QUARTERLY TECHNICAL REPORT

for

October, November, December, 1965

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During the current quarter, the contract work has been done chiefly by
Professor Wesson and Mr. John Edwards. As usual, Professor Shanks' participa-
tion has been reduced substantially because of administrative responsibilities.

However, work has continued on "error stabilizers" under the supervision
of Professor Shanks. A great part of this work has been of a computational
nature in order to get additional information on these stabilizers.

Professor Wesson has continued his investigation of predictor-corrector
processes in the solution of differential equations. A method in which a new
corrector is chosen each step has been developed for several orders, and has
been tested for orders 3 and 5. The investigation included a close look at
the roots of the characteristic equation.

Professor Wesson read a paper outlining his results at the November 12
meeting of the American Mathematical Society. The paper is submitted as part
of this report.

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Respectfully submitted,

E. Baylis Shanks

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A REPORT ON A PREDICTOR-CORRECTOR

PROCESS IN WHICH THE SELECTION OF

AN OPTIMUM CORRECTOR IS MADE EACH STEP [*]

By James R. Wesson, Vanderbilt University

1. Introduction. It is the purpose here to report the development and
use of a predictor-corrector process in which a new corrector is selected
at each step. The purpose of the program is to make a good compromise
between truncation error and propagated error. The new process seems to
be applicable to the numerical solution of a wide variety of differential
equations.

We present in section 2 a one-parameter family of correctors, along
with an examination of the characteristic roots. In section 3 we explain
the method for choosing the optimum corrector from the fifth-order family.
The program is sketched in section 4, and a comparison of the new method
with other methods is given in section 5.

2. A family of stable correctors. The Adams corrector

$$(1) \qquad y_{n+1} = y_n + h \sum_{i=0}^{n+1} B_i y_i'$$

is noted for its favorable stability properties. On the other hand the
Newton-Cotes corrector

$$(2) \qquad y_{n+1} = y_0 + h \sum_{i=0}^{n+1} C_i y_i'$$

has a smaller step error but is on the boundary of the set of stable

correctors. For $h = 0$, the characteristic roots of (1) are $1, 0, \ldots, 0$

and the characteristic roots of (2) are the $(n+1)$-th roots of unity.

We now consider the one-parameter family of correctors obtained by

multiplying equations (1) and (2) by r and $1 - r$ respectively, and

then adding the results. As r varies from 1 to 0, the corrector changes

from (1) to (2).

For $h = 0$ and $0 \le r \le 1$ it is easy to show that no characteris-

tic root is outside the unit circle. For $-x^{n+1} + rx^n + (1-r) = 0$ and

$x \ne 0$ give $|x| \le r + (1-r)|x|^{-n}$. Then $|x| > 1$ is impossible. When

$0 < r < 1$, every root except the single root 1 is within the unit circle.

For any other root would satisfy $(1+a)x^n + x^{n-1} + x^{n-2} + \cdots + x + 1 = 0$,

where $r/(1-r) = a > 0$. Then multiplying by $x - 1$ gives

$$x^{n+1} - 1 = - ax^n(x-1), \quad \text{and}$$

$$x^{-n-1} + ax^{-1} = 1 + a.$$

Suppose $|x| = 1$. Then $\left| x^{-n-1} + ax^{-1} \right| = \left| x^{-n} + a \right| = 1 + a$. The point

x^{-n} is on the unit circle and also on the circle with center $-a$ and

radius $1 + a$. Hence $x^n = 1$. But $x \ne 1$. Then $x^n = 1$ gives

$x^{n-1} + x^{n-2} + \cdots + 1 = 0$, $(1+a)x^n = 0$, and $x = 0$, a contradiction.

3. <u>Choice of a corrector.</u> It is well known that the selection of the

best corrector for solving $y' = f(x,y)$ with stepsize h depends on

$K = h\, f_y$ [2, p.8; 3, p. 197; 4, p. 218]. Recall that each corrector of

the family of section 2 is determined by r, and suppose we use K to

determine $r = r(K)$. Then we may change the corrector as often as we

take time to compute K and $r(K)$.

In this report, the function $r(K)$ has been determined empirically for fifth-order correctors. Note that equations of the form $y' = ay$ present a constant K. For such an equation various correctors (that is, various values of r) were tested and compared. The best one was used to determine $r(K)$. Other values of K were obtained by varying a in $y' = ay$, or by varying h. Each of these was used to determine another best value of r. A least squares smoothing gave the equation $r = 0.57K^2 - 1.18K + 0.18$ for $|K| \leq 0.5$. Then as K varies from -0.5 to 0 to 0.5, r varies from 0.91 to -0.27. The decision to permit r to get outside the interval $[0,1]$ is risky. However, the best results for the equations solved were obtained by using r as defined above.

4. <u>A sketch of the program.</u> The following process by Shanks [6, p. 19] is used to produce three starting points.

$$k_0 = hf(x_0, y_0)$$

$$k_1 = hf(x+h/300, \ y+k_0/300)$$

$$k_2 = hf(x+h/5, \ y+(1/5)(-29k_0+30k_1))$$

$$k_3 = hf(x+3h/5, \ y+(1/5)(323k_0-330k_1+10k_2))$$

$$k_4 = hf(x+14h/15, \ y+(1/810)(-510104k_0+521640k_1-12705k_2+1925k_3))$$

$$k_5 = hf(x+h, \ y+(1/77)(-417923k_0+427350k_1-10605k_2+1309k_3-54k_4))$$

$$y_1 = y_0+(1/3696)(198k_0+0k_1+1225k_2+1540k_3+810k_4-77k_5).$$

Then the predictor

$$y_4 = 10y_1 + 9y_2 - 18y_3 + h(3y_0' + 18y_1' + 9y_2')$$

gives y_4, and y_4' is predicted as $f(x_4, y_4)$. The corrector (take $r = 1$ initially)

$$y_4 = ry_3 + (1-r)y_0 + \frac{h}{720} \Big[(224 + 27r)y_4'$$

$$+ (1024 - 378r)y_3' + (384 - 648r)y_2' + (1024 - 918r)y_1'$$

$$+ (224 - 243r)y_0' \Big]$$

gives a corrected value of y_4, which leads to a corrected value of $y_4' = f(x_4, y_4)$, etc. (In the examples described here, the corrector is applied twice each step.)

Now we compute a new value of r for the next step. Take $K = h(\overline{y_4'} - y_4') / (\overline{y_4} - y_4)$, where $\overline{y_4'}, \overline{y_4}$ are predicted values, and y_4', y_4 are the last corrected values. Then compute $r = 0.57K^2 - 1.18K + 0.18$ if $K \leq 0.5$. In case $\overline{y_4} - y_4 = 0$, use $r = 1$. For $K \leq -0.5$ take r constant. Similarly for $k \geq 0.5$ take r constant.

5. <u>Comparison with other methods</u>. The following table indicates how the method formulated above competes with methods in which a fixed corrector (value of r) is used at each step. Each solution is started at $(0,1)$ with $h = 0.05$ and continued to $x = 10$. The programs are identical in every respect, except in the choice of r.

In the first six columns of the table r is fixed. The first column are the results for the Adams corrector $(r = 1)$. When $K > 0$, values of r close to 0 are used, and this gives a small truncation error with no apparent damage to the numerical stability of the process. For $K < 0$, r must be nearer to 1, or else the process becomes unstable. For all values of K the new process competes very well with any of the others. For $k < 0$ it is on a par with the best of the others, and for $k > 0$ it surpasses the others. It seems to be depend-

TABLE OF RELATIVE ERRORS AT x = 10

EQUATION	VALUE OF r						New r Each Step
	1.0	0.8	0.6	0.4	0.2	0.0	
$y' = xy$	$.56 \times 10^{-2}$	$.37 \times 10^{-2}$	$.25 \times 10^{-2}$	$.16 \times 10^{-2}$	$.97 \times 10^{-3}$	$.45 \times 10^{-3}$	$.11 \times 10^{-4}$
$y' = - xy$	$.15 \times 10^{-1}$	$.39 \times 10^{-2}$	$.42 \times 10^{-1}$	$.33 \times 10^{7}$	---	---	$.49 \times 10^{-2}$
$y' = 5y \cos 5x$	$.72 \times 10^{-3}$	$.52 \times 10^{-3}$	$.31 \times 10^{-3}$	$.17 \times 10^{-3}$	$.10 \times 10^{-3}$	$.11 \times 10^{-4}$	$.68 \times 10^{-4}$
$y' = 10y \cos(x/2)$	$.31 \times 10^{-1}$	$.79 \times 10^{-2}$	$.35 \times 10^{-2}$	$.86 \times 10^{3}$	---	---	$.98 \times 10^{-2}$

able for a broad class of equations.

6. <u>Conclusion.</u> Changing the corrector each step is one way of auto-matically achieving a balance between numerical stability and truncation error. A new corrector each step can be selected without additional functional evaluations and with a relatively small increase in computing time. It is to be expected that the empirical formula for r (see section 3) can be improved. Indeed, the author has experimented with a number of different functions $r = r(K)$, but none have been appreciably superior to the one used.

APPENDIX

The derivation and treatment of formulas (1) and (2) of section 2 are well known for example, $\begin{bmatrix} 1, \text{ p. } 10 \text{ and } 3, \text{ p. } 157 \end{bmatrix}$. The remainder term for the fifth-order corrector given in section 4 is

$-\dfrac{3rh^6 f^{(6)}}{160} - \dfrac{8(1-r)h^7 f^{(7)}}{945}$. For $r = 0$, the corrector is of order six.

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