Positivity-preserving for Runge-Kutta methods

I. Higueras, T. Roldán

Dpto. de I. Matemática e Informática, Univ. Pública de Navarra

higueras@unavarra.es, teo@unavarra.es

Resumen

In this paper we consider IVPs for systems of ODEs that can be written in the form

$$\begin{aligned} \frac{d}{dt} y(t) &= f(y(t))\,, \\ y(t_0) &= y_0\,. \end{aligned} \tag{1}$$

We assume that $f : \mathbb{R}^m \to \mathbb{R}^m$ is a sufficiently smooth function so that for each $t_0 \in \mathbb{R}$ and $y_0 \in \mathbb{R}^m$ the problem (1) has a unique solution $y : [t_0, \infty) \to \mathbb{R}^m$. In the literature much attention has been paid in problems like (1) having monotonicity or positivity properties [1], [4], [7], [8]. For example, if the solution represents concentrations of chemical species, then $y_0 \geq 0$ implies $y(t) \geq 0$ for all $t > 0$.

If we solve (1) numerically, it would be desirable that the numerical method preserves these monotonicity properties. Runge-Kutta methods having these properties have been studied in the last years [2], [3], [4], [6], [8], [9]. Monotonicity and also positivity results have been obtained for the numerical solution under certain step size restriction.

In some cases, the stiffness of the problem makes necessary to solve it with an implicit method. If we solve the IVP with an implicit Runge-Kutta (IRK) method, then the highest computational effort is due the resolution of a nonlinear system in each step. Although there are a number of schemes to solve this nonlinear system, variants of Newton's method are used in all modern ODE codes. The monotonicity results obtained for IRK methods mean that the nonlinear systems are solved exactly, but, in practice, these systems are solved approximately by means of some iterative scheme. Consequently, it is important that the technique used to solve the nonlinear systems maintains the monotonicity properties. In particular, if we deal with positivity and we are using a method to get starting values for the iterations, then it is important that these values are positive

In this work we consider a kind of starting algorithms studied in [5], and analyze the attainable order so that the starting values are positives. We will see how for many positive methods, the optimum predictor cannot be positive.

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Referencias

[1] Bruggeman, J., Burchar, H., Kooi, B., Sommeijer, B. A second-order, unconditionally positive, massconserving integration scheme for biochemical systems. *Applied Numerical Mathematics 57* (2007), 36–58.

[2] Gerisch, A., and Weiner, R. On the positivity of low order explicit Runge-Kutta schemes applied in splitting methods. *Comput. Math. Appl. 45* (2003), 53–67.

[3] S. Gottlieb, C. Shu, E. Tadmor, Strong stability-preserving high order time discretization methods, *SIAM Rev. 43* (2001) 89–112.

[4] I. Higueras, On strong stability preserving time discretization methods, J. Sci. Comput. 21 (2004) 193–223.

[5] I. Higueras and T. Roldán, Starting algorithms for some DIRK methods, *Numerical Algorithms, 23* (2000) 357-369.

[6] Horváth, Z. Positivity of RK and diagonally split RK methods. *Appl. Numer. Math. 28* (1998), 309–326.

[7] W. Hundsdorfer, J. Verwer, Numerical solution of time-dependent Advection-Diffusion-Reaction equations, *Springer Series in Computational Mathematics, 2003.*

[8] Kraaijevanger, J. Contractivity of Runge-Kutta methods. *BIT 31* (1991), 482–528.

[9] M. Spijker, Stepsize restrictions for stability of one-step methods in the numerical solution of initial value problems, *Math. Comp. 45* (1985) 377–392.