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ON SEMI-EXPLICIT RUNGE-KUTTA METHODS AND THEIR STABILITY PROPERTIES

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Abstract. Semi-explicit Runge-Kutta methods of order 3 are discussed and A-stability and L-stability of these methods are studied.

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1. Introduction.

Consider the initial value problem

$$y'(x) = f(x, y(x)), \; y(x_0) = y_0, \tag{1.1}$$

where $f : [a, b] \times \mathbb{R}^m \to \mathbb{R}^m$, $x_0 = a$, $y_0, y \in \mathbb{R}^m$.We discuss implicit Runge-Kutta method for numerical integration of (1.1), having a special form, and called **semi-explicit** or **diagonally implicit.**

This kind of methods have also been investigated by many authors: **J.C. Butcher** [2], [3], **K. Burrage** [1], **J. R. Cash** [4], **E. Hairer, G. Wanner and C. Lubich** [6], [7], **Houwen van der, P. S. Sommeijer** [8], etc.

The aim of this article is the construction of a few classes of semi-explicit Runge - Kutta methods of order 3 with two, three and four stages for the initial value problem (1.1) These methods will be A - stable and L - stable, thus they will be suitable for solving numerically stiff problems. This article is a continuation of the author's work [5].

Without loss of generality, we may assume that (1.1) is a scalar problem.

2. Preliminaries

Let x_n, $n = 0, 1, 2, ..., N$ be equal spaced points in $[a, b]$, with $x_0 = a$, $x_n - x_{n-1} = h$, $n = 0, 1, 2, ..., N$, and let y_n be the approximate value of $y(x_n)$, where $y(x)$ is the exact solution of the local initial value problem

$$y'(x) = f(x, y(x)); \;\; y(x_n) = y_n. \tag{2.1}$$

Definition 2.1. An implicit Runge - Kutta method with s stages for the problem (1.1) is defined by the equations

$$k_{i,n} = hf\left(x_n^i, y_n + \sum_{j=1}^{s} a_{ij} k_{j,n}\right), \quad i = 1, 2, \dots, s \tag{2.2}$$

$$y_{n+1} = y_n + \sum_{i=1}^{s} b_i k_{i,n}; \quad n = 0, 1, 2, \dots \tag{2.3}$$

where $x_n^i = x_n + c_i h$, $i = \overline{1, s}$ and b_i, a_{ij}, c_i are real parameters.

The formulas (2.2) and (2.3) are usually displayed in so called Butcher's tableau

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array}, \tag{2.4}$$

where $c = (c_1, c_2, \dots, c_s)^T$; $b^T = (b_1, b_2, \dots, b_s)$; $A = (a_{ij})$; $i, j = 1, 2, \dots, s$ and we have to have

$$c = Ae, \tag{2.5}$$

whe[illegible] $(1, 1, \dots, 1)^T \in \mathbb{R}^s$.

Definition 2.2. The Runge-Kutta method defined by (2.2) +(2.3) or by (2.4) is called **semi-implicit** if $a_{ij} = 0$ for all $j > i$. A semi-implicit method is called **semi-explicit** method or **diagonally implicit** if we have $a_{ii} = \lambda$ for all $i = 1, 2, \dots s$.

The order conditions for semi-explicit Runge-Kutta methods with s stages can be obtained from general order conditions of implicit methods, which can be found in [2], [7]. For semi-explicit methods of order up to 3, these conditions are:

$$\sum_{i=1}^{s} b_i = 1, \qquad \sum_{i=1}^{s} b_i c_i = 1/2, \tag{2.6}$$

$$\sum_{i=1}^{s} b_i c_i^2 = 1/3, \quad \lambda \sum_{i=1}^{s} b_i c_i + \sum_{i=2}^{s} b_i \sum_{j=1}^{i-1} a_{ij} c_j = 1/6. \tag{2.7}$$

More precisely, when the order is $p = 2$ the necessary conditions are the equations (2.5), (2.6). When the order is $p = 3$ the necessary conditions are the equations (2.6), (2.7) and the equation (2.5).

Remark 2.3. S.P.N Nørset and A. Wolfbrandt A., [9], proved that the maximum order obtained with an s- stages semi- explicit method, is $p = s + 1$.

Definition 2.4. If we apply the Runge-Kutta method defined by (2.2)+(2.3) or generated by the array (2.4), to the test equation

$$y' = \alpha y, \quad y(x_n) = y_n, \quad \alpha \in \mathbb{R}, \tag{2.8}$$

then, we obtain

$$y_{n+1} = R(z) y_n, \quad z = \alpha h, \tag{2.9}$$

where $R(z)$ is a rational function, called the **stability function** of the Runge-Kutta method.

Lemma 2.6. ([2],[9]) For a semi-explicit Runge-Kutta method with s stages, the stability function $R(z)$ depends only on the parameter λ and has the particular form

$$R(z) = \frac{(-1)^s \sum_{j=0}^{s} L_s^{(s-j)}\left(\frac{1}{\lambda}\right)(\lambda z)^j}{(1-\lambda z)^s}, \tag{2.10}$$

where

$$L_s(x) := \sum_{j=0}^{s} (-1)^j \frac{1}{j!} \binom{s}{j} x^j, \tag{2.11}$$

is the Laguerre's polynomial and $L_s^{(i)}(x)$ is the i^{th} derivative of this polynomial.

Definition 2.7. If, for $\lambda > 0$,

$$|R(z)| \le 1, \quad \text{for all } z < 0, \tag{2.12}$$

then the Runge-Kutta method is called **A-stable** and if the method is A-stable and satisfy

$$\lim_{|z| \to \infty} R(z) = 0, \tag{2.13}$$

then the method is called **L-stable**

3. Semi-explicit methods of order 3 with two stages

We discuss first, the semi-explicit Runge-Kutta methods of order 3 with $s = 2$. For $s = 2$ the methods are generated by the tableau

$$\begin{array}{c|cc} c_1 & \lambda & 0 \\ c_2 & a_{21} & \lambda \\ \hline & b_1 & b_2 \end{array} \tag{3.1}$$

and the parameters $c_1, c_2, b_1, b_2, \lambda$ are satisfying the order conditions given by

$$\begin{aligned} b_1 + b_2 &= 1, & b_1 a_{21} c_1 &= 1/6 - \lambda/2, \\ b_1 c_1 + b_2 c_2 &= 1/2, & c_1 &= \lambda, \\ b_1 c_1^2 + b_2 c_2^2 &= 1/3, & c_2 &= a_{21} + \lambda. \end{aligned} \tag{3.2}$$

Theorem 3.1. *There exist only two different semi-explicit Runge Kutta methods of order 3 with $s = 2$ stages. These methods are A-stable and they are generated by the tableaux*

$$\begin{array}{c|cc} \frac{3+\sqrt{3}}{6} & \frac{3+\sqrt{3}}{6} & 0 \\ \frac{3-\sqrt{3}}{6} & -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} \\ \hline & 1/2 & 1/2 \end{array}, \qquad \begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{3-\sqrt{3}}{6} & 0 \\ \frac{3+\sqrt{3}}{6} & \frac{\sqrt{3}}{3} & \frac{3-\sqrt{3}}{6} \\ \hline & 1/2 & 1/2 \end{array}, \tag{3.3}$$

respectively.

Proof. Is not difficult to solve the system (3.2) and to obtain

$$c_1 = \lambda = \frac{3 \pm \sqrt{3}}{6}; c_2 = \frac{3 \mp \sqrt{3}}{6}; a_{21} = \mp\frac{\sqrt{3}}{3}; b_1 = b_2 = \frac{1}{2}. \tag{3.4}$$

The stability functions of these methods are, respectively

$$R(z) = \frac{1 \mp \frac{\sqrt{3}}{6}z - \frac{1 \pm \sqrt{3}}{6}z^2}{\left(1 - \frac{3 \pm \sqrt{3}}{6}z\right)^2} \tag{3.5}$$

It is easy to see that they satisfy the condition of A- stability (2.12)

4. Semi-explicit methods of order 3 with three stages

Let us now consider the case $s = 3$. The methods of this type are generated by the tableau

$$\begin{array}{c|ccc} c_1 & \lambda & 0 & 0 \\ c_2 & a_{21} & \lambda & 0 \\ c_3 & a_{31} & a_{32} & \lambda \\ \hline & b_1 & b_2 & b_3 \end{array} \tag{4.1}$$

When $p = 3$, the order conditions are

$$\begin{aligned} b_1 + b_2 + b_3 &= 1, & c_1 &= \lambda, \\ b_1c_1 + b_2c_2 + b_3c_3 &= 1/2, & c_2 &= a_{21} + \lambda, \\ b_1c_1^2 + b_2c_2^2 + b_3c_3^2 &= 1/3, & c_3 &= a_{31} + a_{32} + \lambda. \\ b_2a_{21}c_1 + b_3(a_{31}c_1 + a_{32}c_2) &= 1/6 - \lambda/2, & & \end{aligned} \tag{4.2}$$

The stability function $R(z)$ of such methods is given by

$$R(z) = \frac{1 + (1 - 3\lambda)z + \left(1/2 - 3\lambda + 3\lambda^2\right)z^2 + \left(1/6 - (3/2)\lambda + 3\lambda^2 - \lambda^3\right)z^3}{(1 - \lambda z)^3}. \tag{4.3}$$

Lemma 4.1. All solutions of the system (4.2) depend on three parameters and they are given by the relations

$$b_1 = \frac{1/3 - (1/2)(c_2 + c_3) + c_2c_3}{(c_2 - c_1)(c_3 - c_1)}, \; b_2 = \frac{-1/3 + (1/2)(c_1 + c_3) + c_1c_3}{(c_2 - c_1)(c_3 - c_2)}, \tag{4.4}$$

$$b_3 = \frac{1/3 - (1/2)(c_1 + c_2) + c_1c_2}{(c_3 - c_1)(c_3 - c_2)}, \tag{4.5}$$

$$a_{32} = \frac{(c_3 - \lambda)(c_3 - c_2)(12\lambda^2 - 9\lambda + 1)}{2(c_3 - \lambda)(2 - 3\lambda - 3c_2 + 6\lambda c_2)} \tag{4.6}$$

$$c_1 = \lambda, \; a_{21} = c_2 - \lambda, \; a_{31} = c_3 - a_{32} - \lambda, \tag{4.7}$$

where λ, c_2 and c_3 are pairwise distinct parameters in $(0,1)$.

Proof. We solve the first three equations from (4.2) as a linear system in the unknowns b_1, b_2, b_3. Then we obtain the other parameters solving the remaining equations (4.2)

Theorem 4.2. *The value $\lambda = 1/6$, replaced in (4.4)-(4.7) provides a subclass of semi-explicit Runge-Kutta methods of order 3 with three stages depending on two parameters $c_2 \neq c_3, c_2, c_3 \in (0,1)$. All these methods are A-stable.*

Proof. To select the value $\lambda = 1/6$, we made many attempts to satisfy the inequality (2.12) for $R(z)$ given by (4.3). We used the Maple 6 package to do this.

Remark 4.4. When $\lambda = 0.4358665215$ in (4.3) and in (4.4)-(4.7) then the stability function is given by

$$R(z) = \frac{1 - 0.3075995664z - 0.237660069z^2}{(1 - 0.4358665215z)^3} \tag{4.8}$$

and all the methods of this subclass satisfy (2.13) i.e. they are L-stable

Example 4.3. For $c_2 = 1/2$, $c_3 = 3/4$ we obtain following semi-explicit Runge-Kutta method belonging to this subclass

$$\begin{array}{c|ccc} 1/6 & 1/6 & 0 & 0 \\ 1/2 & 1/3 & 1/6 & 0 \\ 3/4 & 21/32 & -7/96 & 1/6 \\ \hline & 3/7 & 0 & 4/7 \end{array} \tag{4.9}$$

In the same manner we can discuss the semi-explicit Runge-Kutta methods of order 3 with four stages and we have obtained two subclasses of such A-stable methods but we will propose them into next papers

We give only one example of A-stable semi-explicit Runge-Kutta method of order 3 with four stages belonging to the subclass of semi explicit method corresponding to $\lambda = 1/4$

1/4	1/4	0	0	0
1/3	1/12	1/4	0	0
4/9	7/9	-7/12	1/4	0
2/3	5/3	-5/4	0	1/4
	0	2	-9/4	5/4

(4.10)

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