A Runge-Kutta method for computing guaranteed solutions of ODEs

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Abstract

In this article we present a new approach for the computation of guaranteed solutions of ODEs, based on a classical Runge-Kutta method with a precise error approximation.

The interest in validated methods for solving ODEs has recently increased in many areas, such as state estimation [9] or validation of hybrid systems [6]. In these applications, it is crucial to have guaranteed bounds on the behaviour of the physical environment, which is usually described by non-linear ODEs. Existing validation tools [7] mostly use interval based algorithms to compute these bounds, like COSY Infinity [2] or VNODE [10].

Our method has been developed in order to be used within a validation tool for hybrid systems, and thus focuses more on long-term stability and accuracy than execution time, without however neglecting it. Each computation step consists of two stages: a prediction stage where approximate values for the solution are computed, and a correcting stage where an overapproximation of the global error is calculated. The first stage uses classical RK4 formulae [5] and multiprecision arithmetic in order to get an accurate result. The second stage represents our main contribution. The global error after n steps is expressed as a function of the error after n-1steps and the step size h. An overapproximation of this error is then computed and from this value we modify h in order to keep the global error under user-defined bounds. This separation between the computation of the next step, which uses multiprecision arithmetic, and the computation of the global error using interval arithmetic makes it possible to avoid the well known wrapping effect and then guarantees long term stability of the method.

Basically, the error bound is overapproximated as follows:

$$|y(x+h) - \tilde{y}(x+h)| \le \eta + \chi + \mu \le \epsilon \tag{1}$$

In Equation (1), y is the exact solution of the equation and \tilde{y} the numerical approximation computed without interval arithmetic. The global

error $(|y(x + h) - \tilde{y}(x + h)|)$ can be split into three parts, based on results from [3],[8]: the error η introduced at each step, the propagation of the precedent error χ and the numerical error μ . η and χ are expressed according to the fourth and fifth derivative of the function we want to approximate, and interval arithmetic is then used to compute an overapproximation of these errors as well as μ . However, interval arithmetic is only used for verification and not in the computation of the next value. ϵ is a user-defined parameter.

We have implemented our algorithm in a C++ library called GRKLib for Guaranteed Runge-Kutta library. This library uses the formal derivation tool GiNaC [1] in order to compute the error functions and the MPFR [4] library for multiprecision computations. The interval arithmetic library used is Profil/BIAS. We have compared our results on classical problems with results from VNODE. This comparison showed a better stability and higher precision for our method, while being as fast as it.

References:

- [1] GiNaC Is Not A CAS, http://www.ginac.de.
- [2] M. Berz, J. Hoefkens, and K. Makino, Cosy infinity version 8.1 programming manual., Tech. Report MSUHEP-20703, Michigan State University, 2002.
- [3] L. Bieberbach, On the remainder of the runge-kutta formula., Z.A.M.P., 2:233-248, 1951.
- [4] D. Daney, G. Hanrot, V. Lefvre, P. Plissier, F. Rouillier, and P. Zimmermann, *The MPFR library*, 2005.
- [5] E. Hairer, S. P. Norsett, and G. Wanner, Solving ordinary differential equations II: stiff problems. Springer-Verlag New York, Inc., 1993.
- [6] T. A. Henzinger, P. H. Ho, and H. Wong-Toi, Algorithmic analysis of nonlinear hybrid systems. IEEE Trans. on Automatic Control, 43:540–554, 1998.
- [7] T. A. Henzinger, B. Horowitz, R. Majumdar, and H. Wong-Toi, Beyond HYTECH: Hybrid systems analysis using interval numerical methods. In HSCC, pages 130–144, 2000.
- [8] J. W. Carr, Error bounds for the runge-kutta single-step integration process. Journal of the ACM, 5(1):39–44, 1958.
- [9] M. Kieffer and E. Walter, Guaranteed nonlinear state estimator for cooperative systems. Numerical Algorithms, 37(1-4):187–198, December 2004.
- [10] N. S. Nedialkov and K. R. Jackson, The design and implementation of an object-oriented validated ODE solver, 2001.

Keywords: guaranteed numerical integration, interval arithmetic, Runge-Kutta methods