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Dedicated to Costică MUSTĂŢA on his 60th anniversary

LOW ORDER STABLE SEMI-EXPLICIT RUNGE-KUTTA METHODS

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Abstract. Low order semi-explicit Runge-Kutta methods are discussed and the A-stability and the L - stability of these methods are studied.

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1. Introduction.

Consider the initial value problem

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

where $f : [a, b] \times \mathbb{R}^m \to \mathbb{R}^m$ is sufficiently smooth and $x_0 = a$ and $y_0, y \in \mathbb{R}^m$. 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** [7], [8], **Houwen van der, P. S. Sommeijer** [9], etc.

The aim of this work is the derivation of a few classes of semi-explicit Runge - Kutta methods of order 2 with two and three stages for the initial value problem (1.1) These methods are A - stable and L - stable, thus they are suitable for solving numerically stiff problems.

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

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

We recall now some definitions

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

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

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

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 the Butcher's tableau

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

where

$$c = (c_1, c_2, ..., c_s)^T; b^T = (b_1, b_2, ..., b_s); A = (a_{ij});\ i, j = 1, 2, ..., s$$

and we have to have

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

where $e = (1, 1, ..., 1)^T \in \mathbb{R}^s$.

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 $i = 1, 2, ...s$.

So, the matrix A for a semi-explicit Runge-Kutta method has the form

$$A = \begin{bmatrix} \lambda & 0 & 0 & \cdots & 0 \\ a_{21} & \lambda & 0 & \cdots & 0 \\ a_{31} & a_{32} & \lambda & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{s1} & a_{s2} & a_{s3} & \cdots & \lambda \end{bmatrix}, \tag{2.6}$$

and the equation (2.5) gives.

$$\begin{aligned}
&c_1 = \lambda,\\
&c_2 = a_{21} + \lambda,\\
&c_3 = a_{31} + a_{32} + \lambda\\
&\dots\dots\dots\dots\dots\dots\\
&c_s = a_{s1} + a_{s2} + \dots + a_{s,s-1} + \lambda.
\end{aligned} \tag{2.7}$$

Definition 2.3. The Runge-Kutta methods (2.2), (2.3) has order p if p is the greatest integer such that

$$y_{n+1} - y(x_n + h) = O(h^{p+1}), \quad \text{as} \quad h \to 0 \tag{2.8}$$

The difference $y_{n+1} - y(x_n + h)$ is called the **local error.**

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], [8]. For semi-explicit methods of order 2, these conditions are:

$$\sum_{i=1}^{s} b_i = 1, \tag{2.9}$$

$$\sum_{i=1}^{s} b_i c_i = \frac{1}{2}. \tag{2.10}$$

More precisely, when the order is $p = 2$ the necessary conditions are the equations (2.9), (2.10) and (2.7).

Remark 2.4. S.P.N Nørset and A. Wolfbrandt A,. [11], proved that the maximum order obtained with an s- stages semi- explicit method, is,$p = s + 1$. .

Definition 2.5. If we apply the Runge-Kutta method defined by (2.2)+(2.3) or generated by the array (2.4) to the test problem

$$y' = \alpha y, \;\; y(x_n) = y_n, \;\alpha \in \mathbb{R}, \tag{2.11}$$

then, we obtain

$$y_{n+1} = R(z)y_n, \;\; z = \alpha h, \tag{2.12}$$

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

Remark 2.6. The general expression of $R(z)$ is

$$R(z) = 1 + zb^T(I - zA)^{-1}e, \tag{2.13}$$

where I is the identity matrix of order s and $e = (1, 1, ..., 1) \in \mathbb{R}^s$.

Remark 2.7. As we can see, for example in [2], [11], 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

$$R(z) = \frac{(-1)^s \sum_{j=0}^{s} L_s^{(s-j)} \left(\frac{1}{\lambda}\right) (\lambda z)^j}{(1-\lambda z)^s}, \tag{2.14}$$

where

$$L_s(x) := \sum_{j=0}^{s} (-1)^j \frac{1}{j!} \binom{s}{j} x^j, \tag{2.15}$$

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

Definition 2.8. If

$$|R(z)| \leq 1, \text{ for all } z < 0, \tag{2.16}$$

then the implicit Runge-Kutta method is called **A- stable**. If the method is **A-stable** and satisfy

$$\lim_{|z| \to \infty} R(z) = 0, \tag{2.17}$$

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

3. Semi-explicit methods of order 2 with s = 2 stages

First, we consider the semi-explicit Runge-Kutta schemes of order $p = 2$ with $s = 2$ stages which are generated by the simple tableau

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

We assume that the parameters $c_1, c_2, b_1, b_2, \lambda$ satisfy the order conditions (2.9), (2.10)and the first two equations from (2.8), i.e.

$$\begin{cases} b_1 + b_2 = 1, \\ b_1 c_1 + b_2 c_2 = \dfrac{1}{2}, \\ c_1 = \lambda, \\ c_2 = a_{21} + \lambda. \end{cases} \tag{3.2}$$

Lemma 3.1. The solutions of this system are given by

$$b_1 = \frac{2c_2 - 1}{2(c_2 - \lambda)}, \; b_2 = \frac{1 - 2\lambda}{2(c_2 - \lambda)}, \; c_1 = \lambda, \; a_{21} = c_2 - \lambda. \tag{3.3}$$

where λ and c_2 are arbitrary distinct real numbers in $(0,1)$.

Lemma 3.2. For the class of semi - explicit Runge - Kutta methods of order 2 with $s=2$, provided by (3.3), the stability function $R(z)$, is

$$R(z)=\frac{1+(1-2\lambda)z+\left(\frac{1}{2}-2\lambda+\lambda^2\right)z^2}{(1-\lambda z)^2}. \tag{3.4}$$

Proof. The conclusion follows from (2.14) for $s=2$.

Theorem 3.3. *The choice $\lambda=\frac{1}{4}$ in (3.3) leads to a subclass of semi - explicit Runge - Kutta methods of order 2 with $s=2$ stages depending on one free parameter $c_2\neq\frac{1}{4}, c_2\in(0,1)$. Moreover these methods are generated by the tableau*

$$\begin{array}{c|cc} \frac{1}{4} & \frac{1}{4} & 0 \\ c_2 & c_2-\frac{1}{4} & \frac{1}{4} \\ \hline & \frac{2(2c_2-1)}{4c_2-1} & \frac{1}{4c_2-1} \end{array} \tag{3.5}$$

and have the property of A-stability, that is

$$|R(z)|\leq 1;\ \text{for } z<0. \tag{3.6}$$

Proof. To select the value $\lambda=\frac{1}{4}$, we tried to satisfy the inequality (3.6) with $R(z)$ given by (3.4), for diferent values of λ, usind Maple 6 package. For $\lambda=\frac{1}{4}$ the stability function is

$$R(z)=\frac{1+\frac{1}{2}z+\frac{1}{16}z^2}{\left(1-\frac{1}{4}z\right)^2}, \tag{3.7}$$

and all semi-explicit Runge-Kutta method generated by (3.5) with $c_2\in(0,1), c_2\neq\frac{1}{4}$, are A - stable, because $R(z)$ satisfy (3.6).

Remark 3.4. Another important choice of value for λ in (3.3) and (3.4) is $\lambda=1-\frac{\sqrt{2}}{2}$, which leads to a subclass of L - stable semi-explicit Runge-Kutta methods of order 2 with two stages. All members of this subclass have the stability function

$$R(z)=\frac{1+(\sqrt{2}-1)z}{\left[1+\left(\frac{\sqrt{2}}{2}-1\right)z\right]^2}, \tag{3.8}$$

which satisfies the inequality (3.6). Moreover, we have (2.17), that is all these methods are L - stable.

One example of such L-stable methods of order 2 with two stages is given by

$$\begin{array}{c|cc} 1-\frac{\sqrt{2}}{2} & 1-\frac{\sqrt{2}}{2} & 0 \\ \frac{1}{2} & -\frac{1}{2}+\frac{\sqrt{2}}{2} & 1-\frac{\sqrt{2}}{2} \\ \hline & 0 & 1 \end{array} \tag{3.9}$$

4. Semi-explicit methods of order 2 with s=3 stages

Now, we consider semi-explicit Runge-Kutta methods of order 2 with three stages ($s=3$). These formulas are generated by the tableau

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

The parameters $c_i, b_i, a_{ij}, \lambda$ have to satisfy the equations

$$\begin{cases} b_1+b_2+b_3=1, \\ b_1c_1+b_2c_2+b_3c_3=\dfrac{1}{2}, \\ c_1=\lambda, \\ c_2=a_{21}+\lambda, \\ c_3=a_{31}+a_{32}+\lambda. \end{cases} \tag{4.2}$$

Lemma 4.1. The solutions of the system (4.2) are given by

$$\begin{array}{l} b_2=\dfrac{\frac{1}{2}-c_3-b_1(\lambda-c_3)}{c_2-c_3},\ b_3=\dfrac{-\frac{1}{2}+c_2+b_1(\lambda-c_2)}{c_2-c_3}, \\ c_1=\lambda,\ a_{21}=c_2-\lambda,\ a_{31}=c_3-a_{32}-\lambda, \end{array} \tag{4.3}$$

where $\lambda, c_2, c_3 \in (0,1)$, a_{32} and b_1 are any real numbers, $\lambda \neq c_2 \neq c_3$.

The proof. is immediate.

Lemma 4.2. The solutions (4.3) of the system (4.2) provide a class of semi-explicit Runge-Kutta methods of order 2 with $s=3$. The stability function of all these methods is

$$R(z)=\frac{1+(1-3\lambda)z+\left(\frac{1}{2}-3\lambda+3\lambda^2\right)z^2+\left(\frac{1}{6}-\frac{3}{2}\lambda+3\lambda^2-\lambda^3\right)z^3}{(1-\lambda z)^3}. \tag{4.4}$$

Proof. The statement follows from (2.14) for $s = 3$.

Theorem 4.3. *The choices* $\lambda = \frac{1}{2}, \lambda = \frac{2}{3}, \lambda = \frac{1}{6}$ *in (4.4) and (4.3) provide three subclasses of semi-explicit Runge-Kutta methods of order 2 with* $s = 3$ *stages parametrised by* $c_2, c_3 \in (0, 1)$, $c_2 \neq c_3, a_{32}$ *and* b_1. *All members of these subclasses satisfy (2.16), that is they are A-stable.*

Proof. The conclusion follows by solving the inequality (3.6) for different values of λ in (4.4), using Maple 6 package.

Remark 4.4. The choise $\lambda = \frac{1}{6}$ leads to a subclass of semi-explicit Runge-Kutta methods of order 2 having the stability function

$$R(z) = \frac{1 + \frac{1}{2}z + \frac{1}{12}z^2 - \frac{1}{216}z^3}{\left(1 - \frac{1}{6}z\right)^3}. \tag{4.5}$$

This stability function is considered **optimal** (see[9]) since $\lambda = \frac{1}{6}$ is the minimum value of λ for which these methods of order 2 with $s = 3$ stages are A-stable.

Example 4.5. We present two examples of methods beloging to these subclasses

$$\begin{array}{c|ccc} 1/6 & 1/6 & 0 & 0 \\ 1/2 & 1/3 & 1/6 & 0 \\ 3/4 & 7/12 & 0 & 1/6 \\ \hline & 3/7 & 0 & 4/7 \end{array} \qquad \begin{array}{c|ccc} 1/2 & 1/2 & 0 & 0 \\ 1/6 & -1/3 & 1/2 & 0 \\ 5/6 & 1/3 & 0 & 1/2 \\ \hline & 1/2 & 1/4 & 1/4 \end{array} \tag{4.6}$$

Remark 4.6. Another important choice of value for λ in (4.4) and (4.3) is $\lambda = 0.4358665215...$, selected to vanish the coefficient of z^3 in the numerator of $R(z)$ in (4.4). This leads to a subclass of semi-explicit Runge-Kutta methods all having the following stability function

$$R(z) = \frac{1 - 0.307599564 \cdot z - 0.23766069 \cdot z^2}{(1 - 0.4358665215 \cdot z)^3} \tag{4.7}$$

Note that $R(z)$ satisfies (2.16) and also (2.17) that is, all these methods are L-stable.

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