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Symbolic derivation of Runge–Kutta–Nyström type order conditions and methods for solving $y''' = f(x, y)$

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ABSTRACT

In this work we study the Runge–Kutta–Nyström (RKN) type methods for the solution of a special third order initial value problems. Based on rooted trees the relative order conditions theory is presented introducing a new set of SN-trees named $\mathbb{T}_3$ whose elements' enumeration is given. A Mathematica package, that furnishes instantly order conditions of high orders, is also listed. Finally, a new method of order 8 is constructed that outperforms by far the methods found in the literature.

1. Introduction

We consider the special third order Initial Value Problems (IVPs)

$$\begin{aligned} &y'''(x) = f(x, y(x)), \; x \ge x_0, \\ &y(x_0) = y_0, \; y'(x_0) = y'_0, \; y''(x_0) = y''_0, \end{aligned} \tag{1}$$

where

$$f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n,$$

and

$$y_0, \; y'_0, \; y''_0 \in \mathbb{R}^n.$$

The most popular methods used for the approximate solution for this type of problems. Nevertheless, the special form of (1) enables a different approach. Thus, in the lines of Runge–Kutta–Nyström methods [1,2] for the problem

$$y'' = f(x, y(x)), \; x \ge x_0, \; y(x_0) = y_0, \; y'(x_0) = y'_0,$$

we consider for solving (1) the following explicit $s-$ stage method of algebraic order p

$$y_{n+1} = y_n + h_n y'_n + \frac{h_n^2}{2} y''_n + h_n^3 \sum_{j=1}^{s} b_j f_j,$$

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$$y'_{n+1} = y'_n + h_n y''_n + h_n^2 \sum_{j=1}^{s} b'_j f_j,$$

$$y''_{n+1} = y''_n + h_n \sum_{j=1}^{s} b''_j f_j$$

where

$$f_i = f\left(x_n + c_i h_n, y_n + h_n c_i y'_n + \frac{h_n^2}{2} c_i^2 y''_n + h_n^3 \sum_{j=1}^{i-1} a_{ij} f_j \right),$$

for $i = 1, 2, \ldots, s$ and $h_n = x_{n+1} - x_n$.

Using the same stages with the method above we may get another approximation for $y(x_{n+1})$ of order $p-k,\ k>0$

$$\hat{y}(x_{n+1}) = y(x_n) + h_n y'(x_n) + \frac{1}{2} h_n^2 y''(x_n) + h_n^3 \sum_{j=1}^{s} \hat{b}_j f_j.$$

Then an estimation of the local error $\epsilon = h^{k-1} \| y_{n+1} - \hat{y}_{n+1} \|$ can be used along with a given tolerance δ in order to get the next step [3],

$$h_{n+1} = 0.9 h_n \cdot \left(\frac{\delta}{\epsilon} \right)^{1/p}. \tag{2}$$

In case that $\epsilon > \delta$ the step h_n advancing the approximation of solution from x_n to x_{n+1} is rejected and a smaller step h_n is evaluated by the formula (2).

The Runge–Kutta–Nyström type pairs of methods for the solution of the above special third order initial value problem was studied by Senu et al. [1]. In this particular work the authors have derived pairs of methods of orders 5(4) and 6(5). Moreover, a more theoretical study which a corresponding tree theory and the derivation of constant stepsize schemes of orders up to 5 are presented by You and Chen in [2]. In this study, we do not only present a high orders 8(6) pair that outperforms the methods presented in the literature, but we present the relative order conditions theory, based on the elements of a set of SN-trees named $\mathbb{T}_3$. The enumeration of the specific set of trees is given and programmed in a symbolic programming language of Mathematica. Moreover a Mathematica package, that furnishes instantly order conditions of very high orders, is also listed.

2. Order conditions

The coefficients are tabulated in various matrices. Thus we set

$$A \in \mathbb{R}^{s\times s} \text{ and } b^T, b'^T, b''^T, c \in \mathbb{R}^s.$$

For attaining a specific algebraic order (e.g. eighth) we need to satisfy various order conditions involving these matrices. Setting $I_s \in \mathbb{R}^{s\times s}$ the identity matrix, $C = \mathrm{diag}(c) \in \mathbb{R}^{s\times s}$ and using the simplifying assumptions

$$b = \frac{1}{2} b'' \cdot (I_s - C)^2, \text{ and } b' = b'' \cdot (I_s - C), \tag{3}$$

we conclude to the equations appearing in Table 1 where it is meant that a method is of p th order iff $T_i''^{(j)} = 0$ for $j \le p$. In that table

$$e = [1, 1, \ldots, 1] \in \mathbb{R}^s$$

and multiplication "$*$" may understood component wisely with less priority than dot product. For example if

$$u, v \in \mathbb{R}^s \text{ then } u * v = [u_1 v_1, u_2 v_2, \ldots, u_s v_s]^T \in \mathbb{R}^s.$$

Thus

$$c^2 = c * c = [c_1^2, c_2^2, \ldots, c_s^2]^T \in \mathbb{R}^s,\ c^3 = c^2 * c, \text{ etc.}$$

Considering (3) the corresponding equations of condition involving b and b' are dropped.

For example the third order equation of condition $T_1^{(3)} = be - \frac{1}{6}$, is satisfied automatically since

$$b \cdot e = \frac{1}{2} b'' \cdot (I_s - C)^2 e = \frac{1}{2}\left(b'' \cdot e - 2b'' \cdot c + b'' \cdot c^2 \right) = \frac{1}{2}\left(1 - 2 \cdot \frac{1}{2} + \frac{1}{3} \right) = \frac{1}{6}.$$

Similarly the fifth order equation $T_1'^{(5)} = b'Ae - \frac{1}{120}$ is also satisfied since

$$\begin{aligned} b' \cdot A \cdot e &= b'' \cdot (I_s - C) \cdot A \cdot e = (b'' \cdot A \cdot e - b'' \cdot (c * A \cdot e)) \\ &= \left(\frac{1}{24} - \frac{1}{30} \right) = \frac{1}{120}. \end{aligned}$$

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