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Linearizing Stiff Delay Differential Equations

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Abstract: This paper deals to the study and approximation of stiff delay differential equations based on an analysis of a certain error functional. In seeking to minimize the error by using standard descent schemes, the procedure can never get stuck in local minima, but will always and steadily decrease the error until getting to the solution sought. Starting with an initial approximation to the solution, we improve it, adding the solution of some associated linear problems, in such a way that the error is decreased. The performance is expected very good due to the fact that we can use very robust methods to approximate **linear** stiff delay differential equations.

Keywords: DDEs, variational methods, optimality conditions, approximation, convergence.

1. Introduction

Ordinary differential equations (ODEs) and delay differential equations (DDEs) are used to describe many physical models. While ODEs contain derivatives which depend on the solution at the present value of the independent variable, DDEs contain in addition derivatives which depend on the solution at previous times. For DDEs we must provide not just the value of the solution at the initial point, but also the solution at times prior to the initial point. Despite the obvious similarities between ODEs and DDEs, solutions of DDE problems can differ from solutions for ODE problems in several ways. One important thing is the presence of discontinuities in low-order derivatives. Generally there is a discontinuity in the first derivative of the solution at the initial point. Moreover, if the solution has a discontinuity in a derivative somewhere, there are discontinuities in the rest of the interval at a spacing given by the delays.

A popular approach to solving DDEs is to extend one of the methods used to solve ODEs (see [9–11] and their references). Most of the codes are based on Runge-Kutta methods. The code dde23 [15] takes this approach by extending the method of the Matlab explicit ODE solver ode23. The code RADAR5 is developed in FORTRAN-90 and is based on an adaptation of the 3-stage Radau IIA method to stiff delay differential equations [12]. Stiff systems are prevalent in the study of damped oscillators, chemical reactions and electrical circuits. Although there have been numerous attempts to define stiffness, none seem quite satisfactory. One of them is the following “Stiff equations are problems for which explicit methods don’t work” [14]. On the other hand, implicit schemes need to solve an auxiliary nonlinear system of equations in each step. These systems are approximated via Newton-type iterative methods. In particular, we have to be able to find a good initial guess inside of the ball of convergence of the iterative scheme [4–6].

Recently ([1–3]), a variational approach for the analysis and approximation of Cauchy problems has been introduced. One main step in the procedure relies on a very particular linearization of the problem: in some sense, it is like a globally convergent Newton type method. The performance is astonishingly very good due to the fact that we can use very robust methods to approximate **linear** stiff problems like implicit collocation schemes. As point out in [7, 8], it is not clear if it is possible to cover in a satisfactorily way highly **nonlinear** stiff problems, i.e., problems where also the nonlinear terms are affected by large parameters. Moreover, any result should assume that, in each step, the associated nonlinear system is well approximated. In particular, that we are able to start with a good initial guess for the iterative scheme. This might be very restrictive for many stiff problems, however our variational approach gives good results in these cases, see the numer-

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ical section in [2]. In this paper, we extend this procedure to the case of DDEs.

The rest of the paper is divided in three sections. In Section 2 we introduce our variational approach for the linearization of DDEs. Section 3 introduces the numerical procedure and present a convergence analysis. Finally, we conclude with a small conclusion section including some further research directions.

2. A particular linearization of stiff DDEs via an error minimization problem

Let $C := C^1([-\tau,0],\mathbb{R}^n)$ be the vector space of continuous differentiable functions mapping the interval $[-\tau,0]$ into $\mathbb{R}^n$. The stiff problem we like to analyze can be written as

$$x^{'}(t) = f(x(t), x(t-\tau)), \quad t \in (0,T), \tag{1}$$

$$x(\theta) = \phi(\theta), \quad \theta \in [-\tau,0], \tag{2}$$

where $\phi \in C$ specifies the initial condition and f sufficiently smooth in both variables.

We consider the error functional

$$E(x) = \frac{1}{2}\int_0^T |x'(t) - f(x(t), x(t-\tau))|^2\,dx,$$

to be minimized among the absolutely continuous paths $x : (0,T) \to \mathbf{R}^N$ with square-integrable derivative and such that $x(\theta) = \phi(\theta)$, $\theta \in [-\tau,0]$.

It is straightforward to find the Gâteaux derivative of E at a given feasible x in the direction y with $y(\theta) = 0$, $\theta \in [-\tau,0]$. Namely

$$\begin{aligned} E'(x)y = \int_0^T & (x'(t) - f(x(t), x(t-\tau))) \\ & \cdot\ (y'(t) - \nabla_1 f(x(t), x(t-\tau))y(t) \\ & -\nabla_2 f(x(t), x(t-\tau))y(t-\tau))\,dt, \end{aligned}$$

where ∇_1 and ∇_2 denote the partial derivative with respect $x(t)$ and $x(t-\tau)$ respectively.

This expression suggests a nice possibility to select y from: Choose y such that

$$\begin{aligned} & y'(t) - \nabla_1 f(x(t), x(t-\tau))y(t) \\ & -\nabla_2 f(x(t), x(t-\tau))y(t-\tau) \\ & = f(x(t), x(t-\tau)) - x'(t) \text{ in } (0,T), \end{aligned}$$

with $y(\theta) = 0$, $\theta \in [-\tau,0]$.

We have already pointed out that descent methods can never get stuck on anything but the solution of the problem, under global lipschitzianity hypotheses. The following proposition states that a minimization scheme will work fine as they can never get stuck in local minima, and converge steadily to the solution of the problem, no matter what the initialization is. This is also a fundamental fact for our approach.

Theorem 1. *Let x be a critical point for the error E. Then x is the solution of the problem (1).*

3. Numerical procedure

Our approach is really constructive and an iterative numerical procedure is easily implementable based. Mainly:

1. Start with an initial approximation $x^0(t)$ compatible with the initial conditions.
2. Assume we know the approximation $x^{(j)}(t)$ in $[0,T]$.
3. Compute its derivative $(x^{(j)})'(t)$.
4. Compute the auxiliary function $y^{(j)}(t)$ as the numerical solution of the **linear** problem (by making use of a numerical scheme for DDEs with dense output as RADAR5 [12])
$$\begin{aligned} & y'(t) - \nabla_1 f(x^{(j)}(t), x^{(j)}(t-\tau))y(t) \\ & -\nabla_2 f(x^{(j)}(t), x^{(j)}(t-\tau))y(t-\tau) \\ & = f(x^{(j)}(t), x^{(j)}(t-\tau)) - x'(t) \text{ in } (0,T), \end{aligned}$$
with $y(\theta) = 0$, $\theta \in [-\tau,0]$.
5. Change $x^{(j)}$ to $x^{(j+1)}$ by using the update formula
$$x^{(j+1)}(t) = x^{(j)}(t) + y^{(j)}(t).$$
6. Iterate (3), (4) and (5), until numerical convergence ($||y^{(j)}|| \le TOL$).

Assuming that the problem (1) has a unique solution and following [2], we can derive the convergence of this procedure:

Theorem 2. *The iterative procedure $x^{(j)} = x^{(j-1)} + y^{(j)}$, starting from arbitrary feasible $x^{(0)}$ compatible with the initial conditions, converges strongly in $L^\infty(0,T)$ and in $H^1(0,T)$ to the solution of (1) assuming that f is smooth enough.*

A main different in the solution of delay equations compared to ordinary differential equations is the appearance of breaking points (jump discontinuities in the solution or in its derivatives) even in the presence of smooth functions. If the breaking points are not included in the mesh and a variable step size integration is used, the step sizes may be severely restricted near the low order jump discontinuities. Some algorithms are proposed for the detection and computation of breaking points in [13]. This paper includes theoretical results with regard to errors in the approximation of these important points. By construction, both the original problem (1) and the auxiliary linear equation have the same number of breaking points and in the same position.

If we use the algorithm proposed in [13] for the approximation of the auxiliary linear equation (without including the application of the Newton method since in our case the associated system of equations is linear) and combine the theoretical results of this paper with Theorem 2 we obtain the convergence of our full discretized algorithm:

Theorem 3.*With the notation and hypotheses of Theorem 2, if $\tilde{y}^{(j)}$ is the approximation of the sequence $y^{(j)}$ via RADAR5 with breaking point detection then for all $TOL > O(h^5)$ exists $j \in \mathbb{N}$ such that*

$$||y^{(j)}|| \leq TOL.$$

On the other hand, for the approximation of stiff problems implicit schemes are used [14]. A number of convergence results have been derived for the discretization of nonlinear stiff initial problems. In [7]-[8] the authors extend the B-convergence theory to be valid for a class of nonautonomous weakly nonlinear stiff systems; reference to the (potentially large) one-sided Lipschitz constant is avoided, in particular, including **the linear case**. Unique solvability of the system of algebraic equations is shown, and global error bounds are derived. As point out by the same authors, it is not clear if it is possible to cover in a satisfactorily way highly nonlinear stiff problems, i.e., problems where also the nonlinear terms are affected by large parameters. Moreover, any result should assume that, in each step, the associated nonlinear system is well approximated. In particular, that we are able to start with a good initial guess for the iterative scheme. This might be very restrictive for many stiff problems (see Section 6.2 of our recent work in [2]).

The results, as in the case of stiff ODEs [2], would be very satisfactory. For problems verifying the hypotheses of our theorems we obtain always the convergence to the true solution. Moreover, taking small tolerances (TOL) as stopping criterium, the exact and computed solutions should be indistinguishable in a first look [2]. The computational cost of the direct approximation of the stiff nonlinear DDE with an implicit scheme and with variational approach is similar. In each step of the implicit scheme we use a Newton iterative method to approximate the nonlinear system of equations. In our approach we use an iterative scheme to solve the minimization problem but in each iteration we only approximate linear system of equations.

4. Conclusions

In this paper we have presented a new variational approach of DDEs. The main step in the procedure relies on a very particular linearization of the problem. Therefore, the performance is expected very good due to the fact that we can use very robust methods to approximate **linear** stiff problems like implicit collocation schemes [13].

The main advantage of our approach is that we only need to approximate linear problems. We believe that this procedure can be used in a systematic way to examine other types of DDEs due to its flexibility and its simplicity. In particular, we are interesting in DDEs with multiple lags, in DDEs with non-constant lags and in neutral DDEs with lags in the derivatives.

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