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ALGORITHM FOR CONSTRUCTION OF EXPLICIT n-ORDER RUNGE-KUTTA FORMULAS FOR THE SYSTEMS OF DIFFERENTIAL EQUATIONS OF THE 1ST ORDER

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The purpose of this lecture is to show the transformations of the nonlinear condition equations and also to introduce some relations occurring between the parameters of the RK methods of numerical solutions of the systems of differential equations of the 1st order. The reason of the transformations and the above mentioned relations is the effort to transfer the system of nonlinear condition equations into some linear systems.

In the abstract of this lecture were indicated some fundamental concepts, which will be useful in further considerations.

First of all let us introduce them in a little more extended form:

Problem: It is given a system of differential equations

(1) $y' = f(x, y)$ with initial value conditions $y(x_0) = y_0$.

The well-known solution has the form

$$k = \sum_{i=0}^{s-1} p_i \, k_i \text{ where}$$

$$(2) \quad k_0 = h\, f(x_0, y_0),$$

$$k_i = h\, f(x_0 + a_i h,\ y_0 + \sum_{j=1}^{i} b_{ij}\, k_{j-1}) \text{ for } i = 1,2,\dots,s-1,$$

$$a_i = \sum_{j=1}^{i} b_{ij}$$

here all letters are vectors with the exception of x, which is a scalar. The expressions are the so called s-stages RK formulas. The exact increment K of the unknown functions y(x) is given by the expression

$$(3) \quad K = y(x_0 + h) - y(x_0) = \sum_{l=1}^{\infty} \frac{h^l}{l!} f^{(l-1)}(x_0, y_0)$$

and this relation one can write as follows:

$$(4) \quad K = hf + \frac{h^2}{2!} Df + \frac{h^3}{3!} (D^2 f + f_1 Df) +$$

$$+ \frac{h^4}{4!} (D^3 f + f_1 D^2 f + f_1^2 Df + 3DfDf_1) +$$

$$+ \frac{h^5}{5!} [D^4 f + f_1 D^3 f + f_1^2 D^2 f + f_1^3 Df + 4D^2 fDf_1 + 6DfD^2 f_1 +$$

$$+ 7f_1 Df_1 Df + 3f_2 (Df)^2] + \dots$$

where

(5) $D^r f = \sum_{j=0}^{r} \binom{r}{j} \cdot {}_{r-j}f_j \cdot f^j$, $D^r f_g = \sum_{j=0}^{r} \binom{r}{j} \cdot {}_{r-j}f_{g+j} \cdot f^j$

at the same time denotes

$${}_pf_q = \frac{\partial^{p+q} f}{\partial x^p \, \partial y^q} \text{ and } f_q = {}_of_q .$$

By comparing the coefficients arising from the execution of the operations in (2) with those in (4) we get a system of condition equations of an s-stage method

(6) $[f] \sum_{i=0}^{s-1} p_i = 1,$

(7) $[D^q f] \sum_{i=1}^{s-1} p_i \, a_i^q = \frac{1}{q+1}$ for $q = 1, 2, \ldots, n-1,$

(8) $[D^q f D^r f_1] \sum_{i=2}^{s-1} p_i \, a_i^r \, c(i, 2/q) = \frac{1}{(q+1)(q+r+2)}$

for $q = 1, 2, \ldots, n-2$; $r = 0, 1, \ldots, n-3$ with $q + r \leq n-2$,

(9) $[(Df)^2 D^r f_2] \sum_{i=2}^{s-1} p_i \, a_i^r \, c^2(i, 2/1) = \frac{1}{4(r+5)}$ for $r = 0, 1, \ldots, n-5,$

(10) $[f_1^2 D^r f] \sum_{i=3}^{s-1} p_i \, c(i, 3/o/1, r) = \frac{1}{(r+3)^{[3]}}$ for $r = 1, 2, \ldots, n-3.$

The last equation is

(11) $[f_1^{n-2} Df] \sum_{i=n-1}^{s-1} p_i \, C(i, n) = \frac{1}{n!}$

where C(i, n) is the brief symbolical note of the variable of the highest order n-1 and

(12) $(r+m)^{[m]} = \prod_{j=0}^{m-1} (r+m-j);$

at the same time there holds

(13) $a_i = \sum_{j=1}^{i} b_{ij},$

(14) $c(i, 2/m_1) = \sum_{j=2}^{i} a_{j-1}^{m_1} \, b_{ij},$

(15) $c(i, 3/m_1/m_2, r) = \sum_{j=3}^{i} a_{j-1}^{m_1} \, c^{m_2}(j-1, 2/r) \, b_{ij}.$

The number of the single differential equations $\vartheta(n)$ for the RK formulas of the n-th order and the number of the systems of differential equations N(n) is contained in the following Table I.

Table I.

n	1	2	3	4	5	6	7	8	9	10	11	12	13
$\vartheta(n)$	1	2	4	8	16	31	59	110	201	361	639	1114	1917
N(n)	1	2	4	8	17	37	85	200	486	1205	3047	7813	20299

The numbers N(n) are in reality the numbers r_n that occur in the theory of graphs during the computation of the nodes of rooted trees (Riordan [6]). The numbers $\vartheta(n)$ arise by using the operators (5), the numbers N(n) by using the so called elementary differentials $\mathfrak{f}, \{\mathfrak{f}\}, \ldots$ defined in Butcher's article [1] from 1963.
As one can see from Table I., the numbers N(n) increase faster than $\vartheta(n)$. The equations with the operators D contain sometimes more sums, so that the number of sums in all equation is N(n).
Butcher in his article [2] published a table containing the equivalency of operators D of (5) and elementary differentials. The begin of the mentioned table can be seen in Table II.

Table II.

n	1	2	3	4		
(5)	f	Df	D^2f	f_1Df		etc.
elem. dif.	$\mathfrak{f}$	$\{\mathfrak{f}\}$	$\{\mathfrak{f}^2\}$	$\{_2\mathfrak{f}\}_2$		

The system of the conditional equations (6) till (11) for RK formulas of the n-th order contains equations of "depths" g = 0,1,...,n-1 where the equation of g = 0 contains only parameters p_i for i = 0,1,...,s-1, the equations of g = 1 (the number of which is n-1) contain the parameters p_i and a_i for i = 1,2,...,s-1 etc. The equations for g = k contain the derived variables till C(i, k). At the same time k can attain the values 1,2,...,n-1. The "height" of all these equations is s-1. One can transform the equations by means of the substitution

$$(16)\quad t(i,\ 1/j_1/j_2,\ m_1/j_3,\ m_2,\ m_3,\ m_4) = \sum_{\mu=i+1}^{s-1} p_\mu \cdot a_\mu^{j_1} \cdot c^{j_2}(\mu,\ 2/m_1) \cdot c^{j_3}(\mu,\ 3/m_2/m_3/m_4) \cdot b_{\mu,i+1},$$

the second transformation arises by means of the substitution

$$(17)\quad t(i,\ 2/j_1/j_2,\ m_1/j_3,\ v,\ 1,\ m_2//j,\ 1,\ w) = \sum_{\mu=i+1}^{s-2} a_\mu^{j_1} \cdot c^{j_2}(\mu,\ 2/m_1) \cdot c^{j_3}(\mu,\ 3/v,\ 1,\ m_2) \cdot t(i,\ 1/j/1,\ w) \cdot b_{\mu,i+1}.$$

For the third transformation only one special case is given:

(18) $t(i,\ 3/m//1/j) = \sum_{\mu=i+1}^{s-3} a_\mu^m \cdot t(i,\ 2/1//j) \cdot b_{\mu,i+1}$.

By the introduction of the relations (16) into (6) till (10) we obtain the transformed equations

(19) $\sum_{i=1}^{s-2} a_i^q \cdot t(i,\ 1/r) = \frac{1}{(q+1)(q+r+2)}$ for $q = 1,2,\dots,n-2$,

$r = 0,1,\dots,n-3;\ q+r \leq n-2$,

(20) $\sum_{i=1}^{s-2} a_i \cdot t(i,\ 1/r/1,\ 1) = \frac{1}{4(r+5)}$ for $r = 1,2,\dots,n-3$,

(21) $\sum_{i=2}^{s-2} c(i,\ 2/r) \cdot t(i,\ 1/0) = \frac{1}{(r+3)^{[3]}}$ for $r = 1,2,\dots,n-3$.

The second transformation (18) leads to the equation

(22) $\sum_{i=1}^{s-3} a_i^r \cdot t(i,\ 2/0//0) = \frac{1}{(r+3)^{[3]}}$ for $r = 1,2,\dots,n-3$ etc.

By q-fold transformation of an equation of the height v and depth g there arises an equation of the height v-q and of the depth g-q, so that the span remains unvariable. Only equations with $g \geq 2$ are transformable.

If we denote the number of the condition equations with depth g as $\psi(n,\ g)$, then the number of all condition equations of the n-order RK method is $\varphi(n) = \sum_g \psi(n,\ g)$. The number of the equations with the depth g by i transformations will be $\psi(n,\ g+i)$. The number of all transformation will be n-2. By k-fold transformation of an equation of the highest order variables $C(i,\ k)$ there arises an equation with the variables a_i and obviously with transformed variables $t(i,\ k-1)$.

Under suitable relations between the variables one can reach the state that all derived variable is dependent on a_i. This can be reached by comparing the coefficients of the equations of the system (7) and the coefficients of another system [e.g. (8) or (9) etc.]. In this way we get e.g. the following relations:

(23) $c(i,\ 2/k) = \frac{a_i^{k+1}}{k+1}$,

(24) $c(i,\ 3/0/1,\ k) = \frac{a_i^{k+2}}{(k+2)^{[2]}}$,

(25) $c(i,\ 3/j/1,\ k) = \frac{a_i^{k+j+2}}{(k+1)(k+j+2)}$.

$$(26)\quad c(i,\ 4/0/0/1,\ 0,\ 1,\ 4) = \frac{a_i^{k+3}}{(k+3)^{[3]}}.$$

Some special cases in other notation occur in an article of Hairer [3].

By comparing the coefficients of transformed equations and some linear combinations of equations of system (7) one can obtain the dependence of the transformed variables on the p_i and a_i $(i = 1,2,\ldots,s-1)$.

In this way there arise the following relations:

$$(27)\quad t(i,\ 1/k) = \frac{1}{k+1}\cdot p_i\cdot(1 - a_i^{k+1}),$$

$$(28)\quad t(i,\ 1/k/1,\ 1) = \frac{1}{2}\cdot t(i,\ 1/k+2),$$

$$(29)\quad t(i,\ 2//k) = \frac{1}{(k+1)(k+2)}\cdot p_i\cdot\left[a_i^{k+2} - (k+2)a_i + k + 1\right],$$

$$(30)\quad t(i,\ 2/k//0) = \frac{1}{(k+1)(k+2)}\cdot p_i\cdot\left[(k+1)a_i^{k+2} - (k+2)a_i^{k+1} + 1\right].$$

If the number of variables is greater than the number of the equations (and this can always be reached) then we can choose e.g. $p_i = 0$ for $i = 1,2,\ldots,n-2$. Under these conditions with the relations (23), (24) etc. each equation of the whole system of condition equations will be changed into the system (7) and thus it suffices (if $n > 7$) to choose the parameters a_i $(i = n-1,n,n+1,\ldots,s-2,s-1)$.

Considering the fact that by means of transformations the initial system is transfered into linear systems, the solution can be rational and with the use of rational arithmetic of the computer it can be programable.

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