2 S_2}{S_2 + K_{S_2} + S_2^2/K_{I_2}}\\
\phi &:= C + S_2 - Z + K_{\mathrm{H}}P_{\mathrm{T}} + \frac{k_6\mu_2(S_2)X_2}{k_{\mathrm{L}}a}\\
P_{\mathrm{C}} &:= \frac{\phi - \sqrt{\phi^2 - 4K_{\mathrm{H}}P_{\mathrm{T}}(C + S_2 - Z)}}{2K_{\mathrm{H}}}\\
q_{\mathrm{C}} &:= k_{\mathrm{L}}a(C + S_2 - Z - K_{\mathrm{H}} * P_{\mathrm{C}})
\end{aligned}$$

where X_1, X_2 and S_1, S_2 denote biomass and organic substrate concentrations for the two reactions, respectively; C and Z denote inorganic carbon concentration and total alkalinity, respectively. We consider a dilution rate of $D = 0.4\ \mathrm{day}^{-1}$ and the values for all the other parameters are the same as in [1].

Enclosures of the reachable set obtained with 2nd- and 3rd-order Taylor models with ellipsoidal remainders are shown in Fig. 1, for uncertain initial values given by $X_1(0) \in 0.5 \times [0.98, 1.02]$, $X_2(0) \in [0.98, 1.02]$, $S_1(0) = 1$, $S_2(0) = 5$, $Z(0) = 50$, and $C(0) = 40$. 3rd-order (or higher-order) Taylor models successfully stabilize the reachable set enclosure here, whereas 2nd-order Taylor models fail to do so for this level of uncertainty. In the latter case, stabilizing the enclose would require reducing the uncertainty set further.

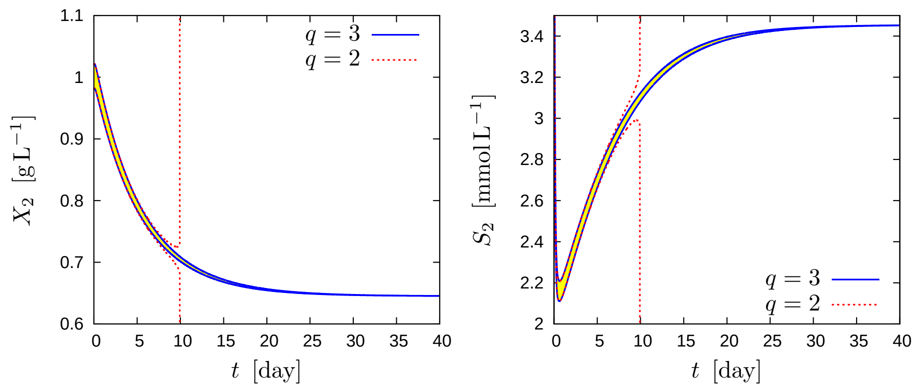

Figure 1: Reachable set enclosure projections for the variables X_2 and S_2.

4. Accounting for ODE Invariants

In order to improve the stability of the enclosures as well as to tighten them further, suppose now that an invariant for the parametric ODE system is known, namely a function $h : \mathbb{R}^{n_x} \times \mathbb{R}^{n_p} \to \mathbb{R}$ such that $h(x(t,p),p) = 0$ for any solution $x(t,p)$ of (1). Given an affine-parameterization basis $\mathbb{E}_{n_p}$, it follows that an extension $h^{\mathbb{E}_{n_p}}$ of h should satisfy

$$\forall t \geq 0, \quad \mathrm{Im}_{\mathbb{E}_{n_p}}\left(h^{\mathbb{E}_{n_p}}(Q_x(t), Q_p)\right) = \{0\}\,,$$

for given parameterizations Q_p and $Q_x(t)$ of the parameter and reachable sets.

Consider the special case of qth-order Taylor models with ellipsoidal remainders, such that $[\mathcal{P}_x(t), \mathcal{R}_x(t)] := Q_x(t)$ and $[\mathcal{P}_h(t), \mathcal{R}_h(t)] := h^{\mathbb{E}^{\mathrm{pol}(q)}_{n_p} \times \mathbb{E}^{\mathrm{ball}}_{n_p}}(Q_x(t), Q_p)$. The polynomial part $\mathcal{P}_h(t)$ is trivially equal to zero by construction. On application of Algorithm 1 in [6], the ellipsoidal remainder is constructed such that:

$$\mathrm{Im}_{\mathbb{E}^{\mathrm{ball}}_{n_p}}\left(\mathcal{R}_h(t)\right) \supseteq \mathrm{Im}_{\mathbb{E}^{\mathrm{ball}}_{n_p}}\left(A_h(t)\,\mathcal{R}_x(t)\,A_h(t)^{\mathrm{T}}\right) \oplus N_h(t)\,, \tag{4}$$

where $A_h(t)$ is the Jacobian matrix of h evaluated along the solution trajectory for some $\hat{p} \in P$, and $N_h(t)$ is an interval nonlinearity bounder. For linear invariants in particular, we have $N_h(t) = \{0\}$ and the ellipsoidal remainder $\mathrm{Im}_{\mathbb{E}^{\mathrm{ball}}_{n_p}}\left(\mathcal{R}_h(t)\right)$ can be thus be safely intersected with the hyperplane $\mathcal{H}_h(t) := \{x \in \mathbb{R}^{n_x} \mid A_h(t)^{\mathrm{T}} x = 0\}$. This intersection is simply repeated multiple times when several invariants are known.

Case Study: Reversible Chemical Reactions Consider the reversible reactions $\mathsf{A} + \mathsf{B} \rightleftharpoons \mathsf{C}$ and $\mathsf{A} + \mathsf{C} \rightleftharpoons \mathsf{D}$ in a batch reactor, as described by the following dynamic model:

$$\begin{aligned}
\dot{x}_{\mathsf{A}} &= -r_1(x_{\mathsf{A}}, x_{\mathsf{B}}, x_{\mathsf{C}})\\
\dot{x}_{\mathsf{B}} &= -r_1(x_{\mathsf{A}}, x_{\mathsf{B}}, x_{\mathsf{C}})\\
\dot{x}_{\mathsf{C}} &= r_1(x_{\mathsf{A}}, x_{\mathsf{B}}, x_{\mathsf{C}}) - r_2(x_{\mathsf{A}}, x_{\mathsf{C}}, x_{\mathsf{D}})\\
\dot{x}_{\mathsf{D}} &= r_2(x_{\mathsf{A}}, x_{\mathsf{C}}, x_{\mathsf{D}})
\end{aligned}
\quad\left|\quad
\begin{aligned}
&\text{with:}\\
&r_1(x_{\mathsf{A}}, x_{\mathsf{B}}, x_{\mathsf{C}}) := k_1^{\mathrm{f}} x_{\mathsf{A}} x_{\mathsf{B}} - k_1^{\mathrm{r}} x_{\mathsf{C}}\\
&r_2(x_{\mathsf{A}}, x_{\mathsf{B}}, x_{\mathsf{C}}) := k_2^{\mathrm{f}} x_{\mathsf{A}} x_{\mathsf{B}} - k_2^{\mathrm{r}} x_{\mathsf{C}}
\end{aligned}\right.$$

Based on mass-conservation considerations, it is not hard to see that the functions $h_1(x) := x_{\mathsf{B}} + x_{\mathsf{C}} + x_{\mathsf{D}}$ and $h_2(x) := x_{\mathsf{A}} - x_{\mathsf{B}} + x_{\mathsf{D}}$ are both linear solution invariants for the ODE system, i.e., $\dot{h}_1(x) = \dot{h}_2(x) = 0$ for all $t \geq 0$. Such invariants are typical in chemical reaction systems [e.g., 10, 11]. Mixed uncertainty in the initial values and kinetic parameters is considered here, with $x_{\mathsf{A}}(0) = 1$, $x_{\mathsf{B}}(0) \in [0.95, 1.05]$, $x_{\mathsf{C}}(0) = x_{\mathsf{D}}(0) = 0$, $k_1^{\mathrm{f}} \in [50, 60]$, $k_2^{\mathrm{f}} = 20$, and $k_1^{\mathrm{r}} = k_2^{\mathrm{r}} = 1$.

Enclosures of the reachable set obtained with 3rd-order Taylor models with ellipsoidal remainders are shown in Fig. 2, with and without accounting for the invariants. On account of the invariants the set-valued integrator is able to stabilize the reachable set enclosure, whereas it fails to do so for this level of uncertainty when the invariants are ignored.

5 Conclusions

This paper was concerned with discrete-time, set-valued integration for computing parameterized enclosures of the reachable set of nonlinear parametric ODEs. Special emphasis has been on the stability properties of the enclosures, giving conditions under which the set-valued integrator inherits the asymptotic stability property of the original dynamic

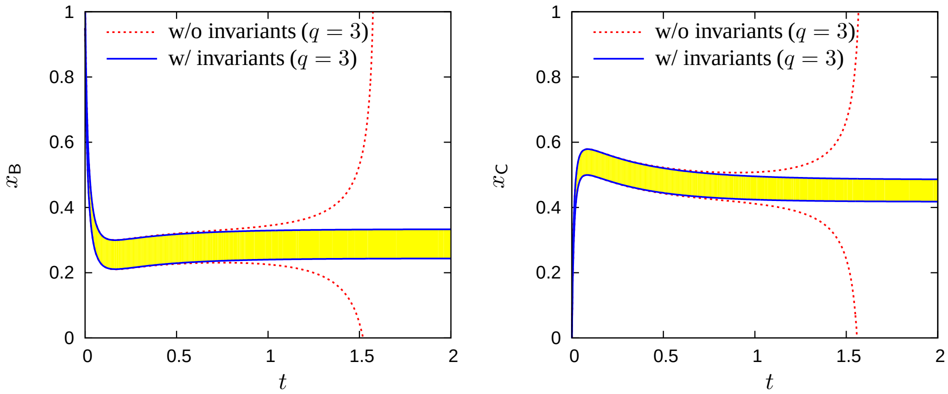

Figure 2: Reachable set enclosure projections for the variables x_A and x_B.

system. The key requirement here is that the underlying set arithmetic constructs extensions of factorable functions that are at least quadratically convergent. This stability property has been illustrated with the case study of an anaerobic digester, using Taylor model arithmetic with ellipsoidal remainders. Another contribution has been incorporating ODE invariants in order to further improve the stability of the algorithm. Future work will focus on taking into account a priori enclosures derived from physical insight, and applying this generic bounding capability in global and robust dynamic optimization.

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