Computers and Chemical Engineering 35 (2011) 844–857

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

Convex/concave relaxations of parametric ODEs using Taylor models

A.M. Sahlodin[a], B. Chachuat[a,b,*]

[a] Department of Chemical Engineering, McMaster University, 1280 Main Street West, Hamilton, ON L8S 4L7, Canada
[b] Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, South Kensington Campus, London SW7 2AZ, United Kingdom

ARTICLE INFO

Article history:
Received 1 October 2010
Received in revised form
25 December 2010
Accepted 17 January 2011
Available online 26 January 2011

Keywords:
Interval analysis
Taylor models
Convex relaxations
Ordinary differential equations
Global optimization
Dynamic optimization

ABSTRACT

This paper presents a discretize-then-relax method to construct convex/concave bounds for the solutions of a wide class of parametric nonlinear ODEs. The algorithm builds upon Taylor model methods recently developed for verified solution of parametric ODEs. To enable the propagation of convex/concave state bounds, a new type of Taylor model is introduced, in which convex/concave bounds for the remainder term are computed in addition to the usual interval bounds. At each time step, a two-phase procedure is applied: a priori convex/concave bounds that are valid over the entire time step are calculated in the first phase; then, pointwise-in-time convex/concave bounds at the end of the time step are obtained in the second phase. This algorithm is implemented in an object-oriented manner using templates and operator overloading. It is demonstrated and compared to other available approaches on a selection of problems from the literature.

1. Introduction

The ability to compute tight enclosures for the solutions $\mathbf{x}$ of parametric ordinary differential equations (ODEs) of the form

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t), \mathbf{p}), \quad t \in (t_0, t_f], \tag{1}$$

$$\mathbf{x}(t_0) = \mathbf{h}(\mathbf{p}), \tag{2}$$

with $\mathbf{p} \in \mathbf{P}$ where $\mathbf{P}:=[\mathbf{p}^L, \mathbf{p}^U] \subset \mathbb{R}^{n_p}$ is an interval vector, is central to many deterministic global optimization methods for dynamic systems. These enclosures are needed to compute lower or upper bounds for general objective or constraint functionals such as

$$\mathcal{F}(\mathbf{p}) = \phi(\mathbf{x}(t_f), \mathbf{p}) + \int_{t_0}^{t_f} \psi(\mathbf{x}(t), \mathbf{p})dt,$$

which in turn can be exploited by branch-and-bound algorithms and their variants (Chachuat & Latifi, 2003; Esposito & Floudas, 2000; Lin & Stadtherr, 2007a; Papamichail & Adjiman, 2002; Singer & Barton, 2006b). Other related applications are in the field of mixed-integer dynamic optimization (MIDO) (Chachuat, Singer, & Barton, 2005), optimization of hybrid discrete/continuous systems (Lee & Barton, 2008), bilevel dynamic optimization (Mitsos, Chachuat, & Barton, 2009b), and guaranteed estimation (Kieffer & Walter, 2010).

Two principal classes of methods have been proposed in the literature to compute an over-approximation of the actual ODE solution set. The first class proceeds by constructing an auxiliary system of ODEs, the solutions of which have the desired properties. General procedures have been developed that build upon Müller's theorem (Walter, 1970) for computing interval bounds (Harrison, 1977; Papamichail & Adjiman, 2002; Scott & Barton, 2010; Singer & Barton, 2006a). Efficient procedures have also been recently devised for constructing auxiliary dynamic systems that describe affine bounds (Singer & Barton, 2006a) or convex/concave bounds (Scott et al., 2010a) with respect to the parameters $\mathbf{p}$, pointwise in the integration variable t. A limitation of these methods, however, is their sensitivity to the wrapping effect and to the dependency problem that ultimately lead to an explosion of the enclosure sizes. Another limitation is tied to the use of non-verified numerical methods for solving the auxiliary dynamic systems, that may result in invalid bounds. Recently, the use of hybrid methods has been investigated to address this latter deficiency (Ramdani, Meslem, & Candau, 2009).

The second class builds upon verified solution methods for ODEs to compute an over-approximation of the actual solution set at discrete grid points $t_k \in [t_0, t_f]$. Here, discretization is performed prior to the bounding step. Traditional interval ODE methods proceed in two phases at each grid point (Nedialkov, Jackson, & Corliss, 1999), namely the computation of an a priori enclosure, followed by the

* Corresponding author at: Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, South Kensington Campus, London SW7 2AZ, United Kingdom.
E-mail addresses: sahlodam@mcmaster.ca (A.M. Sahlodin), b.chachuat@imperial.ac.uk (B. Chachuat).

0098-1354/$ – see front matter
doi:10.1016/j.compchemeng.2011.01.031

computation of a refined enclosure. They have the ability to systematically account for truncation errors as well as built-in capabilities to mitigate the wrapping effect. Recently, Sahlodin and Chachuat (2010) have presented an extension of this approach, which yields convex and concave bounds that are guaranteed to be tighter than the aforementioned interval bounds. Lin and Stadtherr (2007b) have also extended the two-phase approach by using Taylor models (Makino & Berz, 2003) instead of interval bounds, thereby obtaining large improvements. Alternative methods for the verified solution of ODEs that employ Taylor models have been developed by Berz and Makino (2006); see also (Eble, 2007; Neher, Jackson, & Nedialkov, 2007).

Despite these advances, only relatively small dynamic optimization problems can currently be addressed in reasonable computational time using state-of-the-art deterministic global dynamic optimization methods. The lack of reliable and tight bounds for parametric ODEs still appears to be the main bottleneck and calls upon further developments. The focus in this paper is on the second class of methods. A new bounding technique is developed, whereby the two recent extensions of the two-phase approach to propagate Taylor models (Lin & Stadtherr, 2007b) and convex/concave bounds (Sahlodin & Chachuat, 2010) are unified. To enable it, a new type of Taylor model is introduced, in which convex/concave bounds for the remainder term are computed in addition to the usual interval bounds. In so doing, one allies the benefits of both approaches: the ability of Taylor models to mitigate the dependency problem (Makino & Berz, 1999) and to tackle dynamic systems that are highly nonlinear in the parameters on one hand; and the use of convex/concave relaxations that typically greatly enhances convergence speed over simple interval bounds in deterministic global optimization on the other hand (Kearfott, 2006; Tawarmalani & Sahinidis, 2002).

The remainder of the article is organized as follows. In the next section, background on bounding methods is provided, including interval analysis, Taylor models and convex/concave relaxations. The two-phase approach for verified solution of ODEs and its recent extension to the propagation of Taylor models are described in Section 3, and special care is taken to present those approaches in a concise, unified way. In Section 4, a new bounding technique combining Taylor models and convex/concave relaxations is introduced, then this technique is used to develop an improved state-relaxation algorithm for parametric ODEs. This new convex/concave relaxation algorithm is demonstrated and compared to other available approaches for a selection of problems from the literature in Section 5. Finally, Section 6 concludes the paper.

2. Interval analysis, Taylor models, and convex/concave relaxations

2.1. Interval analysis

The closed interval denoted by $[a, b]$ is the set of real variables given by $\{x \in \mathbb{R} : a \le x \le b\}$. Throughout this paper, the term *interval* is understood as *closed interval* and the convention of denoting intervals by capital letters is adopted. The width, the midpoint, and the interior of the interval $X = [a, b]$ are $w(X) = b - a$, $m(X) = (1/2)(a + b)$, and $\mathrm{int}(X) = \{x \in X : a < x < b\}$, respectively.

Vectors are represented in boldface, and equalities/inequalities between vector quantities are understood component-wise. The width of an interval vector is the largest of the widths of any of its component intervals, while the mid-point of an interval vector is the vector of the mid-points of its component intervals.

Basic arithmetic (binary) operations between two interval variables X and Y are defined as $X \Diamond Y = \{x \Diamond y : y \in Y, z \in Z\}$, where $\Diamond$ denotes any of the binary operations $+$, $-$, $\times$ or $\div$. Likewise, univariate intrinsic functions of interval variables can be defined by treating those as unary operations.

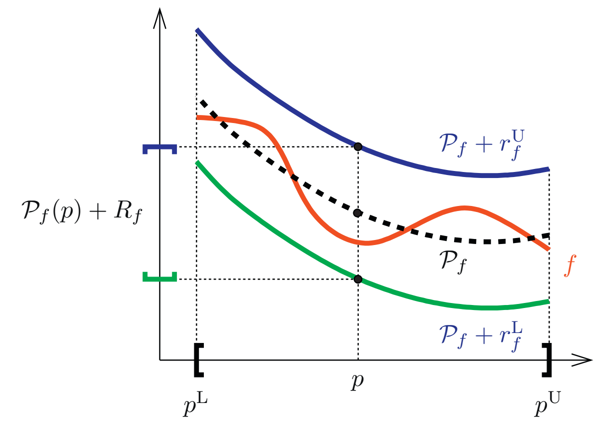

Fig. 1. Illustration of Taylor models.

The class of *factorable functions* (McCormick, 1976), also frequently referred to as the *class FC* of functions in the literature (Moore, Kearfott, & Cloud, 2009), is considered throughout. Factorable functions are those that are defined by a finite recursive composition of binary sums, binary products, and a given library of univariate intrinsic functions. They cover an extremely inclusive class of functions, containing nearly every function which can be represented finitely on a computer by means of a code list or a computational graph.

In interval analysis, *natural interval extensions* can be used for computing bounds on the range of any factorable function for given bounds on their variables; other, more refined, interval forms can also be applied to factorable functions, including the centered and the mean-value forms to name just a few. The interested reader is referred to the literature for a thorough description of interval analysis (Alefeld & Mayer, 2000; Moore et al., 2009).

In performing interval computations, some overestimation is almost always systematic, due to both the wrapping effect and the dependency problem (Moore et al., 2009). The wrapping effect is a result of the actual solution set with an arbitrary shape being wrapped in a box-shaped enclosure. The dependency problem, on the other hand, arises from the inability of interval analysis to recognize multiple occurrences of the same variable in a given expression; as a classical example, consider the natural interval extension of the simple expression $x - x$ with $x \in [-1, 2]$ which is $[-1, 2] - [-1, 2] = [-3, 3]$, while the actual enclosure set is of course $[0, 0]$.

2.2. Taylor models

Taylor models were introduced to reduce the overestimation in interval analysis, by combining interval arithmetic with symbolic computations (Berz, 1997; Makino & Berz, 1999; Makino & Berz, 2003). Consider a function $\mathbf{f}^{[i]}$ defined on the set $\mathbf{P} \subset \mathbb{R}^{n_p}$, and let there be an n_p-variate polynomial $\mathcal{P}_f$ of order q and an interval $R_f := [r_f^L, r_f^U]$ such that:

$$f(\mathbf{p}) \in \mathcal{P}_f(\mathbf{p}) + R_f, \quad \text{for each} \quad \mathbf{p} \in \mathbf{P}.$$

Then, $\mathcal{T}_f := \mathcal{P}_f + R_f$ is called a qth-order Taylor model of f on $\mathbf{P}$. In this context, $\mathbf{P}$ and R_f are known as the *domain interval* and the *remainder interval* of $\mathcal{T}_f$, respectively. Following the work of Neher et al. (2007), no restrictions are imposed on the multivariate polynomial $\mathcal{P}_f$ or on the width of the remainder interval herein. The Taylor model $\mathcal{T}_f$ of a univariate function f on the interval $[p^L, p^U]$ is depicted in Fig. 1; observe, in particular, that $\mathcal{T}_f$ encloses f between two hypersurfaces.