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Pitfalls in fast numerical solvers for fractional differential equations

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Abstract

We consider the problem of implementing fast algorithms for the numerical solution of initial value problems of the form $x^{(\alpha)}(t) = f(t, x(t))$, $x(0) = x_0$, where $x^{(\alpha)}$ is the derivative of x of order α in the sense of Caputo and $0 < \alpha < 1$. We review some of the existing methods and explain their respective strengths and weaknesses. We identify and discuss potential problems in the development of generally applicable schemes.

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1. Introduction

This paper considers the properties of high order methods for the solution of fractional differential equations. There is a growing demand for such methods from modellers whose work leads to linear and nonlinear equations involving derivatives of fractional order and yet there seems to be no well-understood method of reasonably high order that can be used to generate a reliable approximate solution.

Our investigations are motivated by a few classical and many very recent applications of fractional differential equations. Among the classical problems we mention areas like the modelling of the behaviour of viscoelastic materials in mechanics (studied since the 1980s [35]) and applications of Abel–Volterra equations in superfluidity [24]. More recently fractional calculus has been applied to continuum and statistical mechanics for viscoelasticity problems, Brownian motion and fractional diffusion-wave equations [27] and the description of the propagation of a flame [21,23]. Newer studies are also done, among others, in the area of modelling of soft tissues like mitral valves or the aorta in the human heart [15]. It is evident that these applications require not only fast but in particular *reliable* numerical methods.

In our earlier work we have presented (see [5,10,9,12,14]) several methods for the approximate solution of differential equations of fractional order. In the main these have been of low order, but they have nevertheless attracted interest because of the relative ease of application and the reliable results that we have been able to give relating to convergence and stability of the methods. We have also shown (see, e.g., [9,13,14]) that the underlying order of our methods may be improved (through extrapolation schemes) leading to methods of higher order.

In the 1980s there was a surge of interest in developing higher order numerical methods for Abel–Volterra integral equations (of which fractional differential equations form a sub-class) and detailed theoretical results were given for these methods at that time. However these so-called fractional multistep methods have proved to be of more theoretical than practical use over the intervening two decades (although they have been included in the NAG Fortran Library as a method to solve certain Abel–Volterra equations). One purpose of this paper is to assess why this has been the case, and to give a clear direction to further research that will lead to more practical methods for today's applications.

This paper is structured as follows: first we describe in greater detail the class of problems that we seek to solve and we set out clear objectives for a well-behaved numerical scheme, then we review the available algorithms for the solution of these equations against the objectives we have set. We consider the work published in the 1980s on fractional multistep methods and review its strengths from a theoretical viewpoint and show how the methods can be applied very effectively to the types of problems prevalent at that time. We consider more recent model equations and highlight some of the pitfalls in trying to implement fractional multistep methods in this case.

We conclude with some advice to users on the choice of numerical schemes for the solution of particular types of equation. We also give a statement of the issues that we regard as the most important for algorithm developers who wish to produce useful higher order methods for practical application.

2. Objectives

We consider the solution of fractional differential equations of the form

$$x^{(\alpha)}(t) = f(t, x(t)), \quad x^{(k)}(x_0) = x_0^{(k)} \quad (k = 0, 1, \ldots, \lceil \alpha \rceil - 1), \tag{1}$$