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An Investigation Concerning Fifth Order Scalar and Vector Runge - Kutta Processes. (**)

Consider the initial-value problem

$$\text{(I)} \qquad \begin{cases} \dfrac{\mathrm{d}y}{\mathrm{d}x} = f(x, y) \\ y(x_0) = y_0 , \end{cases}$$

where y and f are both either scalar or vector functions.

A fifth order RUNGE-KUTTA formula for the numerical solution of (I) is of the form:

$$\tilde{y}(x_0 + h) = y_0 + \sum_{i=0}^{5} w_i k_i ,$$

where

$$\begin{cases} k_0 = h\, f(x_0, y_0) \\ k_j = h\, f(x + a_j h, \; y + \sum_{n=0}^{j-1} b_{j,n} k_n) \qquad (j = 1, \ldots, 5) \end{cases}$$

with

$$a_j = \sum_{n=0}^{j-1} b_{j,n} \qquad (j = 1, \ldots, 5).$$

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It is well known that the number of algebraic equations associated with a fifth order scalar or vector RUNGE-KUTTA process is 16 or 17, respectively. Let S and V designate the systems of 16 and 17 algebraic equations corresponding to the scalar and vector cases, respectively.

The system S is as follows:

(1) $\sum_{i=0}^{5} w_i = 1$,

(2) $\sum_{i=1}^{5} w_i a_i = \frac{1}{2}$,

(3) $\sum_{i=1}^{5} w_i a_i^2 = \frac{1}{3}$,

(4) $\sum_{i=1}^{5} w_i a_i^3 = \frac{1}{4}$,

(5) $\sum_{i=1}^{5} w_i a_i^4 = \frac{1}{5}$,

(6) $\sum_{i=1}^{4} w_{i+1} A_i = \frac{1}{6}$,

(7) $\sum_{i=1}^{4} w_{i+1} B_i = \frac{1}{12}$,

(8) $\sum_{i=1}^{4} w_{i+1} C_i = \frac{1}{20}$,

(9) $\sum_{i=1}^{4} w_{i+1} a_{i+1} A_i = \frac{1}{8}$,

(10) $\sum_{i=1}^{4} w_{i+1} a_{i+1} B_i = \frac{1}{15}$,

(11) $\sum_{i=1}^{4} w_{i+1} a_{i+1}^2 A_i = \frac{1}{10}$,

(12) $\sum_{i=1}^{4} w_{i+1} A_i^2 = \frac{1}{20}$,

(13) $$w_3 A_1 b_{3,2} + w_4 (A_1 b_{4,2} + A_2 b_{4,3}) + w_5 (A_1 b_{5,2} + A_2 b_{5,3} + A_3 b_{5,4}) = \frac{1}{24},$$

(14) $$w_3 B_1 b_{3,2} + w_4 (B_1 b_{4,2} + B_2 b_{4,3}) + w_5 (B_1 b_{5,2} + B_2 b_{5,3} + B_3 b_{5,4}) = \frac{1}{60},$$

(15) $$\begin{cases} w_3 [A_1 b_{3,2} (a_2 + a_3)] + w_4 [A_1 b_{4,2} (a_2 + a_4) + A_2 b_{4,3} (a_3 + a_4)] + \\ + w_5 [A_1 b_{5,2} (a_2 + a_5) + A_2 b_{5,3} (a_3 + a_5) + A_3 b_{5,4} (a_4 + a_5)] = \frac{7}{120}, \end{cases}$$

(16) $$w_4 A_1 b_{3,2} b_{4,3} + w_5 [A_1 b_{3,2} b_{5,3} + (A_1 b_{4,2} + A_2 b_{4,3}) b_{5,4}] = \frac{1}{120},$$

where

(II) $$\begin{cases} A_i = \sum_{j=1}^{i} a_j \; b_{i+1,j} \\ B_i = \sum_{j=1}^{i} a_j^2 \; b_{i+1,j} \\ C_i = \sum_{j=1}^{i} a_j^3 \; b_{i+1,j} \end{cases} \qquad (i = 1, 2, 3, 4).$$

On the other hand, the system V is composed of all the equations of the system S, except equation (15), and of the following two equations

$$\text{(17)} \quad \left\{ \begin{aligned} & w_3 A_1 a_2 b_{3,2} + w_4 [A_1 a_2 b_{4,2} + A_2 a_3 b_{4,3}] + \\ & \qquad + w_5 [A_1 a_2 b_{5,2} + A_2 a_3 b_{5,3} + A_3 a_4 b_{5,4}] = \frac{1}{40}, \end{aligned} \right.$$

$$\text{(18)} \quad \left\{ \begin{aligned} & w_3 A_1 a_3 b_{3,2} + w_4 a_4 [A_1 b_{4,2} + A_2 b_{4,3}] + \\ & \qquad + w_5 a_5 [A_1 b_{5,2} + A_2 b_{5,3} + A_3 b_{5,4}] = \frac{1}{30}. \end{aligned} \right.$$

Thus it appears that a solution of the system V is not necessarily a solution of the system S, which would be a contradiction since the scalar case is included in the vector case. However, this contradiction is more apparent than real.

Indeed the sum of the equations (17) and (18) yields equation (15). Consequently, we can discard (18) by replacing it with (15).

Thus we can consider the system V as composed of all the 16 equations of the system S and of equation (17). It follows then that a solution of the system V, as expected, is also a solution of the system S. However, the converse is not always true, that is, a solution of S is not a solution of V unless it satisfies also the equation (17). In other words, only a subset of the set of all solutions of S constitutes the set of all solutions of V.

We thus can announce the

Theorem I. *Let S_t and V_t constitute the sets of all solutions for the scalar and for the vector fifth order processes, respectively. We have $S_t \supset V_t$.*

At this point, the question naturally arises about the validity for vector processes of formulas such as Nyström's [1], which have been derived by solving the scalar system esclusively. Indeed, according to Theorem I, these formulas may not be valid in the vector case.

The next theorem will clarify this question. We first introduce the following four new equations or conditions on the parameters a's and b's:

$$\text{(III)} \qquad A_i = \sum_{j=1}^{i} a_j b_{i+1,j} = \tfrac{1}{2} a_{i+1}^2 \qquad (i = 1, 2, 3, 4).$$

Lemma. *Conditions* (III) *imply* $a_1 \neq 0$.

Proof. Since $A_1 = a_1 b_{2,1} = \frac{1}{2} a_2^2$, $a_1 = 0$ implies $a_2 = 0$. In like manner $a_1 = a_2 = 0$ imply $a_3 = 0$; $a_1 = a_2 = a_3 = 0$ imply $a_4 = 0$; $a_1 = a_2 = a_3 = a_4 = 0$ imply $a_5 = 0$ which contradicts equation (2).

Theorem II. *With conditions* (III) *in force, the systems S and V reduce, respectively, to two equivalent systems.*

Proof. The substitution from (III) into S permits the elimination of the four equations (6), (9), (11) and (12), since they reduce to (3), (4), (5) and again to (5), respectively. Furthermore the equation (13) becomes, after simplification,

$$w_3 a_2^2 b_{3,2} + w_4 (a_2^2 b_{4,2} + a_3^2 b_{4,3}) + w_5 (a_2^2 b_{5,2} + a_3^2 b_{5,3} + a_4^2 b_{5,4}) = \frac{1}{12}$$

or

$$(13') \qquad w_3 (B_2 - a_1^2 b_{3,1}) + w_4 (B_3 - a_1^2 b_{4,1}) + w_5 (B_4 - a_1^2 b_{5,1}) = \frac{1}{12}\,.$$

The combination of (7) and (13′), on noting that $B_1 = a_1^2 b_{2,1}$, yields:

$$a_1^2 (w_2 b_{2,1} + w_3 b_{3,1} + w_4 b_{4.1} + w_5 b_{5,1}) = 0$$

or

$$(13'') \qquad w_2 b_{2,1} + w_3 b_{3,1} + w_4 b_{4,1} + w_5 b_{5,1} = 0\,.$$

Finally, the substitution from (III) into (17), after simplification, yields

$$(17') \qquad w_3 a_2^3 b_{3,2} + w_4 (a_2^3 b_{4,2} + a_3^3 b_{4,3}) + w_5 (a_2^3 b_{5,2} + a_3^3 b_{5,3} + a_4^3 b_{5,4}) = \frac{1}{20}.$$

The proof of the theorem is completed on noting that the combination of (17′) with (8) yields (13″) and consequently (17) can be discarded as a dependent equation.

Interestingly, all presently employed fifth order Runge-Kutta formulas, such as Nyström's, satisfy conditions (III) (a direct consequence of which is $w_1 = 0$). Thus these formulas can be indiscriminately used in scalar as well as in vector cases.

It appears that Theorems I and II can be generalized for higher order processes. However, it should be pointed out that each process must be treated independently as a case by itself. The author has near completion the investigation of the sixth order seven and eight stage processes; they will be treated at a later date in another paper.

References.

[1] E. J. Nyström, *Über die numerische Integration von Differentialgleichungen*, Acta Soc. Sci. Fennicae **50** (1925) (no. 13, pp. 56).

Résumé.

On sait que le nombre d'équations algébriques associées aux formules Runge-Kutta d'ordre $n \geqslant 5$ varie selon qu'il s'agit d'une équation différentielle unique ou d'un système d'équations différentielles. Par conséquent une formule Runge-Kutta d'ordre $n \geqslant 5$ construite pour une équation différentielle unique peut ne pas être applicable à un système d'équations différentielles. Cet article démontre que si les constantes d'une formule Runge-Kutta d'ordre cinq satisfont un certain nombre de conditions simples à vérifier, cette formule est applicable non seulement pour une équation différentielle unique, mais également pour un système d'équations différentielles.

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