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AN APPROACH TO PREDICTORS EXPERIMENTS AND DETERMINATION OF BETTER METHODS

by

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ABSTRACT

Based on experiments and on the analysis of its results we found new formulae which used as predictors gave us better approximations than the other well known ones.

I. INTRODUCTION

One of the most powerful methods of solving ordinary differential equations numerically is the predictor-corrector method. It consists of predicting a tentative value $y_p^{(0)}$ of y_p and correcting it as many times as necessary.

Therefore we predict a value to the approximation y_p of the exact solution $y(x_p)$ of the differential equation using a predictor formula and, improve this value applying a corretor, in a iterative process, until we have a reasonable margin of error.

II. MULTISTEP METHODS

Predictors and correctors are "linear multistep methods " whose general form is:

Definition 1

A linear multistep method is a formula of the type

(II.1) $$\alpha_p y_{n+p} + \alpha_{p-1} y_{n+p-1} + \dots + \alpha_0 y_n = h\{\beta_p f_{n+p} + \dots + \beta_0 f_n\},$$

where $|\alpha_0| + |\beta_0| > 0$, $\alpha_p \neq 0$;

α_i , β_i real numbers and $f_j = f(x_j, y_j)$.

For particular α_i and β_i the values y_j obtained by (II.1) represent approximations of the true solution $y(x_j)$ of the given differential equation

(II.2) $$y' = f(x,y) \; ; \; y(x_0) = y_0 \quad , \quad x \in [a,b] \;.$$

Definition 2

When $\beta_p = 0$ (II.1) defines a predictor .

As we can easily see a predictor is always an explicit formula in y_{n+p} . This is not true for the correctors which are implicit ones.

Definition 3

When $\beta_n \neq 0$ (II.1) defines a corrector.

III. STABILITY AND CONSISTENCY : CONVERGENCY

When we are interested in using some formula for solving a given problem we must be sure that it is consistent with our problem and, that negligible errors do not accumulate during the computation into relevant ones for the final solution. These two conditions are respectively called consistency and stability conditions.

In order to exam both conditions in detail, we first intro duce the polynomials

$$\text{(III.1)} \quad \begin{aligned} \rho(z) &= \alpha_p z^p + \alpha_{p-1} z^{p-1} + \ldots + \alpha_1 z + \alpha_0 \\ \sigma(z) &= \beta_p z^p + \beta_{p-1} z^{p-1} + \ldots + \beta_1 z + \beta_0 \end{aligned}$$

which are the generator polynomials of (II.1), and the difference

$$\text{(III.2)} \quad L[y(x);h] = \alpha_k y(x + hk) + \ldots + \alpha_0 y(x) - \\ - h\{\beta_k y'(x + hk) + \ldots + \beta_0 y'(x)\}$$

which indicates the margin of precision of substituition of $y' = f(x,y)$ by (II.1). If the solution to (II.1) is equal to that of $y' = f(x,y)$, then

$$y'(x + hk) = f(x_k, y_k) \quad \text{and} \quad L[y(x);h] \equiv 0$$

If $y(x)$ is sufficiently differentiable we can expand (III.2) in Taylor's series as follows:

$$y(x + mh) = y(x) + mhy'(x) + \frac{1}{2} m^2h^2y''(x) + \ldots$$

$$hy'(x + mh) = hy'(x) + mh^2y''(x) + \ldots$$

$$L[y(x);h] = c_0 y(x) + c_1 hy'(x) + \ldots + c_i h^i y^{(i)}(x) + \ldots$$

where

$$c_0 = \alpha_0 + \alpha_1 + \dots + \alpha_k$$

$$c_1 = \alpha_1 + 2\alpha_2 + \dots + k\alpha_k - (\beta_0 + \beta_1 + \dots + \beta_k)$$

$$c_i = \frac{1}{i!}\left[\alpha_1 + 2^i\alpha_2 + \dots + k^i\alpha_k\right] - \frac{1}{(i-1)!}\left[\beta_1 + 2^{i-1}\beta_2 + \dots + k^{i-1}\beta_k\right]$$

Let us introduce other important definitions:

Definition 4

A linear multistep method is said to be stable if the modulus of each root of $\rho(z)$ is less or equal to one and if the roots modulus is exactly one are semple.

Definition 5

A linear multistep method is consistent if $c_0 = c_1 = 0$ e.g. consistency implies:

$$\rho(1) = 0 \quad ; \quad \rho'(1) = \sigma(1)$$

Definition 6

Let $f(x,y)$ be continuous in $G: \{a<x<b\ ; -\infty<y<\infty\}$, such that it satisfies Lipschitz's condition in y and let $y(x)$ be the solution of $y' = f(x,y)\ ;\ y(a) = y_0$ such that

$$\lim_{h\to 0} y_j(h) = y_0 \quad , \quad j = 0,1,\ldots,p-1 \ .$$

Then a linear multistep method is convergent if

$$\lim_{\substack{h\to 0 \\ x_j\to x}} y_j = y(x)$$

for all solutions $y_j(h)$ de (I.2) with the initial values y_j , $j = 0,1,\ldots,p-2$.

Definition 7

A linear multistep method is of degree p if $\rho(z)$ is a polynomial of degree p .

Definition 8

A linear multistep method is of order q if $c_0 = c_1 = \ldots$ $\ldots = c_q = 0 \ , c_{q+1} \neq 0$.

Theorem 1

A linear multistep method is convergent if and only if it consistent and stable.

Examples:

a) Predictor : $y_{n+4} - y_n = \frac{h}{3}\left[8f_{n+3} - 4f_{n+2} + 8f_{n+1}\right]$

b) Corrector : $y_{n+4} - y_{n+2} = \frac{h}{3}\left[f_{n+4} + 4f_{n+3} + f_{n+2}\right]$

As we can see, in order to start the process of application of a given predictor for computing an approximation to y_p we need a set of y_j "a priori" determined. In example (a) initial approximations of y_0, y_1, y_2 and y_3 are needed and may be obtained by some other method, for instance, linear one-step methods. In (b) we use also the value of y_4 calculated by formula (a). This fact makes the linear multistep methods not self-starting, which is centainly a disadvantage.

IV. DEVELOPMENT OF THE RESEARCH

In this paper we are concerned only with the predictors , trying to find formulae that could give better results than those already known.

We started producing unstable methods for testing one statement of P. Henrici in his book "Discrete Variable Methods in Ordinary Differential Equations" which says that some special unstable methods would produce better approximations than the stable ones.

We first found and tested several unstable predictors. These tests showed us that it is really possible to find this kind of formulae.

After that we defined a special predictor with coefficients α_i such that $[\alpha_i] < 1$; $\alpha_p = 1$. We restricted ourselves to there α_i because we realized that sometimes coefficients greater than one produce too much error accumulation. Then we tried to minimize this accumulation minimizing the function $\Theta = \Sigma\, \alpha_i^2$, where α_i represent the coefficients of the method whose polynomial $\rho(z)$ has degree p and the form:

$$(z) = \sum_{m=0}^{p} \left[z - (a_m + b_m i) \right] \quad , \quad a_m \, , \, b_m \text{ real}$$

Solving the system $\frac{\partial\Theta}{\partial b} = \frac{\partial\Theta}{\partial a} = 0$ we obtain predictors with $\alpha_i = -\frac{1}{p}$, $0 \le i < p$, $\alpha_p = 1$, p = order of the formula and whose general form is:

$$\text{(II)} \qquad y_{n+p} - \frac{1}{p} \sum_{i=0}^{p-1} \alpha_i y_{n+i} = h \sum_{i=0}^{p-1} \beta_i f_{n+i}$$

and that gave us better results than the ones called "optimal" by Henrici, for $p = 2, 3$ and 4. These predictors are certainly stable since all roots of $\rho(z)$ satisfy definition 4.

Examples:

a) $p = 2$:

$$y_{n+2} - \frac{1}{2}\left\{y_{n+1} + y_n\right\} = \frac{h}{4}\left\{- f_n + 7f_{n+1}\right\}$$

b) $p = 3$

$$y_{n+3} - \frac{1}{3}\left\{y_{n+2} + y_{n+1} + y_n\right\} = \frac{h}{6}\left\{3f_n - 4f_{n+1} + 13f_{n+2}\right\}$$

We also tried other ways:

1st) by minimizing the coefficient c_{p+1}, of the last predictors, making $p = 2,3$ and 4, and keeping the α_i sufficiently near $-\frac{1}{p}$;
(for $p = 2,3$ see column 4 in tables I and II)

2nd) by considering $c_{p+1} = 0$ and resolving a problem of minimum with "side conditions", that is, trying to find a point of minimum $P = (\alpha_0, \alpha_1, \ldots, \alpha_{p-1}, \beta_0, \ldots, \beta_{p-1})$ for the function

$$\Theta = \sum_{i=0}^{p-1} (\alpha_i + \frac{1}{p})^2$$

with the conditions $c_0 = c_1 = \ldots = c_{p+1} = 0$. The α_i $0 \le i < p$ found are supposed to be reasonably near $-\frac{1}{p}$.

The formulae obtained with this process are unstable, as is proved in [2] . (results in column 3 in tables I an II).

These attempts, although producing satisfatory results in most cases, did not present greater accuracy then the predictor (II).

V. CONCLUSION

Based on the experiments performed, we arrieved at two important conclusions:

1st) It is always possible to find unstable predictors which give satisfatory results;

2nd) Among all predictors tested, the better ones are those whose general form is

$$y_{n+p} - \frac{1}{p}\left\{y_{n+p-1} + \ldots + y_0\right\} = h\left\{\beta_0 f_n + \beta_1 f_{n+1} + \ldots + \beta_{p-1} f_{n+p-1}\right\}$$

where the coefficients β_i are determined such that the resultant predictor has order p.

TABLE I

2^{nd} DEGREE PREDICTORS

FUNCTION	ORDER 2 $\alpha_0 = \alpha_1 = -\frac{1}{2}$ PREDICTOR STABLE (1)	ORDER 2 "OPTIMAL" PREDICTOR STABLE (2)	ORDER 3 PREDICTOR UNSTABLE (3)	ORDER 2 PREDICTOR STABLE (4)
$y' = y \cos x$	$\varepsilon = 0.003418$ $x = 2.0$	$\varepsilon = 0.914844$ $x = 7.7$	$\varepsilon = 0.003782$ $x = 2.0$	$\varepsilon = 0.003448$ $x = 2.0$
$y' = y$	$\varepsilon = 0.000026$ $x = 7.9$	$\varepsilon = -1.376045$ $x = 7.9$	$\varepsilon = 0.000027$ $x = 7.7$	$\varepsilon = 0.000029$ $x = 7.8$
$y' = \frac{-xy}{4x+16}$	$\varepsilon = 0.000153$ $x = 4.4$	$\varepsilon = 0.031122$ $x = 3.0$	$\varepsilon = 0.000152$ $x = 4.4$	$\varepsilon = 0.00015301$ $x = 4.4$

TABLE II

3rd DEGREE PREDICTORS

FUNCTION	ORDER 3 $\alpha_0=\alpha_1=\alpha_2=-\frac{1}{3}$ STABLE (5)	ORDER 3 "OPTIMAL" STABLE (6)	ORDER 4 UNSTABLE (7)	ORDER 2 STABLE (8)
$y' = y \cos x$	$\varepsilon = 0.000438$ $x = 7.9$	$\varepsilon = 0.000541$ $x = 7.9$	$\varepsilon = 0.00012156$ $x = 7.9$	$\varepsilon = 0.004386$ $x = 7.9$
$y' = y$	$\varepsilon = 0.00001526$ $x = 7.8$	$\varepsilon = 0.000014$ $x = 7.8$	$\varepsilon = 0.0000275$ $x = 6.8$	$\varepsilon = 0.00001621$ $x = 7.8$
$y' = \frac{-xy}{4x-16}$	$\varepsilon = 0.0000016$ $x = 0.3$	$\varepsilon = 0.0000017$ $x = 0.3$	$\varepsilon = 0.0000015$ $x = 7.8$	$\varepsilon = 0.0000016$ $x = 0.3$

Notes:

a) ε is the absolute value of the maximun error in each of the predictor used, $0 \le x \le 7{,}9$, in the point x indicated. Number in the column of the tables are referred to the above predictors:

(1) $$y_{n+2} = \frac{1}{2}\left\{y_{n+1} + y_n\right\} + \frac{h}{4}\left\{- f_n + 7f_{n+1}\right\}$$

(2) $$y_{n+2} = y_n + hf_{n+1}$$

(3) $$y_{n+2} = - 4y_{n+1} + 5y_n + h\left\{2f_n + 4f_{n+1}\right\}$$

(4) $$y_{n+2} = \frac{1}{240}\left\{121y_{n+1} + 119y_n\right\} + \frac{h}{480}\left\{839f_{n+1} - 121f_n\right\}$$

(5) $$y_{n+3} = \frac{1}{3}\left\{y_{n+2} + y_{n+1} + y_n\right\} + \frac{h}{6}\left\{3f_n - 4f_{n+1} + 13f_{n+2}\right\}$$

(6) $$y_{n+3} = y_n + \frac{h}{4}\left\{3f_n + 9f_{n+2}\right\}$$

(7) $$y_{n+3} = - 4y_{n+2} + 9y_{n+1} - 4y_n + \frac{h}{3} - \left\{5f_n - 2f_{n+1} + 13f_{n+2}\right\}$$

(8) $y_{n+3} = \frac{1}{3} y_{n+2} + \quad 239y_{n+1} + 241y_n \quad \frac{1}{720} + \quad \frac{h}{2160} \left\{ \frac{18719}{4} f_{n+2} \quad - \right.$

$$\left. - 1438f_{n+1} + \frac{4325}{4} f_n \right\}$$

b) The correctors used were:

1) For the 2nd degree formulae:

$$y_{n+1} = y_n + \frac{h}{2} \left\{ f_n + f_{n+1} \right\}$$

1st degree
2nd order

2) For the 3rd degree:

$$y_{n+2} = y_n + \frac{h}{3} \left\{ f_n + 4f_{n+1} + f_{n+2} \right\}.$$

2nd degree
3rd order

BIBLIOGRAPH

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[2] Dahlquist : " Convergence and Stability in the Numerical Integration of Ordinary Differential Equations" . Math. Scand. 4(1956) 33- B .