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Runge-Kutta Theory and Constraint Programming

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Introduction

There exist many Runge-Kutta methods (explicit or implicit), more or less adapted to a given class of problems. Some of them have interesting properties such as A-stability for stiff problems or symplecticity for problems with energy conservation. Defining a new method, adapted to a given class of problems, has become a challenge. Indeed, the number of stages and the order don't stop to increase. This race to the "best" method is interesting but forgot an important problem. More precisely, the coefficients of a Runge-Kutta method are more and more difficult to compute and the result is often given in floating-point numbers, which may lead to violate their definition rules. We propose a method using interval analysis tools to compute Runge-Kutta coefficients by using a solver based on guaranteed constraint programming. Moreover, with a global optimization process and a well chosen cost function, we propose a way to define some novel optimal Runge-Kutta methods.

One step of a Runge-Kutta integration scheme, applied on an ordinary differential equation $\dot{y} = f(t, y)$, is obtained with

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i k_i, \text{ where } k_i = f\left(t_0 + c_i h, y_0 + h \sum_{j=1}^{s} a_{ij} k_j\right) . \tag{1}$$

The coefficients c_i, a_{ij} and b_i, for $i, j = 1, \cdots, s$, fully characterize the Runge-Kutta methods and they are usually synthesized in a *Butcher*

tableau [1] of the form:

$$\begin{array}{c|ccc} c_1 & a_{11} & \dots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \dots & a_{ss} \\ \hline & b_1 & \dots & b_s \end{array}$$

Main idea

Our approach consists on the generation of constraints defined by the Butcher theory in order to build a Runge-Kutta method. Then we solve these constraints with a Branch&Prune algorithm. We also propose a Branch&Bound approach to define new optimal methods w.r.t. an easy to obtain cost function.

Interval coefficients preserve properties

In a preliminary stage, we can verify that a Runge-Kutta method with interval coefficients preserves the Butcher rule and then that a method given for an order p has really a local truncature error in $O(h^{p+1})$. We also propose three methods using interval tools to check the linear stability, algebraically stability and symplecticity properties.

Main results

First, our Branch&Prune based approach is used to find existing methods and by the way re-discover the Runge-Kutta theory such as i) Gauss-Legendre is the only 2-stages 4-order method; ii) there is no 2-stages 5-order method; etc. Our Branch&Bound method finds the same results as Ralston [2]. Second, both of our methods is used to define new validated Runge-Kutta methods.

References:

[1] Butcher, John C., Coefficients for the study of Runge-Kutta integration processes, *Journal of the Australian Mathematical Society*, 5 (1963), No. 3, pp. 185–201.

[2] Ralston, Anthony, Runge-Kutta methods with minimum error bounds, *Mathematics of computation*, (1962), pp. 431-437.