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Original article

Numerical computation of derivatives in systems of delay differential equations

Simon M. Lenz *, Johannes P. Schlöder, H. Georg Bock

Interdisciplinary Center for Scientific Computing (IWR), Im Neuenheimer Feld 368, 69120 Heidelberg, Germany

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Abstract

This article deals with initial value problem solutions in systems of delay differential equations and their derivatives with respect to parameters, where the parameters may occur in the initial value, the initial function, the right-hand-side function, and the delay. Sufficient conditions for differentiability are given, and an efficient and reliable method for the numerical computation is presented. Emphasis is laid on the treatment of problems with a discontinuity at the initial time, for which it is shown that jumps occur in the derivative at the propagated discontinuity times. An explicit expression for the size of the jumps in the derivative is given. Features are discussed of the implementation of COLSOL-DDE, an experimental solver for initial value problems in delay differential equations that also computes the derivatives of the solution. The performance of the developed method is demonstrated by a comparison to standard techniques for derivative approximation.
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1. Context and goals of this article

Delay differential equations (DDEs) play an important role in many different application areas and have been used, e.g., in chemistry for modeling enzyme kinetics and Belousov–Zhabotinskii reactions [63] as well as for electrochemical cells and diffusion processes [33], in physics for modeling mode-locked semiconductor lasers [73] and road traffic [64], in climate research for describing the El Ninõ phenomenon [35,67] and in mechanical engineering for the description of milling processes [53]. A particular popularity of differential equation models with delays is found in the biosciences. Baker et al. [5] give an extensive overview of the use of DDE models in this field, e.g. for modeling the spread of epidemics, the reactions of immune systems to pathogens, the within-host dynamics of HIV infections, and the human respiratory control system. Some more recent examples of DDE models for biological systems can be found in [4,22,25,37,57,71,72].

The DDE models in these applications typically contain parameters, e.g. in the right-hand-side function of the differential equation (e.g. reaction rates in a model for enzyme kinetics), in the initial values (e.g. the initial virus concentration in an HIV model), but also in the delay itself (e.g. the immunization time in an epidemiological model).

* Corresponding author.
E-mail addresses: simon.lenz@iwr.uni-heidelberg.de (S.M. Lenz), schloeder@iwr.uni-heidelberg.de (J.P. Schlöder), bock@iwr.uni-heidelberg.de (H.G. Bock).

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This motivates to formulate an initial value problem (IVP) in a system of DDEs with multiple constant delays and very general parameter dependencies as follows:

$$\frac{d}{dt}y(t) = f(t, y(t), c, \{y(t-\tau_k(c))\}_{k=1}^{n_\tau}) \tag{1a}$$

$$y(t^{ini}(c)) = y^{ini}(c) \tag{1b}$$

$$y(t) = \phi(t, c) \quad \text{for} \quad t < t^{ini}(c). \tag{1c}$$

In this article, Eq. (1a) is referred to as the *nominal DDE* and the problem (1) is referred to as the *nominal DDE-IVP*, where the attribute "nominal" is used for distinction from the variational DDE and the variational DDE-IVP, which appear later in this article.

The *right-hand-side function f* of the nominal DDE (1a) depends on the independent variable *time* $t \in \mathbb{R}$, the *current state* $y(t) \in \mathbb{R}^{n_y}$, *parameters* $c \in \mathbb{R}^{n_c}$, and n_τ *retarded states* $y(t-\tau_k(c)) \in \mathbb{R}^{n_y}$ at the *retarded times* $t-\tau_k(c)$, where $\tau_k(c) > 0$, $k = 1, \ldots, n_\tau$, are positive *delays*. The *initial time* of the nominal DDE-IVP is given by $t^{ini}(c)$ and the *initial value* is given by $y^{ini}(c) \in \mathbb{R}^{n_y}$. For $t < t^{ini}(c)$ the state $y(t)$ is given by the *initial function* $\phi(t, c) \in \mathbb{R}^{n_y}$. The initial conditions (1b) and (1c) are allowed to be discontinuous in $t^{ini}(c)$, i.e. $y^{ini}(c) \neq \phi(t^{ini}(c), c)$. The time horizon on which the nominal DDE-IVP is considered is $[t^{ini}(c), t^{fin}(c)]$, where $t^{fin}(c)$ is the *final time*. Together, the functions f, τ_k, t^{ini}, y^{ini}, ϕ, and t^{fin} are called the *model functions of the nominal DDE-IVP*, all of which may depend on parameters.

The parameter dependence of the model functions of the nominal DDE-IVP (1) leads to a parameter dependence of the solution. Therefore, the solution of the nominal DDE-IVP is from now on denoted as $y(t; c)$. In many practical applications modelers are not only interested in the solution for a specific choice of the parameters c, but also in the derivative of the solution with respect to c, because the derivative indicates how sensitive the solution is with respect to changes in the parameters. Computation of this derivative is also essential in order to estimate the parameters from experimental data by solving a parameter estimation problem with derivative-based methods.

There is a number of publications that has dealt with sensitivity analysis and derivative-based parameter estimation methods for processes described by DDEs. Early works by Banks and Daniel Lamm [9] and Murphy [54] approach parameter estimation problems in DDEs by a Levenberg-Marquardt method but do not comment on the computation of derivatives. Bocharov and Romanyukha [16] solve a parameter estimation problem in immune response modeling and obtain derivatives by finite differences of highly accurate solutions of DDE-IVPs, which are obtained at high computational costs. Baker and Paul [7] formulate a variational DDE-IVP, but they also report that solving the variational DDE-IVP is in general insufficient for the computation of derivatives because the derivative has discontinuities. For an appropriately restricted problem class where jumps in the derivative do not occur, Horbelt et al. [52] solve a variational DDE-IVP for providing the derivatives to a multiple shooting method for a DDE-constrained parameter estimation problem. Solution of a variational DDE-IVP for computing the derivative is also used in Rihan [62], where this approach is characterized as a "costly numerical problem".

Given the high relevance of computing derivatives of solutions of DDE-IVPs with respect to parameters and the considerable attention this topic has gained, it is surprising that very few efforts have been undertaken to develop efficient numerical methods for this purpose. Furthermore, in contrast to the large number of codes for the solution of DDE-IVPs of the form (1) (see [6,15,20,23,29,40,41,43,51,55,56,58,59,65,66,70]), there is to the authors' knowledge at present only one solver that features computation of the derivatives, DDEM by ZivariPiran [77]. This solver automatically constructs the variational DDE-IVP, solves it piecewise together with the nominal DDE-IVP and accounts for possible jumps in $\partial y(t; c)/\partial c$. DDEM is based on a continuous explicit Runge–Kutta method called CRK6X developed by Enright and Yan [32], but ZivariPiran and Enright [78] describe the design of DDEM as a "unified approach", which is to be used with any IVP solver.

This article contributes to the existing research on derivatives of solutions of DDE-IVPs with respect to parameters as follows.

- A theorem is formulated that asserts the differentiability of the solution under suitable sufficient conditions (Section 3). Despite an extensive literature review on this subject, which is summarized in this article, the authors did not find any existing differentiability result for the general case that a discontinuity occurs in the initial time, i.e. in the case $y^{ini}(c) \neq \phi(t^{ini}(c), c)$. It turns out that in order to have differentiability the delays have to be pairwise distinct, and that the derivative is given piecewise as the solution of a variational DDE-IVP but with jumps at certain time points.

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