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Runge–Kutta pairs of order 5(4) satisfying only the first column simplifying assumption

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ABSTRACT

Among the most popular methods for the solution of the Initial Value Problem are the Runge–Kutta pairs of orders 5 and 4. These methods can be derived solving a system of nonlinear equations for its coefficients. To achieve this, we usually admit various simplifying assumptions. The most common of them are the so-called row simplifying assumptions. Here we neglect them and present an algorithm for the construction of Runge–Kutta pairs of orders 5 and 4 based only in the first column simplifying assumption. The result is a pair that outperforms other known pairs in the bibliography when tested to the standard set of problems of DETEST. A cost free fourth order formula is also derived for handling dense output.

1. Introduction

We consider the numerical solution of the non-stiff initial value problem,

$$y' = f(x, y), \qquad y(x_0) = y_0 \in \mathbb{R}^m, \quad x \in [x_0, x_f] \tag{1}$$

where the function $f : \mathbb{R}\times\mathbb{R}^m \to \mathbb{R}^m$ is assumed to be as smooth as necessary. Traditionally, explicit embedded Runge–Kutta methods produce an approximation to the solution of (1) only at the end of each step.

The general s-stage embedded Runge–Kutta pair of orders $p(p-1)$, for the approximate solution of the problem (1) can be defined by the following Butcher scheme [1,2]

$$\begin{array}{c|c} c & A \\ \hline & b \\ & \hat{b} \end{array}$$

where $A \in \mathbb{R}^{s\times s}$, is strictly lower triangular, $b^T, \hat{b}^T, c \in \mathbb{R}^s$ with

$$c = A \cdot e, \quad e = [1, 1, \dots, 1]^T \in \mathbb{R}^s.$$

The vectors $\hat{b}$, b define the coefficients of the $(p-1)$-th and p-th order approximations respectively.

Starting with a given value $y(x_0) = y_0$, this method produces approximations at the mesh points $x_0 < x_1 < x_2 < \cdots < x_f$. Throughout this paper, we assume that local extrapolation is applied, hence the integration is advanced using the p-th order approximation. To estimate the error, two approximations are evaluated at each step x_n to $x_{n+1} = x_n + h_n$. These are:

$$\hat{y}_{n+1} = y_n + h_n \sum_{j=1}^{s} \hat{b}_j f_j \quad \text{and} \quad y_{n+1} = y_n + h_n \sum_{j=1}^{s} b_j f_j,$$

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where

$$f_i = f\left(x_n + c_i h_n, y_n + h_n \sum_{j=1}^{i-1} a_{ij} f_j\right), \quad i = 1, 2, \ldots, s.$$

The local error estimate $E_n = \|y_n - \hat{y}_n\|$ of the $(p-1)$-th order Runge–Kutta pair is used for the automatic selection of the step size. Given a Tolerance TOL $> E_n$, the algorithm

$$h_{n+1} = 0.9 \cdot h_n \cdot \left(\frac{\text{TOL}}{E_n}\right)^{\frac{1}{p}}$$

furnishes the next step length. In case TOL $< E_n$ then we reject the current step and try again with the left side of the above formula being h_n.

In case that $c_s = 1, a_{s,j} = b_j$ for $j = 1, 2, \ldots, s-1$ and $b_s = 0 \neq \hat{b}_s$ then the First Stage of each step is the same As the Last one of the previous stage. This device was possibly first used in [3, pg. 22] and it is called FSAL. The pair shares effectively only $s-1$ stages per step then.

Let $y_n(x)$ be the solution of the local initial value problem

$$y'(x) = f(x, y_n(x)), \quad x \geq x_n,\ y_n(x_n) = y_n.$$

Then E_{n+1} is an estimate of the error in the local solution $y_n(x)$ at $x = x_{n+1}$. The local truncation error t_{n+1} associated with the higher order method is

$$t_{n+1} = y_{n+1} - y_n(x_n + h_n) = \sum_{q=1}^{\infty} h_n^q \sum_{i=1}^{\lambda_q} T_{qi} P_{qi} = h_n^{p+1} \Phi(x_n, y_n) + O(h_n^{p+1})$$

where

$$T_{qi} = Q_{qi} - \xi_{qi}/q!$$

with Q_{qi} algebraic functions of A, b, c and ξ_{qi} positive integers. P_{qi} are differentials of f evaluated at (x_n, y_n) and $T_{qi} = 0$ for $q = 1, 2, \ldots, p$ and $i = 1, 2, \ldots, \lambda_q$. λ_q is the number of elementary differentials for each order and coincides with the number of rooted trees of order q. It is known that

$$\lambda_1 = 1, \lambda_2 = 1, \lambda_3 = 2, \lambda_4 = 4, \lambda_5 = 9, \lambda_6 = 20, \lambda_7 = 48, \ldots, \text{etc. [4]}.$$

The set $T^{(q)} = \{T_{q1}, T_{q2}, \ldots, T_{q,\lambda_q}\}$ is formed by the q-th order truncation error coefficients. It is the usual practice for a $(q-1)$-th order method to have minimized

$$\|T^{(q)}\|_2 = \sqrt{\sum_{j=1}^{\lambda_q} T_{qj}^2}.$$

2. Derivation of RK pairs of orders 5(4)

The construction of an effectively 6-stage FSAL Runge–Kutta pair of orders 5(4) requires the solution of a nonlinear system of 25 order conditions. $\lambda_1 + \cdots + \lambda_5 = 17$ equations for the higher order formula and $\lambda_1 + \cdots + \lambda_4 = 8$ equations for the lower order formula. There are 28 unknowns. Namely $c_2 - c_6$, $b_1 - b_6$, $\hat{b}_1 - \hat{b}_7$, $a_{32}, a_{42}, a_{43}, a_{52}, a_{53}, a_{54}$ and $a_{62} - a_{65}$.

We proceed setting $c_6 = 1$ and an arbitrary value for $\hat{b}_7$. Then the only assumption we make is

$$b \cdot (A + C - I_s) = 0 \in \mathbb{R}^{1\times s} \tag{2}$$

with C =diag(c) and $I_s \in \mathbb{R}^{s\times s}$ the identity matrix. This is the minimal set of simplifying assumptions for pairs of orders 5(4). It is worth mentioning that in the family of methods introduced here

$$A \cdot c \neq \frac{c^2}{2}, \quad \text{and} \quad b_2 \neq 0,$$

contrary to the common practice of every 5(4) pair appearing until now [5,3,6]. Expression c^2 is to be understood as component-wise multiplication $c * c$.

The implicit algorithm that derives a pair of the new family follows. A different approach was given in [7].

The algorithm producing the coefficients of the new pair

Set $c_6 = 1$ and get an arbitrary $\hat{b}_7 \neq 0$. Select free parameters c_2, c_3, c_4 and $b_2 \neq 0$. Then

1. Solve $b \cdot e = 1, b \cdot c = \frac{1}{2}, b \cdot c^2 = \frac{1}{3}, b \cdot c^3 = \frac{1}{4}, b \cdot c^4 = \frac{1}{5}$ for b_1, b_3, b_4, b_5 and b_6.
2. Solve $\hat{b} \cdot e = 1, \hat{b} \cdot c = \frac{1}{2}, \hat{b} \cdot c^2 = \frac{1}{3}, \hat{b} \cdot c^3 = \frac{1}{4}$ for $\hat{b}_1, \hat{b}_3, \hat{b}_4$, and $\hat{b}_5$.