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Economical Runge-Kutta methods

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RIASSUNTO: *In questo lavoro si presenta un'elegante idea per risparmiare una valutazione funzionale in una classe di metodi di Runge-Kutta. Ciò viene fatto considerando informazioni del passo precedente. Si determinano formule del terzo, quarto e quinto ordine. Si studia la stabilità e la stima dell'errore di troncamento, mediante formule immerse. Infine si considerano esempi numerici che mostrano la competitività di questi metodi con i migliori attualmente esistenti.*

ABSTRACT: *For the numerical solution of the Cauchy problem, this paper presents an elegant idea of saving one function call for a special class of Runge-Kutt methods by using information from the previous step. The stability analysis and practical error estimation by embedded formulas of order (3,2), (5,4) are studied. Numerical examples are, also, considered, which proved that these methods are in competition with the best methods now exist.*

1 – Introduction

For the numerical solution of the initial value problem

$$\begin{cases} y'(x) = f(x, y(x)) \\ y(x_0) = y_0 \quad y : [x_0, b] \to \mathbb{R}^M , \quad f : [x_0, b] \times \mathbb{R}^M \to \mathbb{R}^M \end{cases} \tag{1.1}$$

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explicit Runge-Kutta methods (R.K. in what follows) are well-known:

$$(1.2)\qquad \begin{cases} y_{n+1} = y_n + h_n \sum_{i=1}^{s} b_i K_i^n & n = 0, 1, \ldots, N-1 \\ y_0 = y(x_0) \end{cases}$$

where

$$h_n = x_{n+1} - x_n = \sigma_n h\,, \quad \sigma_n < +\infty$$

$$y_n \doteq y(x_n)$$

$$K_i^n = f\Big(x_n + c_i h_n, y_n + h_n \sum_{j=1}^{i-1} a_{ij} K_j^n\Big) \quad i = 1, \ldots, s$$

$$c_1 = 0\,, \qquad \sum_{j=1}^{0} \ldots \equiv 0\,.$$

With the papers of Butcher ([1], [2]) it became customary to symbolize method (1.2) by the table (1.3)

Table 1.3 - *Coefficients for an explicit R.K. method.*

0					
c_2	a_{21}				
$\vdots$	a_{31}	a_{32}			
$\vdots$	$\ldots$	$\ldots$	$\ddots$		
c_s	a_{s1}	a_{s2}	$\ldots$	$a_{s,s-1}$	
	b_1	b_2	$\ldots$	$\ldots$	b_s

and it is also called an s-stage explicit R.K. method.

Usually the c_i satisfy the conditions $c_i = \sum_{j=1}^{i-1} a_{ij}$ $i = 2, \ldots, s$.

It is known that if s is the number of the stages, related to the cost of the method, and p is the order, we have

$$s \geq p \quad \text{and} \quad p = s \quad \text{iff} \quad p = 2, 3, 4\,.$$

In this paper we will derive a R.K. method, called economical, which requires a number of stages lesser by one, for $p = 3, 4, 5$, after the first step.

2 – Preliminary definitions

Definition 1. *A R.K. method* (1.1) *with order* $p \geq 3$ *belongs to the class* A^p *iff*

$$b_1 = 0 \qquad c_s = 1\,.$$

For the class A^p we have the table (2.1).

Table 2.1 - *Coefficients for an explicit R.K. method in the class* A^p.

0					
c_2	a_{21}				
$\vdots$	a_{31}	a_{32}			
$\vdots$	$\dots$	$\dots$	$\ddots$		
1	a_{s1}	a_{s2}	$\dots$	$a_{s,s-1}$	
	0	b_2	$\dots$	$\dots$	b_s

Definition 2. *Let*

$$(2.2)\qquad \begin{cases} y_{n+1} = y_n + h_n \sum\limits_{i=2}^{s} b_i K_i^n & n = 0,1,\dots,N-1 \\ y_0 \quad = y(x_0) \end{cases}$$

a method of the class A^p*, we define economical R.K. method* (*Ec. R.K. in what follows*) *the method*

$$(2.3)\qquad \begin{cases} y_{n+1} = y_n + h_n \sum\limits_{i=2}^{s} b_i \widetilde{K}_i^n & n = 0,1,\dots,N-1 \\ y_0 \quad = y(x_0) \end{cases}$$

where

$$\widetilde{K}_i^n = f\Big(x_n + c_i h_n\,, y_n + h_n \Big(\sum_{j=2}^{i-1} a_{ij} \widetilde{K}_j^n + a_{i1} \widetilde{K}_s^{n-1}\Big)\Big)$$

$$\widetilde{K}_s^{-1} = K_1^0 = f(x_0, y_0)\,.$$

3 – The main theorems

Now we prove that the class A^p, $p = 3,4,5$, is not empty and that the Ec. R.K. method (2.3) has the same order as R.K. method (2.2).

THEOREM 1. *The class A^p, $p = 3, 4, 5$, is not empty.*

PROOF. I) Only one method belongs to the class A^p. In fact, if we add the condition $b_1 = 0$ to the equations for order 3 ([7], p. 144) we have the method in the table (3.1).

Table 3.1 - *Coefficients for an explicit method in the class A^3*

0			
$\frac{1}{3}$	$\frac{1}{3}$		
1	-1	2	
	0	$\frac{3}{4}$	$\frac{1}{4}$

II) There exist infinitely many methods of the class A^4. According to BUTCHER ([2], p. 179) we have the family

Table 3.2 - *Coefficients for the family of explicit methods in the class A^4*

$$c_1 = 0\,, \qquad c_3 \neq 0, 1, \frac{1}{3}, \frac{1}{2}\,, \qquad c_2 = \frac{-1 + 2c_3}{-2 + 6c_3}\,, \qquad c_4 = 1$$

$$b_1 = 0\,, \quad b_2 = \frac{2c_3 - 1}{12c_2(c_3 - c_2)(1 - c_2)}\,, \quad b_3 = \frac{1 - 2c_2}{12c_3(c_3 - c_2)(1 - c_3)}\,,$$

$$b_4 = \frac{3 - 4(c_2 + c_3) + 6c_2c_3}{12(1 - c_2)(1 - c_3)}$$

$$a_{21} = c_2\,, \qquad a_{31} = \frac{c_3(3c_2 - c_3 - 4c_2^2)}{2c_2(1 - 2c_2)}\,, \qquad a_{32} = \frac{c_3(c_3 - c_2)}{2c_2(1 - 2c_2)}$$

$$a_{41} = \frac{c_3^2(12c_2^2 - 12c_2 + 4) - c_3(12c_2^2 - 15c_2 + 5) + (4c_2^2 - 6c_2 + 2)}{2c_2c_3\left[3 - 4(c_2 + c_3) + 6c_2c_3\right]}$$

$$a_{42} = \frac{(-4c_3^2 + 5c_3 + c_2 - 2)(1 - c_2)}{2c_2(c_3 - c_2)\left[3 - 4(c_2 + c_3) + 6c_2c_3\right]}\,,$$

$$a_{43} = \frac{(1 - 2c_2)(1 - c_3)(1 - c_2)}{c_3(c_3 - c_2)\left[3 - 4(c_2 + c_3) + 6c_2c_3\right]}\,.$$

Furthermore, in A^4 we have also the method of the table (3.3).

Table 3.3 - *Coefficients for a method of class A^4: Simpson formula.*

0				
$\frac{1}{2}$	$\frac{1}{2}$			
0	$-\frac{1}{2}$	$\frac{1}{2}$		
1	$-\frac{3}{2}$	$\frac{3}{2}$	1	
	0	$\frac{2}{3}$	$\frac{1}{6}$	$\frac{1}{6}$

We note that the coefficients c_is and b_is of the table (3.3) are the nodes and the weights of the Simpson quadrature formula while by $c_3 = (4 \pm \sqrt{6})/10$ in table (3.2), we have the Radau quadrature formula of the table (3.4).

Table 3.4 - *Coefficients for a method of class A^4: Radau formula.*

0				
$\frac{4 \pm \sqrt{6}}{10}$	$\frac{4 \pm \sqrt{6}}{10}$			
$\frac{4 \mp \sqrt{6}}{10}$	$\frac{-11 \pm 4\sqrt{6}}{25}$	$\frac{42 \mp 13\sqrt{6}}{50}$		
1	$\frac{1 \mp 5\sqrt{6}}{4}$	$\frac{-3 \pm 2\sqrt{6}}{2}$	$\frac{9 \pm \sqrt{6}}{4}$	
	0	$\frac{16 \pm \sqrt{6}}{36}$	$\frac{16 \mp \sqrt{6}}{36}$	$\frac{1}{9}$

III) There exist infinitely many methods of the class A^5. Adding the condition $b_1 = 0$, to the equations for order 5, we have the solutions

Table 3.5 - *Coefficients for the class* A^5.

$$c_1 = 0\,, \quad c_3 = \frac{3-5(c_4+c_5)+10c_4c_5}{5\Big[1-2(c_4+c_5)+6c_4c_5\Big]}\,, \quad c_6 = 1\,, \quad b_1 = b_2 = 0$$

$$b_3 = \frac{3-5(c_4+c_5)+10c_4c_5}{60c_3(1-c_3)(c_4-c_3)(c_5-c_3)}\,, \quad b_4 = \frac{3-5(c_3+c_5)+10c_3c_5}{60c_4(1-c_4)(c_3-c_4)(c_5-c_4)}$$

$$b_5 = \frac{3-5(c_3+c_4)+10c_3c_4}{60c_5(c_4-c_5)(1-c_5)(c_3-c_5)}$$

$$b_6 = \frac{-12+15(c_3+c_4+c_5)-20(c_3c_4+c_3c_5+c_4c_5)+30c_3c_4c_5}{60(c_3-1)(c_4-1)(c_5-1)}$$

$$a_{21} = c_2\,, \quad a_{31} = \frac{c_3(2c_2-c_3)}{2c_2}\,, \quad a_{32} = \frac{c_3^2}{2c_2}$$

$$a_{41} = \frac{c_4(2c_2-c_4)}{2c_2} + \frac{c_3-c_2}{c_2}a_{43}\,, \quad a_{42} = \frac{c_4^2}{2c_2} - \frac{c_3}{c_2}a_{43}$$

$$a_{52} = \frac{-c_5\Big\{c_4(c_3-c_4)(5c_3c_4-3c_5-10c_3c_4c_5+5c_5^2)+2c_3(c_3-c_5)\Big[3-5(c_3+c_5)+10c_3c_5\Big]a_{43}\Big\}}{2c_2c_4(c_3-c_4)\Big[3-5(c_3+c_4)+10c_3c_4\Big]}$$

$$a_{53} = \frac{-c_5(c_5-c_3)\Big\{c_4(c_4-c_5)(2-5c_4)+2c_3\Big[3-5(c_3+c_5)+10c_3c_5\Big]a_{43}\Big\}}{2c_3c_4(c_3-c_4)\Big[3-5(c_3+c_4)+10c_3c_4\Big]}$$

$$a_{54} = \frac{c_5(2-5c_3)(c_4-c_5)(c_3-c_5)}{2c_4(c_4-c_3)\Big[3-5(c_3+c_4)+10c_3c_4\Big]}$$

$$a_{62} = \frac{c_4(c_4-c_3)(3-5c_3c_4-5c_5+10c_3c_4c_5)-2c_3(1-c_3)\Big[3-5(c_3+c_5)+10c_3c_5\Big]a_{43}}{2c_2c_4(c_3-c_4)\Big[12-15(c_3+c_4+c_5)+20(c_3c_4+c_3c_5+c_4c_5)-30c_3c_4c_5\Big]}$$

$$a_{63} = \frac{1-c_3}{2c_3c_4(c_4-c_3)(c_5-c_3)\Big[12-15(c_3+c_4+c_5)+20(c_3c_4+c_3c_5+c_4c_5)-30c_3c_4c_5\Big]}\cdot$$
$$\cdot\Big\{c_4(c_4-1)\Big[10c_4+c_3(2-5c_4)-6+10c_5^2(2c_4-1)-c_5(25c_4-14)\Big]+$$
$$+2c_3(c_3-c_5)\Big[3-5(c_3+c_5)+10c_3c_5\Big]a_{43}\Big\}$$

$$a_{64} = \frac{(1-c_3)(1-c_4)\Big[6+5c_3(c_4-2)-2c_4+c_5(25c_3+10c_5-20c_3c_5-14)\Big]}{2c_4(c_3-c_4)(c_5-c_4)\Big[12-15(c_3+c_4+c_5)+20(c_3c_4+c_3c_5+c_4c_5)-30c_3c_4c_5\Big]}$$

$$a_{65} = \frac{(1-c_3)(1-c_4)\Big[3-5(c_3+c_4)+10c_3c_4\Big](1-c_5)}{c_5(c_3-c_5)(c_4-c_5)\Big[12-15(c_3+c_4+c_5)+20(c_3c_4+c_3c_5+c_4c_5)-30c_3c_4c_5\Big]}$$

$$a_{51} = c_5 - a_{52} - a_{53} - a_{54}\,, \quad a_{61} = 1 - a_{62} - a_{63} - a_{64} - a_{65}\,.$$

We note that for

$$c_2 = \frac{1}{2}\,, \quad c_4 = \frac{5 \mp \sqrt{5}}{10}\,, \quad c_5 = 0$$

we have the coefficients in the table (3.6), which are those of Lobatto quadrature formula. ∎

Table 3.6 - *Coefficients for a method of class* A^5: *Lobatto formula.*

0						
$\frac{1}{2}$	$\frac{1}{2}$					
$\frac{5\pm\sqrt{5}}{10}$	$\frac{1}{5}$	$\frac{3\pm\sqrt{5}}{10}$				
$\frac{5\mp\sqrt{5}}{10}$	$\frac{1}{5}\pm\frac{\sqrt{5}}{5}a_{43}$	$\frac{3\mp\sqrt{5}}{5}-\frac{5\pm\sqrt{5}}{5}a_{43}$	a_{43}			
0	$-\frac{1}{2}-\frac{1\pm\sqrt{5}}{2}a_{43}$	$-1+(3\pm\sqrt{5})a_{43}$	$\frac{3\mp\sqrt{5}}{4}-\frac{5\pm\sqrt{5}}{2}a_{43}$	$\frac{3\pm\sqrt{5}}{4}$		
1	$-\frac{3}{2}+\frac{1\mp\sqrt{5}}{2}a_{43}$	$-2+2a_{43}$	$\frac{7\mp\sqrt{5}}{4}-\frac{5\mp\sqrt{5}}{2}a_{43}$	$\frac{7\pm\sqrt{5}}{4}$	1	
	0	0	$\frac{5}{12}$	$\frac{5}{12}$	$\frac{1}{12}$	$\frac{1}{12}$

Remark 1 For $p = 2$ we also have an Ec. R.K. method but the condition $c_2 = 1$ it not satisfied. It is given in table (3.7) and appeared in [3].

Table 3.7 - *Coefficients for Ec. R.K. for p=2*

0		
$\frac{1}{2}$	$\frac{1}{2}$	
	0	1

With no lost of generality we can transform (1.1) to autonomous form ([7], p. 142).

Theorem 2. *Let*

$$\begin{cases} y_{n+1} = y_n + h_n \sum_{i=2}^{s} b_i K_i^n \quad n = 0, 1, \ldots, N-1 \\ y_0 \quad = y(x_0) \end{cases} \tag{3.8}$$

a method of the class A^p $3 \leq p \leq 5$, *then also the economical method defined in (2.3) has order* p *and for it we have*

$$y_{n+1} - y(x_{n+1}) = \frac{h_n^{p+1}}{(p+1)!} \sum \alpha(t) e(t) F(t)(y(x_n)) + O(h^{p+2}) \tag{3.9}$$

where $\alpha(t)$ *is the number of ways of labelling* t *with a given totally ordered set* L *with* $\#L = \rho(t), F(t)(y(x_n))$ *is the elementary differential corresponding to the tree* t *and*

$$e(t) = 1 - \phi(t) \tag{3.9a}$$

with

$$\phi(t) = \phi^{(1)}(t) + \theta_{n-1}^{p-2}\phi^{(2)}(t) \quad \textit{with} \quad \theta_{n-1} = \frac{\sigma_{n-1}}{\sigma_n} \tag{3.9b}$$

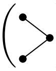
where $\phi^{(1)}(t)$ *and* $\phi^{(2)}(t)$*, for the methods* (3.1), (3.3), (3.4) *and* (3.6)*, will be defined in the tables* (3.8), (3.9), (3.10) *and* (3.11)[(1)].

PROOF. For a method belonging to the class A^P we have

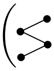
$$\begin{aligned} h_n K_s^{n-1} &= h_n f\Big(y_{n-1} + \theta_{n-1} h_n \sum_{j=1}^{s-1} a_{sj} K_j^{n-1}\Big) \\ h_n K_1^n &= h_n f(y_n) \end{aligned}$$

hence, from the B-series' theory, remembering that $\sum_{j=1}^{s-1} a_{sj} = c_s = 1$,

(3.10)

$$h_n K_s^{n-1} = h_n K_1^n + \theta_{n-1}^2 h_n^3 6\Big(\sum_{j=1}^{s-1} a_{sj} c_j - \frac{1}{2}\Big) F\Big($$  $$\Big) +$$

$$+ \theta_{n-1}^3 h_n^4 24\Big(\frac{1}{2}\sum_{j=2}^{s-1} a_{sj} c_j^2 - \sum_{j=2}^{s-1} a_{sj} c_j + \frac{1}{3}\Big) F\Big($$  $$\Big) +$$

$$+ \theta_{n-1}^3 h_n^4 24\Big(\sum_{j=2}^{s-1} a_{sj} \sum_{k=1}^{j-1} a_{jk}(c_k - 1) + \frac{1}{3}\Big) F\Big($$  $$\Big) + O(h^5)\,.$$

Let $s = 3$ we have $p = 3$ and by (3.10) the method (2.3) becomes

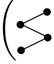
$$y_{n+1} = y_n + h_n \sum_{i=2}^{3} b_i K_i^n + O(h^4) \tag{3.11}$$

(1)For furthermore details about the calculation of $\phi(t)$ you can get in touch with the authors.

from which the thesis follows.

If $s = 4$ we have $p = 4$ and by (3.10) the method (2.3) becomes

$$y_{n+1} = y_n + h_n \sum_{i=2}^{4} b_i K_i^n + X_n \sum_{i=2}^{4} b_i a_{i1} + O(h^5) \tag{3.12}$$

where $X_n = 24\theta_{n-1}^2 h_n^4 \Big(\sum_{j=1}^{3} a_{sj} c_j - \frac{1}{2} \Big) F\Big($  $\Big)$.

Then for the so called simplifying assumptions ([2], p. 178)

$$\sum_{i=1}^{s} b_i a_{ij} = b_j(1 - c_j) \quad j = 1, \dots, 4 \tag{3.13}$$

we have

$$\sum_{i=1}^{4} b_i a_{i1} = 0 \tag{3.14}$$

and by (3.12) the thesis follows.

If $s = 6$ we have $p = 5$ and for the class of 5-order methods ([2], p. 195) we have

$$\sum_{j=1}^{5} a_{sj} c_j = \frac{1}{2}\,.$$

Furthermore for the class A^p we have

$$\sum_{i=1}^{6} b_i a_{i1} = 0$$

and so the method (2.3), by (3.10) gives

$$y_{n+1} = y_n + h_n \sum_{i=2}^{6} b_i K_i^n + O(h^6) \tag{3.15}$$

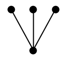
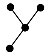
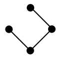
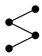
from which the thesis follows. ∎

4 – The local error

The local error for Ec. R.K. method is given by (3.9) and we observe that it depends by the previous step. Now we'll derive $\phi^{(1)}(t)$ and $\phi^{(2)}(t)$ in (3.9b), for each order.

For Ec. R.K. method of order 3 given in table (3.1) we have:

Table 3.8 - *Error functions for method in table* (3.1)

t	$1-\phi^{(1)}(t)-\theta_{n-1}\phi^{(2)}(t)$
	$-\frac{1}{9}$
	$\frac{1}{3}$
	$-\frac{1}{3}$
	1

For Ec. R.K. methods of order 4 given in table (3.3) and in table (3.4) we have:

Table 3.9 - *Error functions for method in table* (3.3)

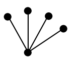
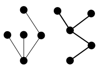
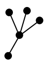
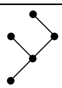
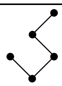
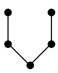
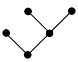
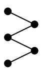
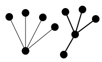
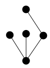
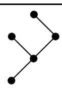
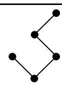
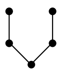
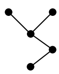
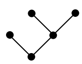
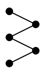
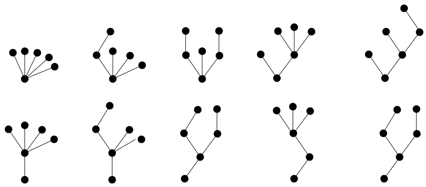
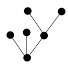
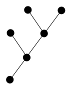
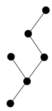
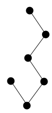
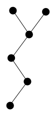
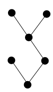
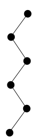
t	$1-\phi^{(1)}(t)-\theta_{n-1}^2\phi^{(2)}(t)$
	$-\frac{1}{24}$
	$-\frac{1}{4}$
	$\frac{1}{6}$
	1
	$-\frac{1}{4}-\frac{1}{48}\theta_{n-1}^2$
	$-\frac{13}{12}$
	$\frac{1}{16}$
	$1+\frac{1}{48}\theta_{n-1}^2$

Table 3.10 - *Error functions for method in table* (3.4)

t	$1-\phi^{(1)}(t)-\theta_{n-1}^2\phi^{(2)}(t)$
	0
	$-\frac{2\pm\sqrt{6}}{24}$
	$\frac{2\pm\sqrt{6}}{6}$
	$-\frac{1}{4}-\frac{3\pm\sqrt{6}}{96}\theta_{n-1}^2$
	$-\frac{19\pm 8\sqrt{6}}{24}$
	$\mp\frac{\sqrt{6}}{4}$
	$\pm\frac{\sqrt{6}}{16}$
	$1+\frac{3\pm\sqrt{6}}{96}\theta_{n-1}^2$

For Ec. R.K. method of order 5 given in table (3.6), for $a_{43} = \mp\dfrac{\sqrt{5}}{15}$, we have:

Table 3.11 - *Error functions for method in table* (3.6)

t	$1 - \phi^{(1)}(t) - \theta_{n-1}^2\phi^{(2)}(t)$
	0
	$\dfrac{25 \pm 3\sqrt{5}}{10}$
	$\pm\dfrac{\sqrt{5}}{20}$
	$\mp\dfrac{\sqrt{5}}{10}$
	$-\dfrac{25 \pm 3\sqrt{5}}{5}$
	$\dfrac{25 \pm 7\sqrt{5}}{10} - \theta_{n-1}^2\dfrac{15 \pm \sqrt{5}}{10}$
	$\dfrac{37 \pm 15\sqrt{5}}{4}$
	$\pm\dfrac{\sqrt{5}}{5}$
	$-\dfrac{25 \pm 7\sqrt{5}}{10} + \theta_{n-1}^2\dfrac{15 \pm \sqrt{5}}{2}$

REMARK 2 For the global error $e_n = y_n - y(x_n)$ by (3.9) with standard techniques we can show that

$$e_n = O(h^p) \qquad n > 0\,.$$

5 – Stability regions

In order to study the stability regions for Ec. R.K. we consider the test differential equations

$$\begin{cases} y' = \lambda y \quad \lambda \in \mathbb{C}\,, \quad \operatorname{Re}\lambda < 0 \\ y(0) = y_0 \end{cases} \tag{5.1}$$

where λ is a complex constant.

Then we have

THEOREM 3. *If we apply the method*

$$\begin{cases} y_{n+1} = y_n + h \sum\limits_{i=2}^{s} b_i \widetilde{K}_i^n \\ h\widetilde{K}_i^n = hf\Big(x_n + c_i h\,, y_n + h\sum\limits_{j=2}^{i-1} a_{ij}\widetilde{K}_j^n + ha_{i1}\widetilde{K}_s^{n-1}\Big) \end{cases} \tag{5.2}$$

to the test problem we have

$$\begin{cases} y_{n+1} = P(z) y_n + hQ(z)\widetilde{K}_s^{n-1} \\ h\widetilde{K}_s^n = L_s(z) y_n + hM_s(z)\widetilde{K}_s^{n-1} \end{cases} \tag{5.3}$$

where $z = h\lambda$*,*

$$\begin{cases} P(z) = 1 + \sum\limits_{i=2}^{s} b_i L_i(z) \\ Q(z) = \sum\limits_{i=2}^{s} b_i M_i(z) \end{cases} \tag{5.4}$$

and

$$\begin{cases} L_2(z) = z \\ M_2(z) = L_2(z) a_{21} \\ L_i(z) = L_2(z)\Big[1 + \sum\limits_{j=2}^{i-1} a_{ij} L_j(z)\Big] \qquad i = 3, \dots, s \\ M_i(z) = L_2(z)\Big[a_{i1} + \sum\limits_{j=2}^{i-1} a_{ij} M_j(z)\Big] \quad i = 3, \dots, s\,. \end{cases} \tag{5.5}$$

PROOF. The proof follows by induction on i. ∎

THEOREM 4. *The stability region for method* (5.2) *is* $S = \{z \in \mathbb{C} : |\lambda_i(z)| \leq 1\}$ *where* $\lambda_i(z)$ $i = 1, 2$ *are the zeros of the characteristic polynomial*

$$\lambda^2 - [P(z) + M_s(z)]\lambda - L_s(z)Q(z) = 0\,.$$

PROOF. Let

$$u_n = [y_n, hK_s^{n-1}]^T$$

by (5.3) we have

$$u_{n+1} = Cu_n$$

where

$$C = \begin{pmatrix} P(z) & Q(z) \\ L_s(z) & M_s(z) \end{pmatrix}\,.$$

If $\lambda_i(z)$ $i = 1, 2$ are the eigenvalues of C the thesis follows easily. ∎

Now we derive the stability region of same Ec. R.K. methods.

p=3 For method of table (3.1) we have the characteristic polynomial

$$\lambda^2 - \left(\frac{7}{6}z^2 + 1\right)\lambda - \left(\frac{1}{3}z^2 + z\right).$$

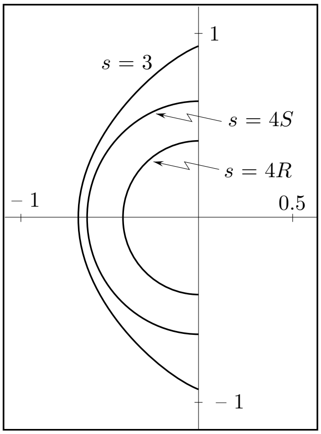
p=4 For method of table (3.3) we have the characteristic polynomial

$$\lambda^2 - \left(\frac{z^3}{3} + \frac{3}{4}z^2 - \frac{1}{2}z + 1\right)\lambda - \left(\frac{1}{3}z^3 + \frac{5}{4}z^2 + \frac{3}{2}z\right).$$

For method of table (3.4) we have the characteristic polynomial

$$\lambda^2 - \left(\frac{13 \mp \sqrt{6}}{24}z^3 - \frac{1 \mp 2\sqrt{6}}{4}z^2 + \frac{5 \mp 5\sqrt{6}}{4}z + 1\right)\lambda + \\ + \frac{z}{12}(3 \mp 15\sqrt{6} - (6 \pm 9\sqrt{6})z - (3 \pm 2\sqrt{6})z^2)\,.$$

The stability regions for the methods (3.1), (3.3), (3.4) are in fig. 1.



$s = 4S$ method (3.3)

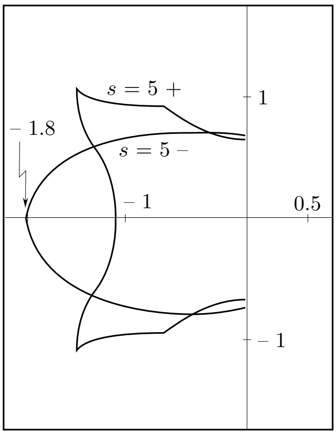
$s = 4R$ method (3.4)

Fig. 1 - *Stability regions of the methods* (3.1), (3.3), (3.4)

p=5 For the method of the table (3.6), with $a_{43} = \pm\dfrac{\sqrt{5}}{15}$ we have the characteristic polynomial

$$\lambda^2 + \left(\frac{105 \pm 49\sqrt{5}}{3600} z^5 - \frac{705 \pm 131\sqrt{5}}{3600} z^4 - \frac{145 \mp 14\sqrt{5}}{600} z^3 + \frac{17 \pm \sqrt{5}}{60} z^2 + \frac{10 \pm \sqrt{5}}{30} z - 1\right)\lambda +$$
$$-\left(\frac{23 \mp 25\sqrt{5}}{720} z^5 + \frac{1385 \pm 3\sqrt{5}}{3600} z^4 + \frac{2475 \pm 102\sqrt{5}}{1800} z^3 + \frac{127 \pm 3\sqrt{5}}{60} z^2 + \frac{40 \pm \sqrt{5}}{30} z\right).$$

The stability regions are in fig. 2.



$s = 5+$ method (3.6) $c_3 = \dfrac{5 + \sqrt{5}}{10}$

$s = 5-$ method (3.6) $c_3 = \dfrac{5 - \sqrt{5}}{10}$

Fig. 2 - *Stability regions of the methods* (3.6)

6 – Practical local error estimation

Since practical error estimates are necessary for a step size control we now derive some embedded Ec. R.K. formulas. So we have to determine the coefficients as in the table (6.1)

Table 6.1 - *Coefficients for embedded Ec. R.K. formula.*

0						
c_2	a_{21}					
$\vdots$	a_{31}	a_{32}				
$\vdots$	$\dots$	$\dots$	$\ddots$			
1	a_{s1}	a_{s2}	$\dots$	$a_{s,s-1}$		
	0	b_2	$\dots$	$\dots$	b_s	
	0	$\tilde{b}_2$	$\dots$	$\dots$	$\tilde{b}_s$	α

such that

$$y_{n+1} = y_n + h_n \sum_{i=2}^{s} b_i \widetilde{K}_i^n \tag{6.2}$$

is of order p, and

$$\tilde{y}_{n+1} = y_n + h_n \left(\sum_{i=2}^{s} \tilde{b}_i \widetilde{K}_i^n + \alpha \widetilde{K}_s^{n-1} \right) \tag{6.3}$$

is of order $p-1$. This formula-pair is indicated by $p(p-1)$.

We have the following

THEOREM 5. *The scheme in the table* (6.4) *is an embedded Ec. R.K. formula of order* 3(2)

Table 6.4 - *Coefficients for embedded Ec. R.K. formula* 3(2).

0			
$\frac{1}{3}$	$\frac{1}{3}$		
1	-1	2	
	0	$\frac{3}{4}$	$\frac{1}{4}$
	0	$\frac{3}{4}-\frac{3}{2}\alpha$	$\frac{1}{4}+\frac{1}{2}\alpha$	α

and the local error estimation is

$$T_n = y_{n+1} - \tilde{y}_{n+1} = \alpha h_n \left(\frac{3}{2}\widetilde{K}_2^n - \frac{1}{2}\widetilde{K}_3^n - \widetilde{K}_3^{n-1} \right). \tag{6.5}$$

Proof. The thesis follows by standard techniques [2]. ∎

Theorem 6. *There are not embedded Ec. R.K. methods like* (6.3) *of order* 4(3).

Proof. By Taylor formula we have

$$\begin{aligned} \tilde{y}_{n+1} &= y_n + h_n\left(\sum_{i=2}^{s} \tilde{b}_i K_i^n + \alpha K_1^n \right) + \\ &\quad + h_n h_{n-1}^2 \alpha \left(\sum a_{ij} c_j - \frac{1}{2} \right) F\left({}^{\bullet}_{\bullet}\!\!>\!\bullet \right) + O(h^4) \end{aligned} \tag{6.6}$$

which is of order 3 for $\alpha \neq 0$ iff

$$\sum a_{ij} c_j = \frac{1}{2}\,.$$

But

$$\sum a_{ij} c_j = \frac{1}{2}$$

iff $c_3 = \frac{1}{3}$ or $c_3 = \frac{1}{2}$ which are not compatible with $c_2 = \frac{-1+2c_3}{-2+6c_3}$ necessary condition to belong to the class A^4. ∎

Theorem 7. *The scheme in the table* (6.7) *is an embedded Ec. R.K. formula of order* 5(4)

Inserire tabella 6.7

and the local error estimation is

$$
\begin{aligned}
T_n = y_{n+1} - \tilde{y}_{n+1} = \frac{\alpha h_n}{38}\Big[&(8 \pm 16\sqrt{5})\widetilde{K_2^n} - (5 \pm 10\sqrt{5})(\widetilde{K_3^n} + \widetilde{K_4^n}) + \\
&+ (39 \pm 2\sqrt{5})\widetilde{K_5^n} + (1 \pm 2\sqrt{5})\widetilde{K_6^n} - \widetilde{K_6^{n-1}}\Big].
\end{aligned} \tag{6.8}
$$

PROOF. The thesis follows by standard techniques [2]. □

REMARK 7 The coefficients of the formula of order 5 of the table (6.7) are also in [4] but in different context.

7 – Implementation and numerical examples

Now for the formula-pair (6.2) and (6.3), with practical local error estimation (6.5), we want to write a code which automatically adjustes the step size in order to achieve a prescribed tolerance for the local error. Whenever a starting step size has been chosen, the algorithm computes a new step size according to the formula

$$
h_{n+1} = h_n \min\left(\mathrm{fac\,max}, \max\left(\mathrm{fac\,min}, \mathrm{fac}\left(\frac{\mathrm{eps}}{\|E\|_\infty}\right)^{\frac{1}{p+1}}\right)\right)
$$

where p is the order of the formula, eps is the tolerance, $E = y - \tilde{y}$, fac min and fac max are coefficients which allow that h can't increase or decrease too fast, and for our examples fac min $= 0.5$, fac max $= 1.5$, fac usually equal 0.8 or 0.9 or $(0.25)^{1/(p+1)}$ or $(0.38)^{1/(p+1)}$. To the parameter α in (6.5) is assigned the value $\frac{1}{1000}$. The algorithms described in the tables (6.4), (6.7), with $c_3 = (5 - \sqrt{5})/10$, have been tested on a wide range of problems including those given by HULL et al. ([8]) in the Detest implementation. They are compared with RUNGE-KUTTA-FEHLBERG ([7], pag. 170) and DORMAND-PRINCE ([5]).

Rather than a complete presentation of results over all the problems in Detest, only for the following five problems, which appear in ([9])

$$\text{(P1)}\qquad \begin{cases} y'(x) = -y \qquad y(0) = 1 \\ \text{with solution} \qquad y(x) = \mathrm{e}^{-x} \end{cases}$$

$$\text{(P2)}\qquad \begin{cases} y'(x) = -\dfrac{y^3}{2} \qquad y(0) = 1 \\ \text{with solution} \qquad y(x) = \dfrac{1}{\sqrt{1+x}} \end{cases}$$

$$\text{(P3)}\qquad \begin{cases} y'(x) = \dfrac{y}{4}\Big(1 - \dfrac{y}{20}\Big) \qquad y(0) = 1 \\ \text{with solution} \qquad y(x) = \dfrac{20}{1 + 19\mathrm{e}^{-x/4}} \end{cases}$$

$$\text{(P4)}\qquad \begin{cases} \begin{cases} y_1' = y_3 \\ y_2' = y_4 \\ y_3' = -\dfrac{y_1}{(y_1^2 + y_2^2)^{3/2}} \\ y_4' = -\dfrac{y_2}{(y_1^2 + y_2^2)^{3/2}} \end{cases} \quad \begin{cases} y_1(0) = 1 - \epsilon \;\; \epsilon = 0.5 \\ y_2(0) = 0 \\ y_3(0) = 0 \\ y_4(0) = \sqrt{\dfrac{1+\epsilon}{1-\epsilon}} \end{cases} \\ \text{(two-body gravitational problem)} \\ \text{with solution} \quad \begin{cases} y_1(x) = \cos u - \epsilon \\ y_2(x) = \sqrt{1-\epsilon^2}\sin u \\ y_3(x) = \dfrac{-\sin u}{1 - \epsilon\cos u} \\ y_4(x) = \dfrac{\sqrt{1-\epsilon^2}\cos u}{1 - \epsilon\cos u} \\ \text{where } u - \epsilon\sin u - x = 0 \end{cases} \end{cases}$$

$$\text{(P5)}\qquad \begin{cases} y'(x) = -\dfrac{2}{21} - \dfrac{120(x-5)}{\big(1 + 4(x-5)^2\big)^{16}} \quad y(0) = 1 \\ \text{with solution} \qquad y(x) = 1 - \dfrac{1}{101^{15}} - \dfrac{2}{21}x + \\ \qquad\qquad + \dfrac{1}{\big(1 + 4(x-5)^2\big)^{15}} \end{cases}$$

the numerical results are displayed in figg. 3,4.

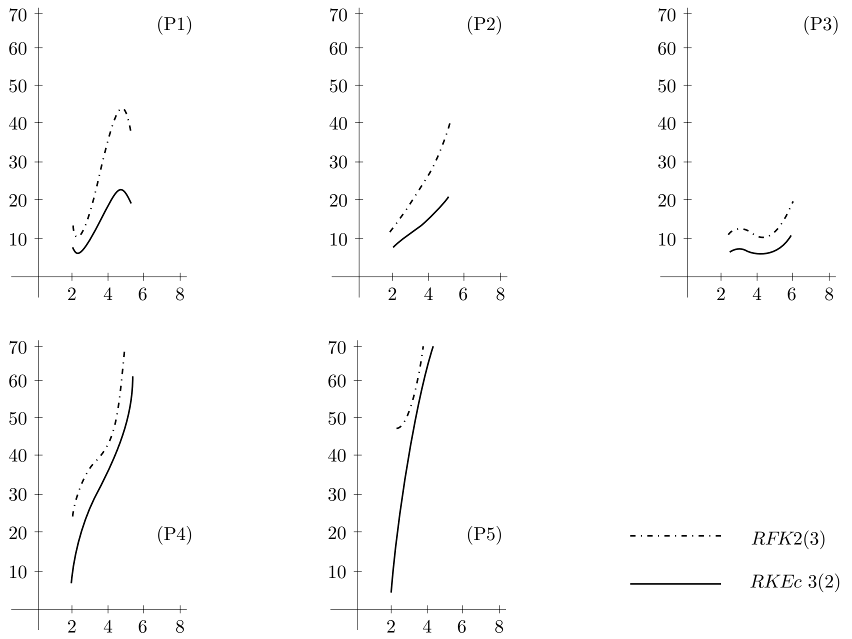


Fig. 3 - *Numerical results for the method in the table* 6.4

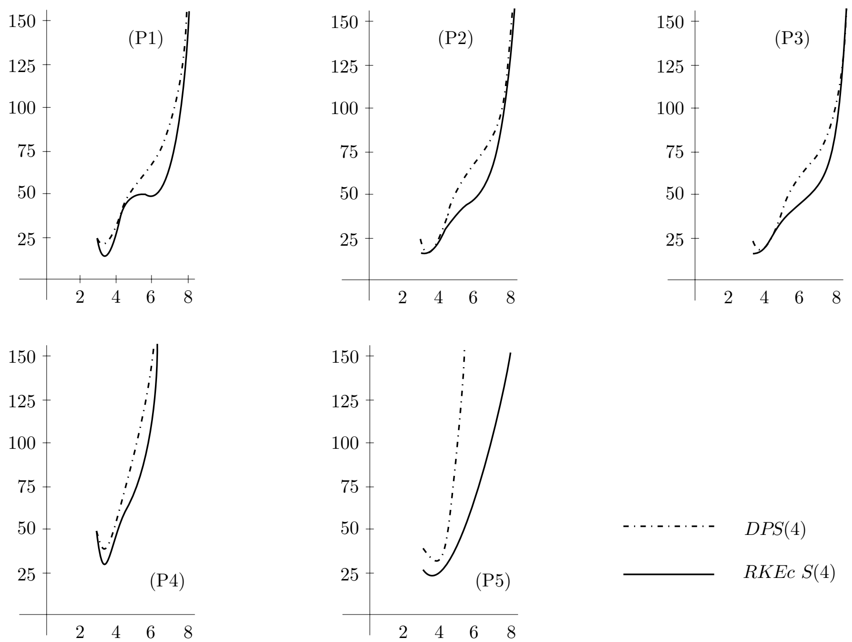


Fig. 4 - *Numerical results for the method in the table* 6.7

The problems P1-P4 are solved for $x \in [x_0, x_0 + 2]$, and the problem P5 is solved for $x \in [x_0, x_0 + 10]$; and tolerance is 10^{-i}, $i = 2, \dots, 5$, for the methods of order 3, and $i = 3, \dots, 8$ for the methods of order 5. The abscissas are $-\log(tol)$, and the ordinates are the number of function evaluations.

It is clear that our methods are quite comparable with the classical methods.

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