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PERFORMANCE CHARACTERISTICS OF HIGHER ORDER APPROXIMATIONS OF RUNGE-KUTTA TYPE

By

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ABSTRACT

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An analysis is given of performance characteristics of higher order approximations of Runge-Kutta type. Performance predictors for the time required on the machine and for the size of the error are developed. These predictors are not supposed to give precise information, but supporting data are given in the note that indicates useful information is obtained from the predictors. The predictors and the data indicate that the usual formulas used should be Shanks' formulas of order six, seven, and eight.

author

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COMPUTATION DIVISION

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1. INTRODUCTION.

The writer of this note has developed higher order formulas for the approximate solution of ordinary differential equations. The previous formulas of this type extended only through the sixth order (two of the sixth order were given by Huta, each requiring eight evaluations of the function). Among the new ones developed by the writer, programmed by Mr. Fred Calhoun, tested, and available for use in the Marshall Space Flight Center Computation Division are several of the sixth order requiring only seven evaluations of the function, several of the seventh order requiring nine evaluations of the function and one of the eight order requiring twelve evaluations of the function.

It is important to know as much as possible about the errors and the time involved in the use of these formulas. In general, one cannot predict such characteristics in a precise manner. However, as shown in this note, useful information can be obtained to serve as a guide.

2. DEVELOPMENT OF PERFORMANCE INDICATORS.

There are three important factors involved in the use of one of these formulas; namely, the formula itself, the differential equation, and the computing machine. In this classification, the programming has been included in the first factor. The pertinent characteristics of the formula are the time τ (in minutes throughout this note) of one step, the order θ of the formula, and the number e of evaluations of the function used in defining the differential equation (for convenience, it is assumed that the differential equation is expressed in the form $y' = f(x,y)$). The characteristics of the machine are the time t_a of one "ideal" arithmetical operation and the time t_e of one evaluation of the function. (t_e obviously depends on the differential equation also).

Let h denote the step size, s the number of steps involved in the solution procedure, $T = ts$ the total time, and $E = es$ the total number evaluations.

For the time of one step, one deduces immediately the (approximate) equation

$$t = et_e + e(e+4)t_a,$$

since $e(e+4)$ is the (approximate) number of arithmetic operations required in the formula (this does not take into account the presence of zero coefficients in the formula). For the total time, one deduces the (approximate) equation

$$T = Et_e + E(e+4)t_a \ . \tag{1}$$

The quantity t_a is (approximately) constant for a given machine and a given type of precision programmed on the machine. The quantity t_e will vary significantly for different differential equations.

Equation (1) leads to the following equivalent

$$T_2 = E_2\left[\frac{T_1}{E_1} + (e_2-e_1)t_a\right] \ , \tag{2}$$

where T_1, E_1, e_1 refer to one formula, T_2, E_2, e_2 refer to another formula and the same differential equation is involved. It is assumed in what follows that the differential equation is fixed, unless the contrary is explicitly stated.

It is seen from equation (2) that t_a may be calculated empirically from the results of two runs on the machine of two formulas with distinct e numbers. This has been done on the IBM 7090 in extended precision and t_a is (approximately) $(45)10^{-7}$. For a particular fixed differential equation, one run on the machine with a particular formula determines T_1, E_1, e_1. Then equation (2) can be used to predict the time T required to make a run with E evaluations for other formulas.

3. SUPPORTING DATA.

Listed below are the results of actual runs on the IBM 7090. All runs are based on the differential equation mentioned previously over the interval from 1-181. In these cases, equation (3) is applicable.

FORMULA	TYPE	PREDICTED TIME (MINUTES)	ACTUAL TIME (MINUTES)	PREDICTED ERROR	ACTUAL ERROR	h	E
1. RUNGE-KUTTA	(4,4)	11.66	9.81	10^{-7}	$.10\ 10^{-5}$	.01	72000
2. RUNGE-KUTTA	(4,4)	3.89	3.27	10^{-6}	$.31\ 10^{-4}$	.03	24000
3. RUNGE-KUTTA	(4,4)	1.94	1.65	10^{-4}	$.51\ 10^{-3}$	.06	12000
4. SHANKS	(6,7)#1	1.47	1.35	10^{-4}	$.17\ 10^{-4}$	.15	8400
5. SHANKS	(6,7)#2	1.47	1.40	10^{-4}	$.16\ 10^{-3}$	.15	8400
6. SHANKS	(6,7)#3	[illegible]	1.51	[illegible]	$.27\ 10^{-3}$	.15	8400
7. SHANKS	(6,7)#4	3.69	3.66	10^{-7}	$.13\ 10^{-5}$	.06	21000
8. SHANKS	(7,9)#1	2.49	2.53	10^{-6}	$.15\ 10^{-5}$	.12	13500
9. SHANKS	(7,9)#2	2.49	2.52	10^{-6}	$.11\ 10^{-5}$	.12	13500
10. SHANKS	(8,12)	4.75	4.73	10^{-7}	$.11\ 10^{-7}$	.09	24000

The predicted error is taken to be 10^{-n}, where $h^{\theta} = (.d_1 d_2 \ldots)10^{-n}$ and $0 < d_1 \leq 9$.

According to the critical value (4), the various formulas are preferred according to the following table.

(Formula) is preferred over	(formula) when the error is less than (number)
(4,4)	(3,3)	$.14\ 10^{-1}$
(6,7)	(4,4)	$.12\ 10^{-3}$
(7,9)	(6,7)	$.20\ 10^{-5}$
(8,12)	(7,9)	$.20\ 10^{-8}$
(5,6)	(4,4)	$.14\ 10$
(6,7)	(5,6)	$.29\ 10^{-2}$
(7,9)	(4,4)	$.48\ 10^{-4}$

For the particular differential equation expressed in the form

$$y'' = -\frac{xy' + y}{x^2y^2}\ , \quad y' = \frac{1}{xy}\ , \quad x_0 = y_0 = y'_0 = 1,$$

equation (2) becomes (approximately)

$$T = \frac{45E}{10^7}(e + 32)\ . \tag{3}$$

Suppose now that the same interval as well as the same differential equation is used. Without loss of generality, it may be assumed that $\theta > \theta_1$ and $e > e_1$ and that the (θ, e) formula is run for only one step. Suppose further that $h^{\theta+\frac{1}{2}} = (\frac{h}{s_1})^{\theta_1+\frac{1}{2}}$, that is, that the errors in the two formulas are (approximately) equal. Then

$$s_1 = h^{\frac{\theta_1-\theta}{\theta_1+\frac{1}{2}}}\ .$$

and $T_1 \geq t$ if and only if

$$h^{\frac{\theta_1-\theta}{\theta_1+\frac{1}{2}}} = s_1 \geq \frac{t}{t_1}\ .$$

From this inequality, one easily deduces that the (θ, e) formula should be used when the error desired is to be less than the critical value

$$\left(\frac{e_1\left[1 + (e_1 + 4)t_r\right]}{e\left[1 + (e + 4)t_r\right]}\right)^{\frac{(\theta-\theta_1)(2\theta_1+1)}{4(\theta-\theta_1)}}\ , \tag{4}$$

where t_r is defined by the equation $t_r t_e = t_a$.

The equation (2) and the critical value (4) are the useful information referred to in the introduction. Neither should be interpreted as giving <u>precise information</u>. However, as shown by the data given below, in cases where the differential equation involves a function that is "reasonably well-behaved," the predictions may be expected to be reasonably accurate. Moreover, it is reasonable to expect that neither of the two formulas will be good approximations when the predictions are not good.

From these predictions, it follows that there is no need for fifth order formulas since the writer has proved that a fifth order formula must require at least six evaluations. It can also be seen that this preference list is biased toward the <u>lower order formulas</u> by examining runs 1 and 7; runs 3 and 6; runs 7 and 9.

These results clearly indicate that (1) Nystrom's formula and Huta's formulas are out-dated and should not be used, (2) the Runge-Kutta formula should be used only when (relatively) rough approximations are desired, (3) the usual formulas used should be Shanks' formulas of order six, seven, and eight.

These results are shown graphically by the following diagram.

(8,12)	$.2\ 10^{-8}$	(7,9)	$.2\ 10^{-5}$	(6,7)	$.12\ 10^{-3}$	(4,4)	$.1\ 10^{-1}$	(3,3)
	8 place accuracy		5 place accuracy		3 place accuracy		1 place accuracy	

4. SUMMARY

1. Definition of Symbols.

h	step size used in the solution
s	the number of steps
t_a	machine time for one "ideal" arithmetical operation
t_e	machine time for one "ideal" evaluation of the function
e	the number of evaluations in a particular formula
θ	the order of approximation of a particular formula
(θ,e)	a formula of order θ with e evaluations
t	the number of minutes required on machine for one step
T	$T = ts$ is the total time for s steps (time in minutes)
E	$E = es$ is the total number of evaluations for s steps
I	error indicator
t_r	$t_r = \frac{t_a}{t_e}$

2. Fundamental relations (approximate).

$$T_2 = E_2 \left[\frac{T_1}{E_1} + (e_2 - e_1) t_a \right]$$

$t_a = (45)10^{-7}$ for extended precision on IBM 7090

$I = 10^{-n}$, where $h^{\theta} = (\cdot d_1 d_2 \ldots) 10^{-n}$ and $0 < d_1 \leq 9$.

$$\text{Critical Value} = \left(\frac{e_1 \left[1 + (e_1 + 4) t_r \right]}{e \left[1 + (e + 4) t_r \right]} \right)^{\frac{(2\theta + 1)(2\theta_1 + 1)}{4(\theta - \theta_1)}}$$

Use formula (θ, e) when error desired is less than critical value. Critical value for (6,7) and (4,4) formulas is approximately $1.2 \; 10^{-4}$.

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The information in this report has been reviewed for security classification. Review of any information concerning Department of Defense or Atomic Energy Commission programs has been made by the MSFC Security Classification Officer. This report, in its entirety, has been determined to be unclassified.

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Director, Computation Division