Computers and Mathematics with Applications 62 (2011) 2101–2111

Contents lists available at ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

On modified Runge–Kutta trees and methods

Ch. Tsitouras [a], I.Th. Famelis [b,*], T.E. Simos [c,d]

[a] TEI of Chalkis, GR-34400 Psahna, Greece

[b] Department of Mathematics, TEI of Athens, GR-12210 Egaleo, Greece

[c] Department of Mathematics, College of Sciences, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia

[d] Laboratory of Computational Sciences, Department of Computer Science and Technology, University of Peloponnese, GR-221 00 Tripolis, Greece

A R T I C L E I N F O

Article history:
Received 4 May 2011
Accepted 28 June 2011

Keywords:
Rooted trees
Integer partitions
Truncation error
Runge–Kutta methods
Initial value problems
Mathematica

A B S T R A C T

Modified Runge–Kutta (mRK) methods can have interesting properties as their coefficients may depend on the step length. By a simple perturbation of very few coefficients we may produce various function-fitted methods and avoid the overload of evaluating all the coefficients in every step. It is known that, for Runge–Kutta methods, each order condition corresponds to a rooted tree. When we expand this theory to the case of mRK methods, some of the rooted trees produce additional trees, called mRK rooted trees, and so additional conditions of order. In this work we present the relative theory including a theorem for the generating function of these additional mRK trees and explain the procedure to determine the extra algebraic equations of condition generated for a major subcategory of these methods. Moreover, efficient symbolic codes are provided for the enumeration of the trees and the generation of the additional order conditions. Finally, phase-lag and phase-fitted properties are analyzed for this case and specific phase-fitted pairs of orders 8(6) and 6(5) are presented and tested.

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. The general s-stage embedded Runge–Kutta pair of orders $p(p-1)$, for the approximate solution of the problem (1) can be represented using the following Butcher tableau [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, $b^T, \hat{b}^T$, and $c \in \mathbb{R}^s$ with $c = A \cdot e$, $e = [1, 1, \ldots, 1]^T \in \mathbb{R}^s$. The vectors b and $\hat{b}$ define the coefficients of the $(p-1)$th and pth 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 pth order

* Corresponding author. Tel.: +301 210 538 5392.
E-mail addresses: tsitoura@teihal.gr (Ch. Tsitouras), ifamelis@teiath.gr (I.Th. Famelis), tsimos@mail.ariadne-t.gr (T.E. Simos).

0898-1221/$ – see front matter © 2011 Elsevier Ltd. All rights reserved.
doi:10.1016/j.camwa.2011.06.058

approximation. For estimating the error, two approximations are evaluated at each step from x_n to $x_{n+1} = x_n + h_n$. These are

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

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 parameter *TOL*, if $TOL > E_n$, the algorithm

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

provides the next step length. Whereas if $TOL < E_n$ we reject the current step and evaluate another smaller one using the same formula but with h_{n+1} now being h_n.

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

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

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

$$t_{n+1} = y_{n+1} - y_n(x_n + h_n) = \sum_{q=1}^{\infty} h_n^q \sum_{i=1}^{\lambda_q} \sigma_{qi} T_{qi} P_{qi} = h_n^{p+1} \Phi(x_n, y_n) + O(h_n^{p+2})$$

where

$$T_{qi} = \left(Q_{qi} - \frac{\xi_{qi}}{q!}\right)$$

and σ_{qi} are real numbers depending on the order of the group of automorphisms on a particular labeling of tree t that corresponds to the elementary differential [3]. This order is known as the 'symmetry group' of the tree The ξ_{qi} are positive integers, Q_{qi} are algebraic functions of A, b, c and P_{qi} are differentials of f evaluated at (x_n, y_n). For a pth order method the order conditions

$$T_{qi} = 0, \quad \text{for } q = 1, 2, \ldots, p \text{ and } i = 1, 2, \ldots, \lambda_q,$$

must hold.

The number of elementary differentials for each order is λ_q and coincides with the number of rooted trees of order q. It is known [4] that

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

More details can be found in [5].

The set $T^{(q)} = \{T_{q1}, T_{q2}, \ldots, T_{q,\lambda_q}\}$ is formed by the qth order truncation error coefficients. It is common practice that a $(q-1)$th order method has

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

minimized.

In this work we are interested on a modification of Runge–Kutta methods called modified Runge–Kutta (mRK). mRK methods can have interesting properties as their coefficients may depend on the step length. By a simple perturbation of very few coefficients we may produce various function-fitted methods and avoid the overload of evaluating all the coefficients in every step. For this class of methods the works of Franco [6] and Vyver [7] can be found in the literature.

When we expand the Runge–Kutta tree theory to the case of mRK methods, some of the rooted trees produce additional trees, called mRK rooted trees, and so additional conditions of order. Here we present the relative theory including a theorem for the generating function of these additional mRK trees and explain the procedure to determine the extra algebraic equations of condition generated for a major subcategory of these methods. Moreover, efficient symbolic codes are provided for the enumeration of the trees and the generation of the additional order conditions. Finally, phase-lag and phase-fitted properties are analyzed for this case and specific phase-fitted pairs are presented and tested.