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A TWO-STEP FIFTH ORDER RUNGE-KUTTA METHOD

Séka Hippolyte, N'gohissé Konan Firmin and
Kouadio Amos Michaêl Akpini

Department of Mathematics and Informatics
Institut National Polytechnique Félix Houphouêt-Boigny
Yamoussoukro, Côte d'Ivoire

Department of Mathematics and Informatics
Université Peleforo Gon Coulibaly
Korhogo, Côte d'Ivoire

Department of Mathematics and Informatics
Université Alassane Ouattara
Bouaké, Côte d'Ivoire

Abstract

In this article, we develop a two-step Runge-Kutta method of order 5 that depends on a free parameter $a_{6,3}$ to solve ordinary differential equation. For $a_{6,3} = 6/7$, the two-step and one-step methods of order

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5 of Butcher are found. An estimation of the error of this two-step method is proposed, and the comparison of the stability region with that of the one-step method is made.

1. Introduction

The Runge-Kutta method is one of the most widely used methods for solving ordinary differential equations. Several single-step methods have been proposed (see literatures [1-9]). However, extending the study of these methods with one-step by the development of two-step methods is not fully presented in the literature. Proposing two-step methods as well as an estimation of the error and their stability pose challenges for scientific research. Khashin has already explored in his article [7] a two-step method of order 4 as well as an estimate of the error. To do this, Khashin presented this two-step method as a one-step method of order 4 with 9 stages. However, Khashin did not study the stability of this two-step method. The two-step Runge-Kutta method of order 5 with the study of its absolute stability is not explained in the literature. We know that the higher the order of the method, the more accurate it is. Therefore, we will go beyond the method of order 4 proposed by Khashin to explore a two-step method of order 5 by including the study of absolute stability. Proposing two-step methods for methods of order $p \geq 5$ is a real complexity problem to solve, given the number of evaluations to be calculated. Thus the two-step method of order 5 can be seen as a one-step method of order 5 with 13 stages. In addition to numerous evaluations to compute, the stability regions of two-step methods are not completely explored in the literature. In our work, we deepen the study of the one-step Butcher's method of order 5 by calculating a two-step method. To do this, a new one-step method of order 5 is proposed, depending on the parameter $a_{6,3}$. For $a_{6,3} = 6/7$, we find the one-step Butcher's method of order 5. The two-step method is found by performing the evaluations $k_1, ..., k_{13}$. An estimate of the error is found by taking the difference of two numerical solutions. We study the regions of stability and show that under certain conditions, the stability region of the two-step method can be better compared to that of the one-step method.

Our work follows the following plan: In Section 2, the new family of methods of order 5 is proposed. The two-step method of order 5 is constructed in Section 3. In Section 4, an error estimation is provided. Afterwards, the stability region and accuracy of the two-step method is compared to that of the one-step method in Section 5. The conclusion is finally given in Section 6.

2. A New Fifth Order Runge-Kutta Method

Let us consider the following Cauchy problem:

$$\frac{dy}{dt} = f(t, y), \quad y(t_0) = y_0. \tag{2.1}$$

A Runge-Kutta method of order 5 allows us to compute an approximation y_{n+1} of $y(t_{n+1})$ from $y_n \approx y(t_n)$ with a step h such that:

$$y_{n+1} = y_n + h\Phi(t_n, y_n, h), \tag{2.2}$$

where Φ is a linear combination of the evaluations of f at intermediate points. The local error is then:

$$y(t_{n+1}) - y_{n+1} = Ch^6 + \mathcal{O}(h^7). \tag{2.3}$$

To find the coefficients of the new method of order 5, we use the 17 equations of Runge-Kutta method of order 5 below (see literatures [2, 4, 5]):

$$\sum_i^s b_i = 1; \quad \sum_i^s b_i c_i = \frac{1}{2}; \quad \sum_{i=1}^s b_i c_i^2 = \frac{1}{3}, \tag{2.4}$$

$$\sum_{i,j=1}^s b_i a_{ij} c_j = \frac{1}{6}; \quad \sum_{i=1}^s b_i c_i^3 = \frac{1}{4}; \quad \sum_{i,j=1}^s b_i c_i a_{ij} c_j = \frac{1}{8}, \tag{2.5}$$

$$\sum_{i,j=1}^s b_i a_{ij} c_j^2 = \frac{1}{12}; \quad \sum_{i,j,k=1}^s b_i a_{ij} a_{jk} c_k = \frac{1}{24}, \tag{2.6}$$

$$\sum_{i=1}^{s} b_i c_i^4 = \frac{1}{5}; \quad \sum_{i,\,j=1}^{s} b_i c_i^2 a_{ij} c_j = \frac{1}{10}, \tag{2.7}$$

$$\sum_{i,\,j,\,k=1}^{s} b_i a_{ij} c_j a_{ik} c_k = \frac{1}{20}; \quad \sum_{i,\,j=1}^{s} b_i c_i a_{ij} c_j^2 = \frac{1}{15}, \tag{2.8}$$

$$\sum_{i,\,j,\,k=1}^{s} b_i c_i a_{ij} a_{jk} c_k = \frac{1}{30}; \quad \sum_{i,\,j=1}^{s} b_i a_{ij} c_j^3 = \frac{1}{20}, \tag{2.9}$$

$$\sum_{i,\,j,\,k=1}^{s} b_i a_{ij} c_j a_{jk} c_k = \frac{1}{40}; \quad \sum_{i,\,j,\,k=1}^{s} b_i a_{ij} a_{jk} c_k^2 = \frac{1}{60}, \tag{2.10}$$

$$\sum_{i,\,j,\,k,\,l=1}^{s} b_i a_{ij} a_{jk} a_{kl} c_l = \frac{1}{120}. \tag{2.11}$$

We solve these 17 equations by using Maple 18 and obtain all the coefficients of the new method of order 5. The identical coefficients to those of the Butcher's method not dependent on $a_{6,3}$ are:

$$b_1 = \frac{7}{90}; \; b_2 = 0; \; b_3 = \frac{16}{45}; \; b_4 = \frac{2}{15}; \; b_5 = \frac{16}{45}; \; b_6 = \frac{7}{90}; \tag{2.12}$$

$$c_2 = \frac{1}{4}; \; c_3 = \frac{1}{4}; \; c_4 = \frac{1}{2}; \; c_5 = \frac{3}{4}; \; c_6 = 1; \tag{2.13}$$

$$a_{2,1} = \frac{1}{4}; \; a_{3,1} = \frac{1}{8}; \; a_{3,2} = \frac{1}{8}; \tag{2.14}$$

$$a_{4,1} = 0; \; a_{5,1} = \frac{3}{16}; \; a_{5,4} = \frac{9}{16}; \tag{2.15}$$

$$a_{6,1} = -\frac{3}{7}; \; a_{6,4} = -\frac{12}{7}; \; a_{6,5} = \frac{8}{7}. \tag{2.16}$$

The other coefficients identical to those of the Butcher method (see literature [2]) depending on the coefficients $a_{6,3}$ are as follows:

$$a_{4,2} = \frac{1}{2} - \frac{7}{12} a_{6,3}; \; a_{4,3} = \frac{7}{12} a_{6,3}, \tag{2.17}$$

$$a_{5,2} = -3/4 + \frac{7}{16} a_{6,3}; \; a_{5,3} = \frac{3}{4} - \frac{7}{16} a_{6,3}, \tag{2.18}$$

$$a_{6,2} = 2 - a_{6,3}. \tag{2.19}$$

The numerical solution is given by

$$y_1 = y_0 + h\left(\frac{7}{90}k_1 + \frac{16}{45}k_3 + \frac{2}{15}k_4 + \frac{16}{45}k_5 + \frac{7}{90}k_6\right), \tag{2.20}$$

where

$$k_1 = f(x_0, y_0),$$

$$k_2 = f\left(x_0 + \frac{1}{4}h,\ y_0 + ha_{2,1}k_1\right),$$

$$k_3 = f\left(x_0 + \frac{1}{4}h,\ y_0 + ha_{3,1}k_1 + ha_{3,2}k_2\right),$$

$$k_4 = f\left(x_0 + \frac{1}{2}h,\ y_0 + ha_{4,1}k_1 + ha_{4,2}k_2 + ha_{4,3}k_3\right),$$

$$k_5 = f\left(x_0 + \frac{3}{4}h,\ y_0 + ha_{5,1}k_1 + ha_{5,2}k_2 + ha_{5,3}k_3 + ha_{5,4}k_4\right),$$

$$k_6 = f(x_0 + h,\ y_0 + ha_{6,1}k_1 + ha_{6,2}k_2 + ha_{6,3}k_3 + ha_{6,4}k_4 + ha_{6,5}k_5). \tag{2.21}$$

Note that for $a_{6,3} = \frac{6}{7}$, we obtain the Butcher method. We can recapitulate the two methods by Butcher's tables:

Table 1. Runge-Kutta method of order 5 dependent of a_{63}

0						
1/4	1/4					
1/4	1/8	1/8				
1/2	0	$1/2 - 7a_{63}/12$	$7a_{63}/12$			
3/4	3/16	$-3/4 + 7a_{63}/16$	$3/4 - 7a_{63}/16$	9/16		
1	−3/7	$2 - a_{63}$	a_{63}	−12/7	8/7	
	7/90	0	16/45	2/15	16/45	7/90

Table 2. Butcher method of order 5 $(a_{63} = 6/7)$

0						
1/4	1/4					
1/4	1/8	1/8				
1/2	0	0	1/2			
3/4	3/16	−3/8	3/8	9/16		
1	−3/7	8/7	6/7	−12/7	8/7	
	7/90	0	16/45	2/15	16/45	7/90

3. Construction of Two Steps Fifth Order Method

According to the construction of the two-step method of order 4 proposed by Khashin which is seen as a one-step method with 9 stages given by the following table [7]:

Table 3. Two-step Runge-Kutta method of order 4

0									
c_2	a_{21}								
c_3	a_{31}	a_{32}							
c_4	a_{41}	a_{42}	a_{43}						
1	b_1	b_2	b_3	b_4					
$1 + c_2$	b_1	b_2	b_3	b_4	a_{21}				
$1 + c_3$	b_1	b_2	b_3	b_4	a_{31}	a_{32}			
$1 + c_4$	b_1	b_2	b_3	b_4	a_{41}	a_{42}	a_{43}		
2	b_1	b_2	b_3	b_4	b_1	b_2	b_3	b_4	
	d_1	d_2	d_3	d_4	d_5	d_6	d_7	d_8	d_9

According to Table 3, we built in the same way a two-step method of order 5 which can be viewed as a one-step method of order 5 with 13 stages according to the following Butcher's table with

$$c_7 = 1; \quad c_8 = 1 + c_2; \quad c_9 = 1 + c_3; \quad c_{10} = 1 + c_4, \tag{3.1}$$

$$c_{11} = 1 + c_5; \quad c_{12} = 1 + c_6; \quad c_{13} = 2. \tag{3.2}$$

Table 4. Two-step Runge-Kutta method of order 5

$$
\begin{array}{c|ccccccccccccc}
0 & & & & & & & & & & & & & \\
c_2 & a_{21} & & & & & & & & & & & & \\
c_3 & a_{31} & a_{32} & & & & & & & & & & & \\
c_4 & a_{41} & a_{42} & a_{43} & & & & & & & & & & \\
c_5 & a_{51} & a_{52} & a_{53} & a_{54} & & & & & & & & & \\
c_6 & a_{61} & a_{62} & a_{63} & a_{64} & a_{65} & & & & & & & & \\
c_7 & b_1 & b_2 & b_3 & b_4 & b_5 & b_6 & & & & & & & \\
c_8 & b_1 & b_2 & b_3 & b_4 & b_5 & b_6 & a_{21} & & & & & & \\
c_9 & b_1 & b_2 & b_3 & b_4 & b_5 & b_6 & a_{31} & a_{32} & & & & & \\
c_{10} & b_1 & b_2 & b_3 & b_4 & b_5 & b_6 & a_{41} & a_{42} & a_{43} & & & & \\
c_{11} & b_1 & b_2 & b_3 & b_4 & b_5 & b_6 & a_{51} & a_{52} & a_{53} & a_{54} & & & \\
c_{12} & b_1 & b_2 & b_3 & b_4 & b_5 & b_6 & a_{61} & a_{62} & a_{63} & a_{64} & a_{65} & & \\
c_{13} & b_1 & b_2 & b_3 & b_4 & b_5 & b_6 & b_1 & b_2 & b_3 & b_4 & b_5 & b_6 & \\
\hline
 & d_1 & d_2 & d_3 & d_4 & d_5 & d_6 & d_7 & d_8 & d_9 & d_{10} & d_{11} & d_{12} & d_{13}
\end{array}
$$

The numerical solution is given by

$$
\begin{aligned}
y_2 = y_0 + h(&d_1k_1 + d_2k_2 + d_3k_3 + d_4k_4 + d_5k_5 + d_6k_6 + d_7k_7 + d_8k_8 \\
&+ d_9k_9 + d_{10}k_{10} + d_{11}k_{11} + d_{12}k_{12} + d_{13}k_{13}),
\end{aligned} \tag{3.3}
$$

$k_1, \ldots, k_6$ are given in (2.21). $x_1 = x_0 + h$ and

$$
\begin{aligned}
k_7 &= f(x_0 + c_7h,\ y_0 + hb_1k_1 + hb_2k_2 + hb_3k_3 + hb_4k_4 + hb_5k_5 + hb_6k_6), \\
&= f(x_1,\ y_1),
\end{aligned} \tag{3.4}
$$

$$
\begin{aligned}
k_8 &= f(x_0 + c_8h,\ y_0 + hb_1k_1 + hb_2k_2 + hb_3k_3 + hb_4k_4 \\
&\qquad + hb_5k_5 + hb_6k_6 + ha_{2,1}k_7), \\
&= f(x_1 + c_2h,\ y_1 + ha_{2,1}k_7),
\end{aligned} \tag{3.5}
$$

$$k_9 = f(x_1 + c_3 h,\ y_1 + ha_{3,1}k_7 + ha_{3,2}k_8), \tag{3.6}$$

$$k_{10} = f(x_1 + c_4 h,\ y_1 + ha_{4,1}k_7 + ha_{4,2}k_8 + ha_{4,3}k_9), \tag{3.7}$$

$$k_{11} = f(x_1 + c_5 h,\ y_1 + ha_{5,1}k_7 + ha_{5,2}k_8 + ha_{5,3}k_9 + ha_{5,4}k_{10}), \tag{3.8}$$

$$\begin{aligned} k_{12} = f(x_1 + c_6 h,\ y_1 &+ ha_{6,1}k_7 + ha_{6,2}k_8 + ha_{6,3}k_9 \\ &+ ha_{6,4}k_{10} + ha_{6,5}k_{11}), \end{aligned} \tag{3.9}$$

$$\begin{aligned} k_{13} = f(x_1 + h,\ y_1 &+ hb_1k_7 + hb_2k_8 + hb_3k_9 + hb_4k_{10} \\ &+ hb_5k_{11} + hb_6k_{12}). \end{aligned} \tag{3.10}$$

To find the coefficients d_i, we solve the 17 equations with Maple 18 and find the coefficients d_i, some of which depend on a_{63}.

4. Error Estimation in the Two-step Butcher Method

Consider a Runge-Kutta method of order p. The local error is defined by $E(h) = y(t_1 + h) - y_2$, where y_2 is the approximate value after a step h. Theoretically,

$$E(h) = C_1 h^{p+1} + O(h^{p+2}) \approx C_1 h^{p+1}. \tag{4.1}$$

So

$$y(t_1 + h) - y_2 = C_1 h^{p+1} + O(h^{p+2}). \tag{4.2}$$

Let us consider a second numerical approximation Y_2 of $y(t_1 + h)$. Then

$$y(t_1 + h) - Y_2 = C_2 h^{p+1} + O(h^{p+2}). \tag{4.3}$$

(4.2) and (4.3) give

$$Y_2 - y_2 \approx (C_1 - C_2)h^{p+1} = (C_1 - C_2)E(h)/C_1 = KE(h). \tag{4.4}$$

The error is proportional to the difference of the numerical solutions $Y_2 - y_2$ which can be used to estimate the error. Empirically, $E(h) \approx Y_2 - y_2$.

To find an estimation of the error of this method with a two-step order 5, let us find using the software Maple 18 the coefficients $d_1, ..., d_{13}$ of the form $d_i = b_i + ß_i$ with $i = 1, ..., 13$ and

$$b = (b_i) = (b_1, b_2, b_3, b_4, b_5, b_6, 0, 0, 0, 0, 0, 0, 0),$$

$$d_1 = \frac{7}{90} - \frac{9}{32}d_{11};\ \ d_2 = 0;\ \ d_3 = \frac{16}{45} + d_{11};\ \ d_4 = \frac{2}{15} - \frac{3}{8}d_{11}; \tag{4.5}$$

$$d_5 = \frac{16}{45} - 3d_{11};\ d_6 = \frac{7}{90} - \frac{35}{32}d_{11};\ d_7 = \frac{205}{32}d_{11};\ d_8 = 0; \tag{4.6}$$

$$d_9 = -3d_{11};\ d_{10} = -\frac{3}{8}d_{11};\ d_{12} = \frac{21}{32}d_{11};\ d_{13} = -\frac{15}{16}d_{11}. \tag{4.7}$$

The coefficients $ß_i$ are

$$ß_1 = -\frac{9}{32}d_{11};\ \ ß_2 = 0;\ ß_3 = d_{11};\ \ ß_4 = -\frac{3}{8}d_{11}; \tag{4.8}$$

$$ß_5 = -3d_{11};\ \ ß_6 = -\frac{35}{32}d_{11};\ \ ß_7 = \frac{205}{32}d_{11};\ \ ß_8 = 0; \tag{4.9}$$

$$ß_9 = -3d_{11};\ \ ß_{10} = -\frac{3}{8}d_{11};\ \ ß_{12} = \frac{21}{32}d_{11};\ \ ß_{13} = -\frac{15}{16}d_{11}. \tag{4.10}$$

An estimate of the error δ of two-step Runge-Kutta method of order 5 for all $d_{11} \neq 0$ is given by

$$\delta = h \sum_{i=1}^{13} ß_i k_i \tag{4.11}$$

$$\delta = h \cdot d_{11}(-9k_1/32 + k_3 - 3k_4/8 - 3k_5 - 35k_6/32 + 205\,k_7/32 - 3k_9$$
$$- 3k_{10}/8 + k_{11} + 21k_{12}/32 - 15k_{13}/16). \tag{4.12}$$

By taking $a_{6,3} = 6/7,$ we find an estimate of the error of Butcher's method of order 5.

5. Comparison of the Stability Regions and Accuracy of One-step and Two-step Methods

Let R_1 be the one-step stability function and R_2 be the two-step stability function. To find the stability functions R_1 and $R_2,$ we use the following Dahlquist equation:

$$u'(t) = \lambda u(t). \tag{5.1}$$

Let us use (2.13), (3.4)-(3.10) and (5.1) to obtain

$$k_s = \lambda\left(y_i + h\sum_{j=1}^{s-1} a_{s,j}k_j\right). \tag{5.2}$$

Here $s = \overline{2,6}$ for the one-step method and $s = \overline{2,13}$ for the two-step method. This gives us the method for one-step

$$y_{i+1} = R_1(h\lambda)y_i \tag{5.3}$$

and for the two-step method, we obtain

$$y_{i+1} = R_2(h\lambda)y_i. \tag{5.4}$$

Let $z = h\lambda.$ Then we find R_1 and R_2 by using the software Maple 18:

$$R_1(z) = 1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4 + \frac{1}{120}z^5 + \frac{7}{7680}a_{6,3}z^6; \tag{5.5}$$

$$R_2(z) = R_1(z) + \gamma(z), \tag{5.6}$$

where

$$\gamma(z) = \left(-\frac{105}{4096}d_{11}a_{6,3} + \frac{5}{128}d_{11}\right)z^6 + \frac{1}{192}d_{11}z^7 + \left(-\frac{7}{8192}a_{6,3} + \frac{5}{3072}\right)d_{11}z^8 + \frac{1}{15360}d_{11}z^9$$

$$+\left(\frac{7}{491520}a_{6,3}-\frac{1}{15360}\right)d_{11}z^{10}$$

$$+\left(-\frac{49}{2621440}a_{6,3}^{2}+\frac{7}{122880}a_{6,3}-\frac{1}{15360}\right)d_{11}z^{11}$$

$$+\left(-\frac{147}{20971520}a_{6,3}^{2}-\frac{7}{491520}a_{6,3}\right)d_{11}z^{12}$$

$$-\frac{49}{62914560}a_{6,3}^{2}d_{11}z^{13}. \tag{5.7}$$

We can notify that if $d_{11}=0$, then $R_2(z)=R_1(z)$. For $a_{6,3}=6/7$, we find the stability functions of the Butcher's method of order 5 with one-step and two steps. The absolute stability regions for one-step and two-step methods are, respectively, the following regions:

$$\{z \in C, |R_1(z)| \leq 1\}, \tag{5.8}$$

$$\{z \in C, |R_2(z)| \leq 1\}. \tag{5.9}$$

We now compare using GNU Octave (GUI), the stability regions of the two-step Butcher method to those of the one-step method. We obtain some representations of the stability regions given by Figures 1 to 10 below:

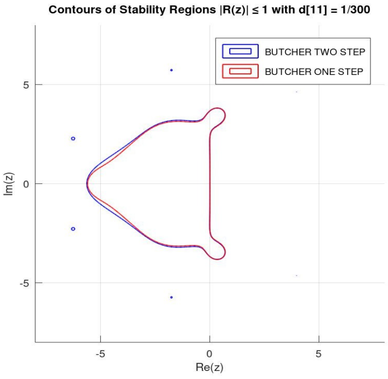


Figure 1

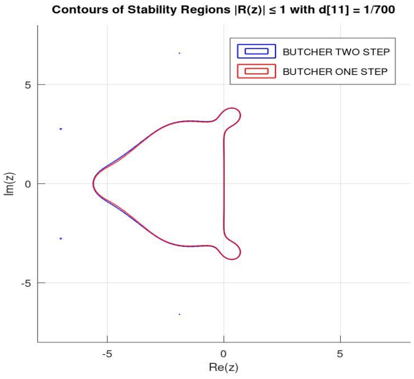


Figure 2

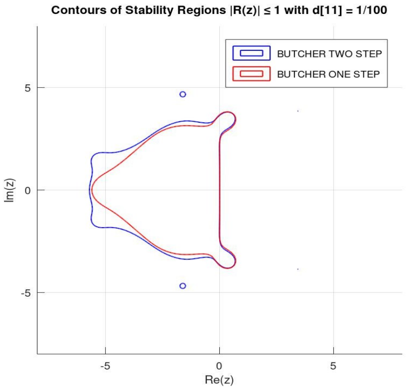


Figure 3

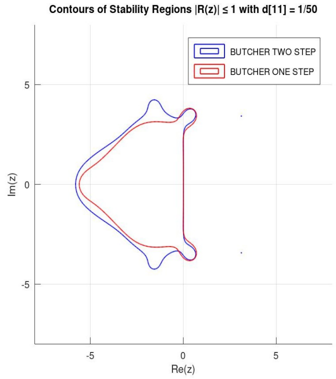


Figure 4

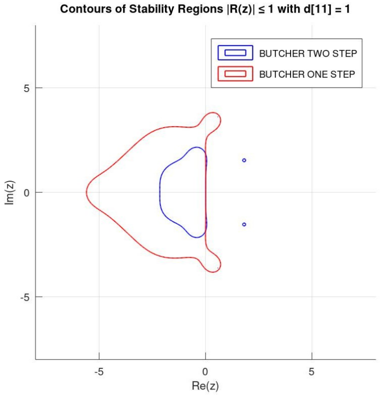


Figure 5

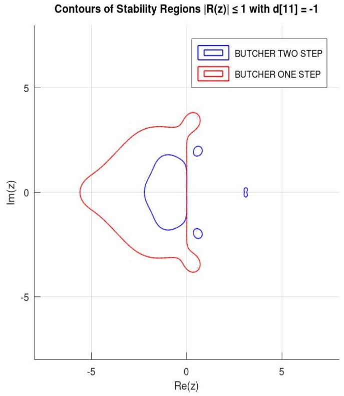
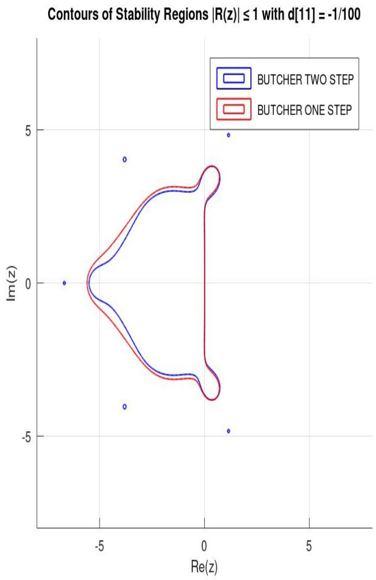
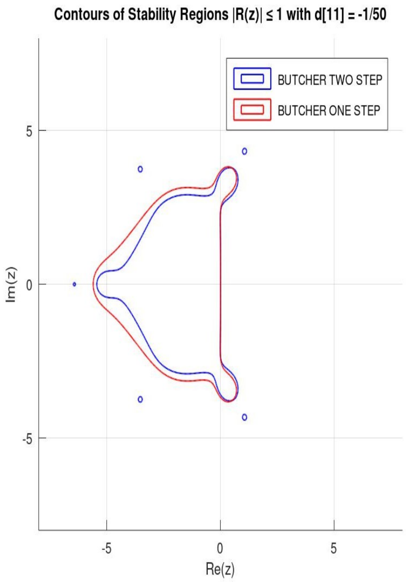


Figure 6



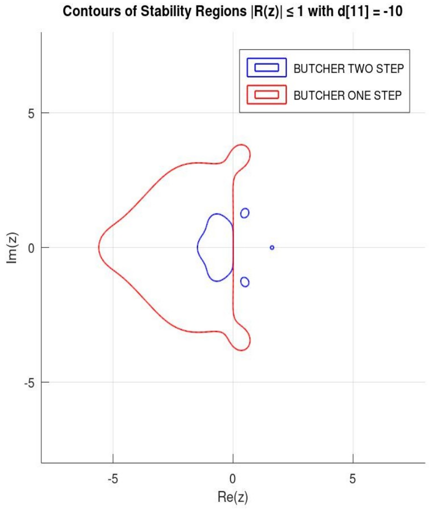
Contours of Stability Regions |R(z)| ≤ 1 with d[11] = -1/100

Figure 7



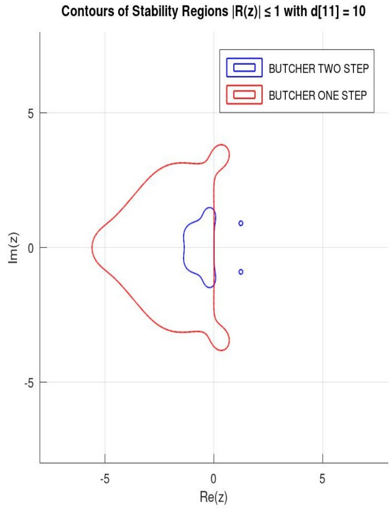
Contours of Stability Regions |R(z)| ≤ 1 with d[11] = -1/50

Figure 8



Contours of Stability Regions |R(z)| ≤ 1 with d[11] = -10

Figure 9



Contours of Stability Regions |R(z)| ≤ 1 with d[11] = 10

Figure 10

$R_1(z) = \sum_{k=0}^{6} \frac{z^k}{k!}$ corresponds exactly to the development of the exponential up to order 6. $R_2(z)$ takes up exactly all the terms from $R_1(z)$, plus correction terms depending on d_{11}. These corrective terms appear in high powers (from z^6 to z^{13}) and are proportional to d_{11}. Some of these corrective terms dampen the amplification in large negative values of z. For large negative values of z, the series $R_1(z)$ diverges very rapidly. On the other hand, in $R_2(z)$, the terms from z^7 to z^{13}, with alternating signs and a factor d_{11}, help to mitigate this divergence. In other words, the modulus $|R_1(z)|$ remains closer to 1 or less than 1 over a larger region of the complex plane, particularly on the negative real axis, which enhances stability. By choosing for example $d_{11} \in]0; 1[$, the stabilizing terms are not too strong (which would prevent an overreach or artificial instability), but they are sufficient to widen the stability area on the negative axis. The stability region for R_2 is larger and encompasses more of the negative real axis than that of R_1.

Let us take a simple example to compare the errors of the one-step and two-step methods. For this, let us take the differential equation as an example $y' = -y$, $y'(0) = 1$. The exact solution of this differential equation is $y(x) = e^{-x}$. Using the software Maple 18, let us evaluate the local error of the one-step and two-step methods by taking an example $d_{11} = \frac{1}{50}$

Value of x_i	Exact value	Local error	
		One-step	Two-step: $d_{11} = \frac{1}{50}$
0.2	0.8187307531	$1.07798185867 \cdot 10^{-9}$	$4.7798185867 \cdot 10^{-9}$
0.4	0.6703200460	$1.73563930074 \cdot 10^{-9}$	$8.3563930074 \cdot 10^{-9}$
0.6	0.5488116361	$2.19402643263 \cdot 10^{-9}$	$9.9402643263 \cdot 10^{-9}$
0.8	0.4493289641	$2.31722159143 \cdot 10^{-9}$	$1.01722159143 \cdot 10^{-9}$
1	0.3678794412	$2.37144232160 \cdot 10^{-9}$	$1.07144232160 \cdot 10^{-9}$

For this example, the two-step method provides a better local error than the one-step method.

6. Conclusion

A new Runge-Kutta method of order 5 for solving ordinary differential equations has been proposed. This method depends on the coefficient $a_{6,3}$. For $a_{6,3} = \frac{6}{7}$, we find one-step Butcher's method of order 5. The two-step method from this family of methods of order 5 is given. An estimate of the error is provided. The stability function of this two-step method depends on the free parameter d_{11}. It is shown that for different values of d_{11}, the stability region of the two-step method is better compared to that of the one-step method. However, if we take $d_{11} < 0$ and $d_{11} \geq 1$, then the stability region of the one-step method is better compared to that of the two-step method. By taking $d_{11} = 0$, the method is reduced to a one-step method of order 5 with 6 stages. With the help of a very simple example, we verify that the two-step method provides a better local error than the one-step method.

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