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NUMERICAL SOLUTION OF DIFFERENTIAL EQUATIONS USING OBRECHKOFF CORRECTOR FORMULAS

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16. Abstract

In this report we are concerned with the solution of differential equations by predictor-corrector formulas which give high-order accuracy. The corrector formulas are obtained from an extension of Obrechkoff's formula. These formulas are characterized by the fact that they contain higher derivatives of the unknown function y(x), and if their derivatives are readily determinable, fewer terms are needed for a given order as compared to other multistep methods which do not involve derivatives. Corresponding to these corrector formulas, certain new predictor, or extrapolation, formulas are suggested. These formulas also make use of the derivatives used in the corrector formulas.

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SUMMARY

In this report we are concerned with the solution of differential equations by predictor-corrector formulas which give high-order accuracy. The corrector formulas are obtained from an extension of Obrechkoff's formula. These formulas are characterized by the fact that they contain higher derivatives of the unknown function $y(x)$, and if their derivatives are readily determinable, fewer terms are needed for a given order as compared to other multistep methods which do not involve derivatives. Corresponding to these corrector formulas, certain new predictor, or extrapolation, formulas are suggested. These formulas also make use of the derivatives used in the corrector formulas.[1]

INTRODUCTION

A class of predictor-corrector formulas of higher-order accuracy for the initial value problem $y' = F(x, y)$ is presented here. The corrector formulas are based on results in a recent article [1] which gives an extension of a formula associated with the name of Obrechkoff [2]. The Obrechkoff formulas are characterized by the fact that they involve the higher derivatives of the unknown function $y(x)$. Corrector formulas with this property are not peculiar to the Obrechkoff formulas alone; less advantageously, corrector formulas can be obtained, for instance, by using the Euler-Maclaurin sum formula which also may be expressed in a form that involves the higher derivatives [2].

The great advantage in using Obrechkoff formulas is that generally correspondingly fewer terms are needed for a given order as compared to other formulas used in multistep methods which do not involve derivatives. This advantage is beneficial only if it is relatively easy to determine some of the higher-order derivatives. In some classes of problems this may be done by obtaining recursive formulas for the derivatives. For instance, this is

1. This work was done at the Computer Sciences Corporation under Contract NAS8-18405 for the NASA Computer Center.

the basis of the one-step method that Fehlberg [3] developed in which he combined a power series expansion for the solution with a Runge-Kutta process.

We should also remember another advantage characteristic of multistep predictor-corrector methods; that is, the difference between prediction and correction gives a reasonable estimate of the local truncation error which can be used for automatic step-size control.

THE EXTENDED FORMULA OF OBRECHKOFF

Let r, m, n be nonnegative integers, $r \leqq m$. Let $f(x) \in C^{m+n}[a,b]$ and suppose $f^{(m+n+1)}(x)$ exists and is R-integrable in $[a,b]$, then for every x in $[a,b]$ we have

$$f(x) - f(a) = \sum_{j=1}^{m} \frac{A_j}{j!} (x-a)^j f^{(j)}(a)$$
$$- \sum_{j=r+1}^{r+n} (-1)^j \frac{B_j}{j!} (x-a)^j f^{(j)}(x) + R(m,n,r) \quad , \tag{1}$$

where

$$A_j = \sum_{k=0}^{r} \frac{\binom{n+r}{k}\binom{m-r}{j-k}}{\binom{m+n}{j}} , \qquad 1 \leqq j \leqq m, \tag{2}$$

$$B_j = \frac{(-1)^r \binom{n+r}{j}\binom{j-1}{r}}{\binom{m+n}{j}} , \qquad r+1 \leqq j \leqq r+n, \tag{3}$$

and

$$R(m,n,r) = \frac{(-1)^n \binom{m+n}{r} \frac{(x-a)^{m+n+1}}{(m+n+1)!} f^{(m+n+1)}(\xi)}{\binom{m+n}{m-r}} \tag{4}$$

for some ξ, $a < \xi < x$.

If we set $y = f(x)$, $a = x_n$, and $x = x_{n+1}$ so that $x - a = h$, then if $y_s = f(x_s)$, equation (1) becomes

$$y_{n+1} - y_n = \sum_{j=1}^{m} A_j \frac{h^j}{j!} y_n^{(j)} - \sum_{j=r+1}^{r+n} (-)^j B_j \frac{h^j}{j!} y_{n+1}^{(j)} + R(m,n,r) \tag{5}$$

where A_j, B_j, and R are given by equations (2), (3), and (4).

For $r = 0$, equation (5) reduces to the formula of Obrechkoff, thus:

$$y_{n+1} - y_n = \sum_{j=1}^{m} A_j \frac{h^j}{j!} y_n^{(j)} - \sum_{j=1}^{n} (-)^j B_j \frac{h^j}{j!} y_{n+1}^{(j)} + R(m,n) \tag{6}$$

where

$$A_j = \frac{m!\,(m+n-j)!}{(m+n)!\,(m-j)!} \quad , \qquad 1 \le j \le m \tag{7}$$

$$B_j = \frac{n!\,(m+n-j)!}{(n-j)!\,(m+n)!} \quad , \qquad 1 \le j \le n \tag{8}$$

and

$$R_{m,n} = (-1)^n \frac{m!\,n!}{(m+n)!\,(m+n+1)!} h^{m+n+1} y^{(m+n+1)}(\xi) \quad , \qquad x_n < \xi < x_{n+1} \quad . \tag{9}$$

Whereas Taylor's expansion gives $f(x_{n+1})$ in terms of $f^{(\nu)}(x_n)$, $\nu = 0, 1, \ldots, m$, the above formula of Obrechkoff gives $f(x_{n+1})$ in terms of $f^{(\nu)}(x_n)$, $0 \le \nu \le m$, and $f^{(\nu)}(x_{n+1})$, $1 \le \nu \le n$. Thus, the formula of Obrechkoff may be looked upon as a two-point Taylor type expression of $f(x_{n+1})$ [4, 5] using the values of the function and its m derivatives at x_m and its first n derivatives at x_{n+1}. As a matter of fact, when $n = 0$, Obrechkoff's formula, equation (6), reduces to the usual Taylor expansion.

The special case where m = n in equation (6) deserves consideration. From equations (7) and (8), we get

$$A_j = B_j = \frac{m!}{2m!} \frac{(2m-j)!}{(m-j)!} \tag{10}$$

so that by equation (6)

$$y_{n+1} - y_n = \frac{m!}{(2m)!} \sum_{j=1}^{m} \frac{(2m-j)!}{(m-j)!} \frac{h^j}{j!} \left[y_n^{(j)} - (-)^j y_{n+1}^{(j)} \right] + R \quad , \tag{11}$$

whereby equation (9)

$$R = (-1)^m \frac{(m!)^2}{(2m)!(2m+1)!} h^{2m+1} y^{(2m+1)}(\xi), \quad x_n < \xi < x_{n+1} \quad . \tag{12}$$

For m = 2 and 3, as examples, equation (11) gives

$$y_{n+1} - y_n = \frac{h}{2} (y'_{n+1} + y'_n) - \frac{h^2}{12} (y''_{n+1} - y''_n) + \frac{h^5}{720} y^{iv}(\xi) \tag{13}$$

and

$$y_{n+1} - y_n = \frac{h}{2} (y'_{n+1} + y'_n) - \frac{h^2}{10} (y''_{n+1} - y''_n) + \frac{h^3}{120} (y'''_{n+1} + y'''_n) - \frac{h^7}{100,800} y^{vii}(\xi) \quad . \tag{14}$$

With appropriate predictor formulas these may be used as corrector formulas. For the application of equations (13) and (14) as predictor formulas in an n-body program see Reference 6.

PREDICTOR FORMULAS

Corresponding to each corrector formula we must find an appropriate predictor, or extrapolation, formula. Thus, as an example, in the corrector formula (13) for y_{s+1}, the unknown quantities y'_{s+1} and y''_{s+1} appear on the right and must be estimated from an appropriate extrapolation formula. Thus, in connection with this corrector formula (13), we can use

$$y_{s+1} = y_{s-1} + 2h\,y'_{s-1} + \frac{2h^2}{3}(2y''_s + y''_{s-1}) + \frac{2h^5}{45}\, y^{V}(\xi) \tag{15}$$

which we shall derive in order to illustrate how we can find predictor formulas to correspond to any Obrechkoff corrector formula. With the approximate value of y_{s+1}, from equation (15), we form $y'(x_{s+1}) = F(x_{s+1}, y_{s+1})$ and then use $y'' = dF/dx = F_x + F_y F$, etc. We can, of course, use recurrence formula where these are feasible [3]. For closer approximations, successive iterations between equations (14) and (15) may be made.

To obtain equation (15) we will use the method of undetermined coefficients. We anticipate the form of the desired formula using undetermined coefficients and then impose appropriate conditions on the formula which lead to a system of linear equations in the solvable coefficients. Thus, we start with

$$y_{s+1} - y_{s-1} = \int_{x_{s-h}}^{x_{s+h}} y'(x)\,dx = h(\alpha_0\, y'_s + \alpha_1\, y'_{s-1}) + h^2(\beta_0\, y''_s + \beta_1\, y''_{s-1}) + R \, , \tag{16}$$

and it is our purpose to obtain the coefficients and remainder in equation (15). We suppose that the remainder R is zero when $y = x^n$, $n = 0, 1, 2, 3,$ and 4 (hence, when $y(x)$ is a polynomial of degree ≤ 4). A simplification without a loss in generality follows if we take $x_n = 0$ and $h = 1$. We get

$$\begin{aligned} \alpha_0 + \alpha_1 &= 2 \\ \alpha_1 - (\beta_0 + \beta_1) &= 0 \\ 3\alpha_1 - 6\beta_1 &= 2 \\ \alpha_1 - 3\beta_1 &= 0 \, . \end{aligned} \tag{17}$$

An interpolation formula [7] is of interest here because, like the corrector formulas of Obrechkoff, it will give predictor formulas not only involving the functional values but as many derivatives as may be desired. When no derivatives are used, the formula reduces to the well-known Lagrange formula. The formulas are given by the following:

Let $f(x)$, together with its first $m+n+1$ derivatives, be continuous in an interval containing $x_0, x_1, \ldots, x_n$, where $x_i \neq x_j$. We define

$$c_i' = \frac{(m+n-i)!m!}{(m+n)!(m-i)!i!}$$

$$S_k = f(x_k) + \sum_{i=1}^{m} c_i' \, f^{(i)}(x_k)\,(x - x_k)^i \quad , \qquad k = 0, 1, 2, \ldots, n \quad . \tag{18}$$

$$R_k = (-1)^n \frac{m!n!(x - x_k)^{m+n+1}}{(m+n)!(m+1)!} \, f^{(m+n+1)}(\theta_k) \quad , \tag{19}$$

where θ_k lies somewhere between x and x_k.

$$R = \sum_{i=0}^{n} \prod_{j \neq i} \frac{x_j - x}{x_j - x_i} \, R_i \quad . \tag{20}$$

Under the conditions stated

$$f(x) = \sum_{i=0}^{n} \prod_{j \neq i} \frac{x_j - x}{x_j - x_i} \, S_i + R \quad . \tag{21}$$

The interpolation formula is obtained by using the right member of equation (21) with R omitted, which is the error due to using the formula.

It should be observed that the S_k as defined by equation (18) need not all contain the same number of derivatives. Thus, S_0 could contain m_0 derivatives, S_1 include m_1 derivatives, etc. However, this generalization does not affect the form of equation (21).

Finally we wish to explain that in actual practice, it is usually possible to estimate the accuracy of the formula by computing one or two of the R_i as indicated by the coefficients in equation (20).

If we assume equal intervals h between $x_0, x_1, \ldots, x_n$ and also that $x = x_{n+1}$, the above formulas are considerably simplified and are useful to our purposes.

A few examples will be given as illustrations. For instance, a fifth-order, three-point formula is obtained if we take $x = x_3$ and $n = m = 2$. Then

$$y_{n+1} = (y_{n-2} - 3y_{n-1} + 3y_n) + \frac{1}{2} h\,(3y'_{n-2} - 6y'_{n-1} + 3y'_n) + \frac{1}{4} h^2\,(3y''_{n-2} - 4y_{n-1} + y''_n) + R \tag{22}$$

where we have set $y = f(x)$ and

$$R = R_0 - 3R_1 + 3R_2$$

and

$$R_k = \frac{1}{5.4}\,(x_3 - x_k)^5\, y^{(v)}(\theta_k) \quad , \qquad k = 0, 1, 2$$

when θ_k lies between x_3 and x_k .

For use with Obrechkoff corrector formulas we would probably prefer a two-point predictor formula (though this is not necessary) in which case we take $n = 1$. Thus, for $x = x_2$ and $n = m = 1$, we get the third-order interpolation formula

$$y_{n+1} = (-y_{n-1} + 2y_n) + h\,(-y'_{n-1} + \frac{1}{2} y'_n) + R \tag{23}$$

where

$$R = -R_0 + 2R_1$$

and

$$R_k = \frac{-(x_2 - x_k)^3}{12} \; y''(\theta_k) \;, \qquad k = 0, 1$$

where θ_k lies between x_2 and x_k.

For $x = x_3$ and $n = 1, m = 3$, we get the fifth-order corrector formula

$$y_{n+1} = (-y_{n-1} + 2y_n) + \frac{1}{2} h(-y_{n-1} + 2y'_n) + \frac{1}{2} h^2(-y''_{n-1} + 2y''_n)$$

$$+ \frac{1}{3} h^3(-y'''_{n-1} + 2y'''_n) + R \qquad (24)$$

where

$$R = -R_0 + 2R_1$$

and

$$R_k = -\frac{(x_2 - x_k)^5}{480} \; y^{V}(\theta_k) \;, \qquad k = 0, 1$$

where θ_k lies between x_2 and x_k, so that

$$R = h^5 \left[\frac{1}{15} \; f^{V}(\theta_0) - \frac{1}{240} \; f^{V}(\theta_1) \right] \;, \qquad \begin{array}{l} x_0 < \theta_0 < x_2 \\ x_1 < \theta_1 < x_2 \end{array} \;. \qquad (25)$$

RECURRENCE FORMULAS FOR DERIVATIVES

As an example of the use of recurrence formulas for the higher derivatives of our differential equation, we will give an illustration using the Kepler problem:

$$\ddot{x} = \left(-\frac{k}{r^3} \right) x \qquad (26)$$

$$\ddot{y} = \left(-\frac{k}{r^3}\right) y \tag{27}$$

where

$$r^2 = x^2 + y^2 \quad . \tag{28}$$

Make the substitution:

$$u = -\frac{k}{r^3} \tag{29}$$

And we obtain the following set of equations:

$$\ddot{x} = u x \tag{30}$$

$$\ddot{y} = u y \tag{31}$$

$$r^2 = x^2 + y^2 \tag{32}$$

$$\dot{u} r + 3 \dot{r} u = 0 \quad , \tag{33}$$

where equation (33) is obtained by differentiating equation (29) with respect to t.

We now introduce the following power series expansions:

$$x = \sum_{n=0}^{\infty} X_n \, (t - t_0)^n \tag{34}$$

$$y = \sum_{n=0}^{\infty} Y_n \, (t - t_0)^n \tag{35}$$

$$u = \sum_{n=0}^{\infty} U_n \, (t - t_0)^n \tag{36}$$

$$r = \sum_{n=0}^{\infty} R_n \, (t - t_0)^n \tag{37}$$

where the coefficients are $X_n = \frac{1}{n!} \frac{dx^n}{dt^n}$, etc.

Introducing equations (34) and (36) into equation (30) and equating like powers of $(t - t_0)$ on both sides, we get a recurrence formula for the coefficients of equation (34). Proceeding in this way, we get the following set of recurrence formulas

$$
\begin{aligned}
X_{n+2} &= \frac{1}{(n+1)(n+2)} \left(\sum_{k=0}^{n} U_k X_{n-k} \right) \\
Y_{n+2} &= \frac{1}{(n+1)(n+2)} \left(\sum_{k=0}^{n} U_k Y_{n-k} \right) \\
R_n &= \frac{1}{2R_0} \left(\sum_{k=0}^{n} X_k X_{n-k} + \sum_{k=0}^{n} Y_k Y_{n-k} - \sum_{k=1}^{n-1} R_k R_{n-k} \right) \\
U_{n+1} &= - \frac{1}{(n+1) R_0} \left(\sum_{k=1}^{n} k U_k R_{n+1-k} + 3 \sum_{R=1}^{n+1} k R_k U_{n+1-k} \right)
\end{aligned}
\tag{38}
$$

A similar, but somewhat more complex, example may be found in Reference 3.

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Marshall Space Flight Center, Alabama 35812, September 3, 1969
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