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The numerical simulation of the qualitative behaviour of Volterra integro-differential equations

John T. Edwards, Neville J. Ford and Jason A. Roberts
j.edwards@chester.ac.uk, njford@chester.ac.uk, j.roberts@chester.ac.uk

Chester College, Parkgate Road, Chester, CH1 4BJ, UK.

Abstract

We consider the qualitative behaviour of exact and approximate solutions of integral and integro-differential equations with fading memory kernels. Over long time intervals the errors in numerical schemes may become so large that they mask some important properties of the solution. One frequently appeals to stability theory to address this weakness, but it turns out that, in some of the model equations we have considered, there remains a gap in the analysis.

We consider a linear problem of the form

$$y'(t) = -\int_0^t e^{-\lambda(t-s)} y(s)\,ds, \qquad y(0) = 1,$$

and we solve the equation using simple numerical schemes. We outline the known stability behaviour of the problem and derive the values of λ at which the true solution bifurcates. We give the corresponding analysis for the discrete schemes and highlight that, for particular stepsizes, the methods give unexpected behaviour and we show that, as the step size of the numerical scheme decreases, the bifurcation points tend towards those of the continuous scheme. We illustrate our results with some numerical examples.

1 Introduction

The qualitative behaviour of numerical approximations to solutions of functional differential equations is an important area for analysis. We aim to investigate whether the behaviour of the numerical solution reflects accurately that of the true solution. We are particularly concerned with the behaviour of the solution over long time periods when (in particular) the convergence *order* of the method gives us limited insight, since the error depends on a constant that grows with the time interval. Many authors are concerned with stability of solutions and of their numerical approximations. We have considered elsewhere (see [7]) the stability of numerical solutions of equations of this type (and of non-linear extensions). This analysis raised a number of questions, which we consider here, about just how well the full range of qualitative behaviour of even quite a simple equation is understood.

Bifurcations (by which we shall mean any change in the qualitative behaviour of solutions) frequently arise only for systems or for higher order problems and therefore

one is particularly interested in finding suitable simple equations as the basis for analysis. In this paper, we consider the solution by numerical techniques of the integro-differential equation

$$y'(t) = -\int_0^t e^{-\lambda(t-s)} y(s) ds, \ y(0) = 1. \tag{1.1}$$

The equation is a linear convolution equation with separable fading memory convolution kernel and therefore is a simple example from an important class of problems familiar in applications. It is also possible to analyse the equation in the form of a second order ordinary differential equation.

The equation has several key properties that make it an ideal basis for our analysis:

1. it depends on the value of the *single* parameter λ,

2. when λ varies through real values, four distinctive qualitative behaviours in the solution can be detected, and

3. equations with exponential convolution kernels frequently arise in applications and elsewhere in the literature.

For λ real and positive, the kernel is of fading memory type. For λ real and negative, the kernel has a growing memory effect. This linear equation displays surprisingly rich dynamical behaviour for real values of the parameter λ and it is this behaviour that we want to consider for the numerical scheme. We note that the classical test equation

$$y'(t) = g(t) + \xi y(t) + \eta \int_0^t y(s) ds, \quad \eta \neq 0 \tag{1.2}$$

([1, 2]) displays the same range of qualitative behaviour possibilities as (1.1) for varying values of the *two* real parameters ξ, η.

This motivates us to consider equation (1.1) as a prototype problem that is interesting in its own right and that will also provide insight into the behaviour of more complicated equations. We propose to give a further analysis, where we consider the boundaries along which bifurcations occur for equation (1.2) in a sequel [3].

We consider the following questions.

1. Does the numerical scheme display the same four qualitatively different types of long term behaviour as are found in the true solution?

2. Are the interval ranges for the parameter λ that give rise to the changes in behaviour of the solution the same as in the original problem?

2   Behaviour of the exact solution

We consider the equation (1.1) which can be shown to have a unique continuous solution (see, for example, [10]). One can easily establish (by considering, for example, an equivalent ordinary differential equation) the general solution

$$y(t) = A e^{\frac{-\lambda + \sqrt{\lambda^2 - 4}}{2} t} + B e^{\frac{-\lambda - \sqrt{\lambda^2 - 4}}{2} t} \tag{2.1}$$

where A, B are constants. For real values of λ the solution to (1.1) bifurcates (or changes qualitative behaviour) at $\lambda = 0, \pm 2$. We have the following qualitative behaviour.

A1. When $\lambda \geq 2$, $y \to 0$ as $t \to \infty$, with no oscillations.

A2. When $0 < \lambda < 2$, $y \to 0$ as $t \to \infty$, with infinitely many oscillations.

A3. When $\lambda = 0$, $y(t) = \cos(t)$ (persistent oscillations).

A4. When $-2 < \lambda < 0$, the solutions contain infinitely many oscillations of increasing amplitude.

A5. When $\lambda \leq -2$, the solution grows (in magnitude) without any oscillations.

3   Numerical analysis

To apply a numerical method to an integro-differential equation of the type

$$y'(t) = f\left(t, y(t), \int_0^t k(t, s, y(s))ds\right), \quad y(0) = y_0, \tag{3.1}$$

we write the problem in the form

$$y'(t) \quad = \quad f(t, y(t), z(t)) \tag{3.2}$$

$$z(t) \quad = \quad \int_0^t k(t, s, y(s))ds. \tag{3.3}$$

We solve (3.2), (3.3) numerically using a linear multistep method for solving equation (3.2) combined with a suitable quadrature rule for deriving approximate values of z from equation (3.3) (see [2]). Such a method is sometimes known as a *DQ-method*. For linear k-step methods, one also needs to provide a special starting procedure to generate the additional $k-1$ initial approximations to the solution that are not given in the equation but are needed by the multistep method on its first application. It turns out that one needs to choose the quadrature, multi-step method and starting schemes carefully to ensure that the resulting method is of an appropriate order of accuracy for the work involved. One should try to choose schemes of the same orders as one another since the order of the overall method is equal to the lowest of the orders of the three separate methods (the multistep formula, the starting value scheme and the quadrature) used to construct it. In this paper we have chosen to focus on one-step methods. There are two reasons for this: we have thereby avoided the need to construct special starting procedures which would make our analysis more complicated; as Wolkenfelt showed in [11], methods with a *repetition factor* of 1 (such as the ones we consider) are always stable and we also draw attention (see [9] for example), to the fact that the trapezoidal rule is an A-stable 1-step method.

For a well-behaved numerical scheme for (3.2), (3.3), we would anticipate four intervals (as with the continuous problem) of λ-values where the solutions to the discrete scheme behave qualitatively differently. However we know from investigation of bifurcation points for numerical solution of delay differential equations (see [12]) and indeed from stability analysis of integro-differential equations, that the points at which the qualitative behaviour of the solution changes may arise at the *wrong* values of the parameter. Based on previous experience (see [6]) we would expect this difference to be dependent upon the stepsize h of the numerical method and on the choice of method itself. Furthermore (see, for example [8], [12]), one might expect the bifurcation points of the discrete

scheme to approach the bifurcation points of the continuous problem as $h \to 0$ and one could anticipate that, for a method of overall order p, the approximation of the true bifurcation point by the bifurcation point of the numerical scheme would also be to $\mathcal{O}(h^p)$. We will show in this paper that (for $h \to 0$) the approximation of the bifurcation points in the methods we have chosen is at least to the order of the method.

To keep the analysis reasonably simple, we consider the following discrete form of (3.2). We use a linear θ-method in each case so that we solve the system

$$y_{n+1} = y_n + h(\theta_1 F_n + (1 - \theta_1)F_{n+1}), \, n = 0, 1, \ldots, \tag{3.4}$$

$$F_n = f(nh, y_n, z_n), \tag{3.5}$$

$$z_n = h\left(\theta_2 k(nh, 0, y_0) + \sum_{j=1}^{n-1} k(nh, jh, y_j) + (1 - \theta_2)k(nh, nh, y_n)\right). \tag{3.6}$$

One could choose any combination of $\theta_i, 0 \leq \theta_i \leq 1$ and a natural choice could be $\theta_1 = \theta_2$. However, in order to start with a simple method where the algebraic problem is tractable we have considered first the cases where $\theta_1 = 0$ and we consider a range of values of θ_2.

One solves equations of the form

$$y_{n+1} - y_n = -h^2\left(\theta_2 e^{-\lambda(n+1)h}y_0 + \sum_{j=1}^{n} e^{-\lambda h(n+1-j)}y_j + (1 - \theta_2)y_{n+1}\right), \, y_0 = y_1 = 1. \tag{3.7}$$

Note that we have used a simple procedure to find the additional starting value $y_1 = 1$. We have observed from the integro-differential equation that $y'(0) = 0$ and have deduced that $y(h) = y(0)$ will provide a reasonable order 1 starting approximation. This choice of formula implies that we are combining a backward Euler scheme to discretise the differential equation, with, respectively, (for $\theta_2 = 1$) the forward rectangular (Euler) rule, (for $\theta_2 = \frac{1}{2}$) the trapezoidal rule and (for $\theta_2 = 0$) the backward rectangular rule for the quadrature. We will return to consider other combinations of θ_1, θ_2 later.

The equation (3.7) is equivalent to

$$\left(1 + h^2(1 - \theta_2)\right) y_{n+2} + \left(h^2\theta_2 e^{-\lambda h} - 1 - e^{-\lambda h}\right) y_{n+1} + e^{-\lambda h}y_n = 0. \tag{3.8}$$

The behaviour of the solution as $t \to \infty$ depends on the roots of the characteristic equation

$$\left(1 + h^2(1 - \theta_2)\right) k^2 + \left(h^2\theta_2 e^{-\lambda h} - 1 - e^{-\lambda h}\right) k + e^{-\lambda h} = 0. \tag{3.9}$$

Any solution of (3.8) will be asymptotically stable if both roots of (3.9) are of magnitude less than one and unstable if either root of (3.9) has magnitude greater than one. The solutions will contain (stable or unstable) oscillations when the roots of (3.9) are complex or, indeed, when at least one root is negative. It follows from this (see [4]) that the bifurcations occur as follows (for reasonably small $h > 0$).

B1. When $\lambda \geq -\frac{1}{h} \ln \left(\frac{1+2h^2-h^2\theta_2-2\sqrt{-h^2(h^2\theta_2-1-h^2)}}{h^4\theta_2^2-2h^2\theta_2+1} \right)$, $y_n \to 0$ as $n \to \infty$ with no oscillations. This condition can be written in the simpler form

$$\lambda \geq \frac{1}{h} \ln \left(1 + 2h^2 - h^2\theta_2 + 2\sqrt{-h^2\left(h^2\theta_2 - 1 - h^2\right)} \right)$$

and we thank the anonymous referee for pointing out this simplification.

B2. When $\frac{1}{h} \ln \left(\frac{1}{1+h^2(1-\theta_2)} \right) < \lambda < \frac{1}{h} \ln \left(1 + 2h^2 - h^2\theta_2 + 2\sqrt{-h^2\left(h^2\theta_2 - 1 - h^2\right)} \right)$, $y_n \to 0$ as $n \to \infty$, with infinitely many oscillations.

B3. When $\lambda = \frac{1}{h} \ln \left(\frac{1}{1+h^2(1-\theta_2)} \right)$ we obtain persistent oscillations.

B4. When $\frac{1}{h} \ln \left(1 + 2h^2 - h^2\theta_2 - 2\sqrt{-h^2\left(h^2\theta_2 - 1 - h^2\right)} \right) < \lambda < \frac{1}{h} \ln \left(\frac{1}{1+h^2(1-\theta_2)} \right)$, the solutions contain infinitely many oscillations of increasing amplitude.

B5. When $\lambda \leq \frac{1}{h} \ln \left(1 + 2h^2 - h^2\theta_2 - 2\sqrt{-h^2\left(h^2\theta_2 - 1 - h^2\right)} \right)$, the solution grows (in magnitude) without any oscillations.

4   Bifurcation points of the numerical scheme as approximations to true bifurcation points

We consider now the way in which the bifurcation points of the discrete scheme approximate those of the original problem. We are using a numerical scheme of order 1.

First we consider the value of $\lambda_1 = \frac{1}{h} \ln \left(1 + 2h^2 - h^2\theta_2 + 2\sqrt{-h^2\left(h^2\theta_2 - 1 - h^2\right)} \right)$ as θ_2 varies and $h \to 0$. It is easy to see that, as $h \to 0$, the value λ_1 satisfies $\lambda_1 \to 2$. In fact we can give greater precision to this. We can show that $\lambda_1 = 2 - \theta_2 h + \mathcal{O}(\ell^\epsilon)$ as $h \to 0$. This means that, for θ methods in general, the approximation by our scheme approximates the true value (-2) to order 1 (the order of the method), as $h \to 0$. In the particular case $\theta_2 = 0$ the approximation is to order 2.

For $\lambda_2 = \frac{1}{h} \ln \left(\frac{1}{1+h^2(1-\theta_2)} \right)$ it is straightforward to show that stability is lost at a value of λ that approximates the true value (0) to order 1 in general. In fact, for $\theta_2 = 1$, the forward Euler scheme, the approximation is exact for all values of h.

The analysis of $\lambda_3 = \frac{1}{h} \ln \left(1 + 2h^2 - h^2\theta_2 - 2\sqrt{-h^2\left(h^2\theta_2 - 1 - h^2\right)} \right)$ follows in exactly the same way as for λ_1 and leads to an identical conclusion: the approximation of the bifurcation point $\lambda = -2$ is in general to order 1 as $h \to 0$ and to order 2 if $\theta_2 = 0$.

We illustrate our results graphically. Each of the plots shown in Figure 1 illustrate, for varying h, the ranges for the parameter λ where

1. the solutions are unstable due to at least one real root greater than unity in magnitude (the darkest region in the figures) (exponential growth if the root is positive, growing oscillations if the root is negative),
2. the solutions are unstable due to growing oscillations (the next darkest region in the figures),
3. the solutions are stable with asymptotically stable oscillations (the lightest region in the figure), and

4. the solutions are stable with exponentially stable decay.

We can compare with the right hand plot in Figure 2 which shows the true regions for the original problem and we can make the following observations.

1. As $h \to 0$ the values of λ at which changes in the behaviour occur approach the true values. This coincides with our previous experience in delay equations (see [8]).
2. There is some extremely surprising behaviour for some values of $h > 0$.
   (a) For the two values $\theta_2 = 0.5$ and $\theta_2 = 1$ we can see that the darkest region is in two parts: in the upper part there is a negative real root of magnitude greater than unity leading to exponentially growing oscillations in the solution; in the lower part there is a positive real root of modulus greater than unity leading to exponential growth in the solutions.
   (b) There can be a critical value of $h > 0$ ($h = \frac{1}{\sqrt{\theta_2}}$ when $\theta_2 > 0$) at which, for apparently arbitrarily large $\lambda < 0$ the numerical solution displays oscillatory behaviour.
   (c) There can be an additional thin region (visible only in larger scale versions of the plots) between the darkest and lightest regions in which there is a real negative root of magnitude less than unity leading to decaying oscillations.
   (d) For $\theta_2 = 0.5$ and $\theta_2 = 1$ the upper part of the darkest region indicates some really strange behaviour: spurious oscillations may arise for arbitrarily large negative values of λ and even (see figure 1) for some positive values of λ. Thus we can have the situation (for example for λ small and positive) where the true solution tends to zero while the approximate solution exhibits oscillations of growing magnitude. Alternatively, (for λ large and negative) the true solution could exhibit high index exponential growth while the approximate solution exhibits oscillations. We draw attention also to the fact that, for $\theta_2 = 0.5$ and $\theta_2 = 1$ the stability boundary of the method is made up of parts of the boundaries of two regions, making the prediction of behaviour for varying $h > 0$ particularly difficult.

We believe that these observations justify our view that more attention needs to be paid to changes in qualitative behaviour other than stability in reaching a good understanding of the behaviour of numerical methods for problems of this type.

We can consider next whether these observations are equally true for other choices of numerical method. We present in Figures 2 plots revealing the qualitative behaviour of solutions to equations (3.2), (3.3) with other choices of θ-method. It is easy to see that, even for combinations such as using the trapezium rule for both parts of the discretisation (a method characterised by $\theta_1 = \theta_2 = 0.5$ and known to do very well at preserving the stability boundary) there are problems in the preservation of other types of qualitative behaviour when h is not very small. Similarly, we can see that the choice $\theta_1 = \theta_2 = 1$ leads to a shrinking range (as h increases) for λ that lead to stable oscillatory solutions.
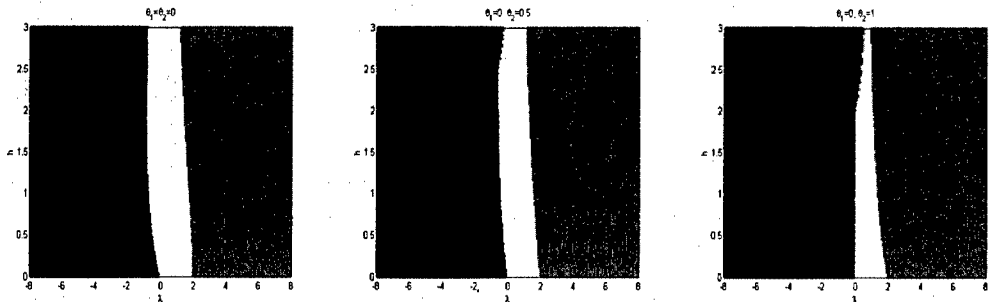
FIG. 1. Bifurcation points as h varies for $\theta_1 = 0, \theta_2 = 0, .5, 1$ respectively.
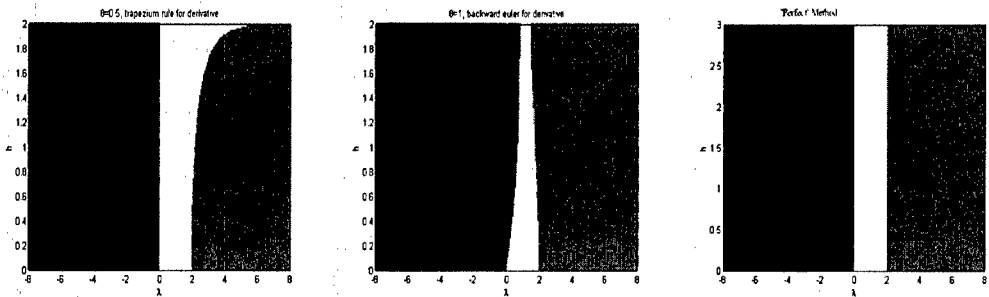

FIG. 2. Bifurcation points as h varies for, respectively, $\theta_1 = \theta_2 = 0.5, 1$ and for the analytical problem.

5   Alternative approaches

The particular equation we have considered can be formulated as an integro-differential equation, as an integral equation or as a second order differential equation. We have shown in [4] that the interesting and somewhat surprising observations about numerical behaviour that we made in the previous section also apply in these other formulations.

6   Closing remarks

The results presented in this paper show that the well-established stability theory based on the analysis of equation (1.2) gives only a very limited insight into the qualitative behaviour of solutions of the class of convolution equations with exponential memory kernel that we have considered here. We have observed elsewhere (see [5, 6, 7]) that the qualitative behaviour of numerical solutions to equations of this type may have surprising features and our consideration here of the prototype problem (1.1) illustrates how this unexpected behaviour may arise. We have seen in this paper how oscillations may arise in the numerical schemes when they should not, and how in other cases the numerical schemes may supress genuine oscillatory behaviour. When one seeks good methods based on a stability analysis, the desire is to focus on those methods where the step-length $h > 0$ is not subject to some upper bound to ensure the stability of the method. However our initial observations in this paper have shown that this may well prove an unreasonable

expectation when one is investigating these other changes in qualitative behaviour.

We believe that this paper introduces a range of worthwhile investigations in a field that is still quite open. Space restrictions have prevented us from considering the behaviour of more general methods in this paper and also from extending our analysis to consider other problems. The results we have presented here show that, for these simple methods at least, the bifurcation parameters are approximated in the numerical scheme to at least the order of the method, for sufficiently small $h > 0$. It is also very clear that, even for what appears to be a simple problem, the choice of numerical scheme and the form in which the problem is presented provide us with a rich source of example behaviour.

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