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Validated solutions of initial value problems for parametric ODEs

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Abstract

In initial value problems for ODEs with interval-valued parameters and/or initial values, it is desirable in many applications to be able to determine a validated enclosure of all possible solutions to the ODE system. Much work has been done for the case in which initial values are given by intervals, and there are available software packages that deal with this case. However, less work has been done on the case in which parameters are given by intervals. We describe here a new method for obtaining validated solutions of initial value problems for ODEs with interval-valued parameters. The method also accounts for interval-valued initial values. The effectiveness of the method is demonstrated using several numerical examples involving parametric uncertainties.
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1. Introduction

Initial value problems (IVPs) for ordinary differential equations (ODEs) arise naturally in many applications in science and engineering. It is often the case that the problem involves parameters and/or initial values that are not known with certainty but that can be expressed as intervals. For this situation it is desirable to be able to determine an enclosure of all possible solutions to the ODEs. Traditional approximate solution methods for ODEs are not useful in this context, since, in essence, they would have to solve infinitely many systems to determine such an enclosure. Interval methods [25] for ODEs, on the other hand, provide a natural approach for computing the desired enclosure. Even in the case in which the initial values and parameters are known exactly, standard numerical methods for solving ODEs only compute an approximate solution to some tolerance, without guaranteed error bounds, and so it is of interest to determine an enclosure of the true solution. Interval methods (also called validated methods or verified methods) not only can determine a guaranteed error bound on the true solution, but can also verify that a unique solution to the problem exists. An excellent review of interval methods for IVPs has been given by Nedialkov et al. [28]. Much work has been done for the case in which the initial values are given by intervals, and there are several available software packages that deal with this case. However, relatively little work has apparently been done on the case in which parameters are given by intervals. We concentrate here on the case of such parametric ODEs. However, the method developed will also account for interval-valued initial values.

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Traditional interval methods usually consist of two processes applied at each integration step [28]. In the first process, existence and uniqueness of the solution are proven, and a rough enclosure of the solution is computed. In the second process, a tighter enclosure of the solution is computed. This can be regarded as similar to the familiar predictor-corrector procedure employed in many standard methods for obtaining an approximate solution. In general, both processes are realized by applying interval Taylor series (ITS) expansions with respect to time, and using automatic differentiation to obtain the Taylor coefficients. A major difficulty in interval methods is the overestimation of bounds caused by the dependency problem of interval arithmetic and by the wrapping effect [25]. The accumulation of overestimations at successive time steps may ultimately lead to an explosion of enclosure sizes, causing the integration procedure to abort. Several schemes for reducing the overestimation of bounds have been proposed. For example, Lohner's AWA package employs a QR-factorization method which features efficient coordinate transformations to tackle the wrapping effect [15]. Nedialkov's VNODE package employs QR together with an interval Hermite–Obreschkoff method [27,29], which can be viewed as a type of generalized Taylor method, and improves on AWA. Janssen et al. [7] have introduced a constraint satisfaction approach to these problems, which enhances traditional interval methods with a pruning step based on a global relaxation of the ODEs. Another approach for addressing the dependency problem and the wrapping effect has been described by Berz and Makino [3] and implemented in the beam dynamics package COSY INFINITY. This scheme is based on expressing the dependence on initial values and time using a Taylor model (i.e., a Taylor polynomial and an interval remainder bound). Neher et al. [30] have recently described this Taylor model approach in some detail and compared it to traditional interval methods. We will also use Taylor models in the new method described here, though they will be determined and used in a different way, and a new type of Taylor model will be introduced.

Available general-purpose validated ODE solvers are focused on dealing with uncertainties in the initial values. Some solvers, including VNODE [26], can take interval parameters as input. These solvers, however, can become very inefficient in the presence of interval parameters because this tends to exacerbate the wrapping effect; thus the size of the enclosure can grow so quickly that the integration must be stopped. An alternative approach is to treat time-invariant interval parameters as additional state variables, with zero first-order derivatives, as suggested by Lohner [16]. Since the parameters are now treated as independent variables, tighter enclosures can be obtained using this approach. However, the increase in the number of state variables can result in a significant increase in the computational expense. For example, in a problem with n states and p parameters, an $(n + p) \times (n + p)$ matrix, instead of an $n \times n$ matrix, must be factored at each time step in the usual approach for controlling the wrapping effect. In the work described here, we will develop a method for efficiently determining validated solutions of ODEs with parametric uncertainties, where instead of increasing the number of state variables, we will treat the parametric uncertainties directly. The method follows the traditional two-phase interval approach, but makes use, in a novel way, of Taylor models.

Singer and Barton [35] have recently suggested another approach for bounding the solutions of parametric ODEs. They use convex underestimators and concave overestimators to construct two bounding IVPs, which are then solved to obtain the lower and upper bounds on the trajectories. However, as implemented [34], the bounding IVPs are solved using standard numerical methods that do not provide guaranteed error estimates. Thus, this approach cannot be regarded as providing rigorously guaranteed enclosures.

The remainder of this paper is organized as follows. Section 2 describes the problem we are addressing and the notation used. Section 3 provides background on interval analysis and a brief introduction to the use of Taylor models, based on the Taylor model arithmetic (remainder differential algebra) described by Makino and Berz [20,23]. Section 4 presents the new interval method for obtaining guaranteed enclosures of the solutions of parametric ODEs. Then, in Section 5 we present the results of several numerical experiments that demonstrate the effectiveness of the new method.

2. Problem description

In this section we describe the problem to be solved, and introduce our notation. We consider validated numerical methods for solving the set of parametric autonomous IVPs

$$y'(t) = f(y, \theta), \quad y(t_0) = y_0 \in Y_0, \quad \theta \in \Theta, \tag{1}$$

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