THE CORRECTION DIFFERENCE METHOD FOR NON-LINEAR BOUNDARY VALUE PROBLEMS OF CLASS M.

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1. INTRODUCTION

A thouroug discussion on the practical aspects of the difference correction method can be found in Fox [1957] and Fox [1961], where the method is applied to a wide variety of problems. Considering boundary value problems for the Poisson equation in two dimensions Bickley, Michaelson and Osborne [1961] have pointed out some theoretical aspects of the difference correction when applied to that problem.

This paper will deal with the theory and application of the correction difference method to boundary value problems of class M, i.e.,

$$(1.1) \qquad y'' = f(x, y), \quad y(a) = \alpha, \quad y(b) = \beta$$

with some additional hypotheses on $f(x, y)$.

In Henrici's book, "Discrete variable methods in ordinary differential equations" [1962], p. 377, it is indicated that, if a difference correction is added to an approximate solution of (1.1) then the order of the discretization error is improved in two units. After giving some notation in Section 2, the asymptotic behavior of the discretization error is discussed in Section 3, folowing the lines of Henrici with certain changes which make it more general, and allow us to introduce several ways of performing the difference correction.

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In Section 4 the h^2 improvement property of a generalized difference correction is proved.

In Section 5 two possibilities (different from the classical) are investigated for the case $p = 2$, and in Section 6 numerical results and comparisons with other methods are presented.

2. NOTATION AND KNOWN RESULTS

As we want to use several results by Henrici [1962] Chapter 7, and we prefer to avoid repeated references, we will adopt its notation and we will give a summary of these results.

A non linear boundary value will be called of class M, if it is of the form (1.1) and, a) the initial value problem $y' = f(x, y)$ $y(a) = \alpha$ $y'(a) = A$, with A arbitrary, has a unique solution. b) $f_y(x, y)$ is continuous and

$$(2.1) \qquad f_y(x,y) > 0 \quad \text{for} \quad a \leqq x \leqq b, \quad -\infty \leqq y \leqq \infty .$$

It is proved then that a problem of class M always has an unique solution.

The finite difference approximations that we will discuss are of the form

(2.2)

$$-y_{n-1} + 2y_n - y_{n+1} + h^2 \{ \beta_0 f_{n-1} + \beta_1 f_n + \beta_2 f_{n+1} \} = 0$$
$$n = 1, 2, \ldots, N-1$$

where $\beta_0 + \beta_1 + \beta_2 = 1$, $\beta_0 = \beta_2$, $h = (b-a)/N$ (N integer)

$y_0 = \alpha$, $y_N = \beta$ and the rest is standard notation. The limitation of taking this kind of equations appears naturally if we do not want to consider grid points outside of the interval $[a, b]$. By introducing some special matrices and vectors, part of the following discussion can be simplified. In fact, let the symbols y, f (y) and α represent the vectors whose components are $(y_1, y_2 \ldots\ldots, y_{n-1})$, $(f(x_1, y_1), f(x_2, y_2), \ldots, f(x_{n-1}, y_{n-1}))$

and $(\alpha - \beta_0 h^2 f(x_0, \alpha), 0, \ldots, 0, \beta - \beta_0 h^2 f(x_N, \beta))$

respectively; furthermore let the symbol J represent the matrix where all the main diagonal elements are equal to 2, all the elements of the adjacent diagonals are equal to —1 and the rest of the elements equal to zero and let B be the matrix where the elements of the main diagonal ar e equal to β_1, the elements of the lower adjacent diagonal are equal to β_2, those of the upper adjacent diagonal are equal to β_2 and the rest of the elements equal to zero. Finally let F (y) be the diagonal matrix whose non zero elements are equal to $f'(x_1, y_1)$, $f'_y(x_2, y_2), \ldots,$ $f'_y(x_{n-1}, y_{n-1})$

Formula (2 .2) can now be written,

$$\text{(2.4)} \qquad \mathrm{J}\mathrm{y} + h^2\,\mathrm{B}\mathrm{f}(\mathrm{y}) - \mathrm{a} = 0$$

where the vector a takes care for the boundary values.

A Newton type iteration used to solve the system of non-linear equations (2.4) is insured to be convergent under certain restrictions, mainly on the first approximation and on the step length h (Henrici, Th. 7.7, p. 373). If the first approximation is called $\mathrm{y}^{(0)}$, then the formulas for Newton method are in this case,

$$\text{(2.5)} \qquad \mathrm{r}(\mathrm{y}^{(i)}) = \mathrm{J}\mathrm{y}^{(i)} + h^2\,\mathrm{B}\mathrm{f}(\mathrm{y}^{(i)}) - \mathrm{a}$$

$$\text{(2.6)} \qquad \Delta\mathrm{y}^{(i)} = -\,(\mathrm{J} + h^2\,\mathrm{B}\mathrm{F}(\mathrm{y}^{(i)}))^{-1}\,\mathrm{r}(\mathrm{y}^{(i)})$$

and finally,

$$\text{(2.7)} \qquad \mathrm{y}^{(i+1)} - y^{(i)} + \Delta\mathrm{y}^{(i)}$$

If the computed approximation is called y*, and the exact solution of (1.1) is called y, then theorem 7.8, p. 374 gives for the components of the discretization error, e = y* — y the following bound,

$$\text{(2.8)} \qquad |\,\mathrm{e}_n\,| \leq \frac{(x_n - a)\ \ (b - x_n)}{2}\,(c\ h^p + K\,h^q)$$

where c is a constant which depends on the method and on the problem itself, and p is the order of the method. K and q are arbitrary non negative constants which stem from the assumption that the Newton iteration is stopped when the components of the residual vector satisfy

$$(2.9) \qquad | r_n | \leqq K h^{q+2}$$

This is a very important practical fact, because it permits us to perform an incomplete iteration (the only possible kind in actual computation) before applying the difference correction technique. We will assume that $q > p + 4$ in order to avoid interference of this term in the discussion of the discretization error.

A difference operator $L[y(x);h]$ is naturally associated with the difference scheme (2.2),

$$(2.10) \qquad L[y(x) ;h] = -y(x_{n-1}) + 2y(x_n) - y(x_{n-1}) + \\ + h^2 \{\beta_0 y''(x_{-1}) + \beta_1 y''(x_n) + \beta_2 y''(x_{n+1}) \}.$$

$L[y(x);h]$ operates on all functions $y(x)$ sufficiently differentiable. By expanding in Taylor series all the terms of (2.10) it is possible to find,

$$(2.11) \qquad L[y(x) ;h] = h^{p+2}C_{p+2}\, y^{(p+2)}(x) + \\ + h^{p+4}C_{p+4}\, y^{(p+4)}(x) + 0(h^{p+6}),$$

where p is called the order of the method.

3. ASYMPTOTIC BEHAVIOR OF THE DISCRETIZATION ERROR

Following the lines of Henrici, pp. 375-377, we will now derive an expression for the discretization error which will be useful in the discussion of the difference correction method.

We recall that, if formula (2.2) is used as a finite difference approximation to problem (1.1), and y is the approximate solution of the systems of equations, then the discretization error, $e_n = y_n - y(x_n)$ $(n = 0,1, \ldots, N)$ satisfies 2.8). We will assume that $p \geqq 2$ and that the exact solution $y(x)$ is $(p+6)$ times continuously differentiable.

Therefore

$$f(x_n, y_n) - f(x_n, y(x_n)) = f_y(x_n, y(x_n)) \, (y_n - y(_n)) + 0(h^{2p})$$

or, by calling $g_n = f_y(x_n, y(x_n))$,

$$f(x_n, y_n) - f(x_n, y(x_n)) = g_n \cdot e_n + 0(h^{2p}). \tag{3.1}$$

As $\beta_0 + \beta_1 + \beta_2 = 1$ and $\beta_0 = \beta_2$ we get,

(3.2)

$$y^{(p+2)}(x_n) = \beta_0 \, y^{(p+2)}(x_{n-1}) + \beta_1 \, y^{(p+2)}(x_n) + \beta_2 \, y^{(p+2)}(x_{n+1}) \\ - \beta_0 \, h^2 \, y(^{(p+4)}(x_n) + 0(h^4).$$

Now we will construct a difference equation for the discretization error, by subtracting (2.11) from (2.2)

$$- y_{n-1} + 2\, y_n - y_{n+1} + h^2 (\beta_0 \, f_{n-1} + \beta_1 \, f_n + \beta_2 \, f_{n+1}) - \\ - L[y(x), h] = - h^{p+2} \, C_{p+2} \, y^{(p+2)} \, (x) - h^{p+4} \, C_{p+4} \, y^{(p+4)} \, (x) + \\ + 0 \, (h^{p+6}).$$

Or

$$- e_{n-1} + 2\, e_n - e_{n+1} + h^2 \{ \beta_0 \, (f_{n-1} - f(x_{n-1}, y(x_{n-1}))) + \\ + \beta_1 \, (f_n - f(x_n, y(x_n))) + \beta_2 (f_{n+1} - f\,(x_{n+1}, \, y\,(x_{n+1}))) \} = \\ = - h^{p+2} \, C_{p+2} \, y^{(p+2)} \, (\mathrm{x}) - h^{p+4} \, C_{p+4} \, y^{(p+4)} \, (x) + 0 \, (h^{p+6}).$$

Using now the relation (3.1), dividing through by h^p and defining *the magnified error* $\bar{e}_n = h^{-p} \, e_n$ we get,

$$- \bar{e}_{n-1} + 2\, \bar{e}_n - \bar{e}_{n+1} + h^2 \{ \beta_0 \, g_{n-1} \, \bar{e}_{n-1} + \beta_1 \, g_n \, \bar{e}_n + \\ + \beta_2 \, g_{n+1} \, \bar{e}_{n+1} + 0(h^p) \} = - h^2 \, C_{p+2} \, y^{(p+2)} \, (x) - \\ - h^4 \, C_{p+4} \, y^{(p+4)} (x) + 0(h^6). \tag{3.3}$$

Introducing now (3.2) and defining,

$$\Phi_n = g_n \, \bar{e}_n + y^{(p+2)}(x_n) \, C_{p+2} \tag{3.4}$$

(3.3) is transformed in,

$$- \bar{e}_{n-1} + 2\, \bar{e}_n - \bar{e}_{n+1} + h^2 \, (\beta_0 \, \Phi_{n-1} + \beta_1 \, \Phi_n + \beta_2 \, \Phi_{n+1}) = \\ = h^4 \, (C_{p+2} \, \beta_0 - C_{p+4}) \, y^{\,(p+4)} \, (x_n) + 0 \, (h^6). \tag{3.5}$$

If we solve the boundary value problem of class M,

$$(3.6) \qquad e''(x) = g(x)\, e(x) + C_{p+2}\, y^{(p+2)}(x)$$
$$e(a) = e(b) = 0$$

by the method (2.2), we will obtain equations (3.5) with zeros in the right hand sides. Then, by (2.8) we get,

$$(3.7) \qquad e_n = e(x_n)\, h^p + 0(h^{p+2}), \text{ or}$$

$$(3.8) \qquad y(x_n) = y_n - h^p\, e(x_n) + 0(h^{p+2})\,.$$

4. THE DIFFERENCE CORRECTION

In this section we will establish a sharper formula for the discretization error which will allow us to write,

$$y(x_n) = y_n - h^p\, e_n^* + 0(h^{p+2})\,.$$

where e_n^* is a computable quantity.
We will show that, if in (3.5) $y^{(p+2)}(x_n)$ is replaced by an approximate expression $A(x_n)$, which satisfies,

$$(4.1) \qquad y^{(p+2)}(x_n) = A(x_n) + B(x_n)\, h^2 + 0(h^4)\,,$$

where $B(x)$ is a sufficiently differentiable function, then it is possible to write,

$$(4.2) \qquad y(x_n) = y_n - h^p\, e_n^* + h^{p+2}\, \eta(x_n) + 0(h^{+}{}_{4})$$

in which

$$\eta(x_n) = (e_n^* - e(x_n))\, h^{-2} + 0(h^2)$$

and e_n^* is the solution of (3.5) whit $A(x_n)$ instead of $y^{(p+2)}(x_n)$ and the right hand side equal to zero.

First we define $\Phi_n^* = f_y(x_n, y_n)\, e_n^* + C_{p+2}\, A(x_n)$ and

(4.3)

$$- e^*_{n-1} + 2\, e^*_n - e^*_{n+1} + h^2\, (\beta_0\, \Phi^*_{n-1} + \beta_1\, \Phi^*_n + \beta_2\, \Phi^*_{n+1}) = 0\,.$$

We can also write,

$$(4.4)\quad -e(x_{n-1}) + 2\,e(x_n) - e(x_{n+1}) + h^2\,(\beta_0\,\Phi_{n-1} + \beta_1\,\Phi_n + \\ + \beta_2\,\Phi_{n+1}) = h^4(C_{p+2}\,\beta_0\,y^{(p+4)}(x_n) - C_{p+4}\,y^{(p+4)}\,(x_n)) + 0(h^6)$$

where

$$\Phi_n = f_y(x_n, y(x_n))\; e(x_n) + C_{p+2}\,y^{p+2}(x_n)\;.$$

Since,

$$f_y(x_n, y_n)\; e_n^* - f_y(x_n, y(x_n)) - f(x_n, y(x_n)))e(x_n) = \\ = f_y(x_n, y_n)\;(e_n^* - e(x_n)) + f_y(x_n, y_n)\,e(x_n) = \\ = f_y(x_n, y_n)\;\tilde{\eta}_n + f_{yy}(x_n, y(x_n))\;h^p\,e^2(x_n) + 0(h^{p+2})$$

with $\qquad \tilde{\eta}_n = e_n^* - e(x_n)\;,$

By subtracting (4.3) from (4.4) we get

(4.5)

$$-\tilde{\eta}_{n-1} + 2\,\tilde{\eta}_n - \tilde{\eta}_{n+1} + h^2 \sum_{i=-1}^{1} \beta_{i+1}\,\{\,f_y(x_{n+i}, y_{n+i})\;\tilde{\eta}_{n+i} + \\ + f_{yy}(x_{n+i}, y(x_{n+i}))\;h^p\,e^2(x_{n+i}) - C_{p+2}\,B(x_{n+i})h^2\,\} = \\ = -\,h^4\,y^{(p+4)}\,(x_n)\;\;(C_{p+2}\,\beta_0 - C_{p+4}) + 0\;(h^6)\;.$$

As we do not want terms in h^4 on the right hand side of (4.5), we will further transform it. Dividing through by h^2 and defining $\eta_n = \tilde{\eta}_n/h^2$, we get

$$-\eta_{n-1} + 2\,\eta_n - \eta_{n+1} + h^2 \sum_{i=-1}^{1} \beta_{i+1}\,[f_y(x_{n+i},\; y_{n+i})\;\eta_{n+i} + \\ + f_{yy}\,(x_{n+i}, y_{n+i})\;h^{p-2}\;\;e^2(x_{n+i}) - C_{p+2}\;\;B(x_{n+i})] = \\ = -\,h^2\,y^{(p+4)}\,(x_n)\;\;(C_{p+2}\,\beta_0 - C_{p+4}) + 0(h^4)\;.$$

By the properties of β_i, we van write,

$$y^{(p+4)}\,(x_n) = \beta_0\,y^{(p+4)}\,(x_{n-1}) + \beta_1\,y^{(p+4)}\,(x_n) + \\ + \beta_2\,y^{(p+4)}\,(x_{n+1}) + 0(h^2)$$

Finally, (4.5) becomes

(4.6)

$$-\eta_{n-1} + 2\eta_n - \eta_{n+1} + h^2 \sum_{i=-1}^{1} \beta_{i+1} [f_y (x_{n+i}, y_{n+i}) \eta_{n+i} + \\ + f_{yy} (x_{n+i}, y_{n+i}) h^{p-2} e^2 (x_{n+i}) - C_{p+2} B(x_{n+i}) + \\ + (C_{p+2} \beta_0 - C_{p+4}) y^{(p+4)} (x_{n+i})] = 0(h^4) .$$

Consequently, the continuous function $\eta(x)$, which satisfies the boundary value problem of class *M*,

(4.7)

$$\eta''(x) = f_y (x, y) \eta + f_{yy} (x, y) h^{p-2} e^2(x) - C_{p+2} B(x) + \\ + (C_{p+2} \beta_0 - C_{p+4}) y^{(p+4)} (x) , \eta(a) = \eta(b) = 0$$

differs in $0(h^2)$ from η_n, the solution of (4.6) with the right hand side equal to zero. Thus,

$$e_n^* - e(x_n) = \bar{\eta}_n = \eta_n h^2 = \eta(x_n) h^2 + 0(h^4)$$

or

$$e(x_n) = e_n^* - \eta(x_n) h^2 + 0(h^4)$$

and

$$y(x_n) = y_n - h_p e_n^* + h^{p+2} \eta(x_n) + 0(h^{p+4})$$

as we wanted to prove.

Summarizing, the complete procedure to obstain an h^{p+2} order in the discretization error is,

1) Compute y_n $(n = 0,1, \ldots, N)$ by the method of order p given by formula (2.2). The iteration in Newton method can be stopped when the residuals are less than $K h^{p+2}$.
2) Compute $-h^p e_n^*$ by using (4.3), and add this quantity to y_n. The new approximation will hold (4.2).

The remaining discussion will deal with some possible choices for the approximation (4.1).

The classical choice is,

$$(4.8) \qquad A(x_n) = h^{-p-2} \quad \delta^{p+2}\, y_{n+q+1} \quad (p = 2q)$$

By (3.8)

$$\delta^{p+2}\, y_{n+q+1} = h^{p+2}\, y^{(p+2)}\,(x_n) + h^{p+4}\, B^{(p+2)}\,(x_n + 0(h^{p+6})$$

where we have assumed enough differentiability on $y(x)$.

In this case the quantity $h^p\, e_n{}^*$ is called the difference correction by Fox [1957].

By extension we will keep calling difference correction to any quantity computed in this way, whatever the approximation $A(x)$ be.

In the next Section we will give two more expressions for $A(x)$ in the case $p = 2$. We will also show there, that the use of the difference correction instead of a direct formula with the same order, results in less computational work for the same accuracy. There are two reasons for this saving; on one side the formula used in the Newton iteration is much simpler and on the other side, the number of iterations needed is smaller. That is explained since, when the difference correction is used, the q of (2.9) has only to be equal to $p + 2$, while in the other case it has to be at least $p + 4$.

5. TWO EXPRESSIONS FOR THE CORRECTION TERM

As we are considering the equation,

$$y'' = f(x, y)$$

and we want to approximate $y^{(4)}\,(x)$ $(p = 2)$, a natural idea is to consider,

$$(5.1) \qquad y^{(4)}\,(x) = \frac{d^2 f(x, y(x))}{dx^2}$$

which immediately gives place to two new forms for $A(x)$. We will prove they are valid expressions, in the sense that they satisfy (4.1).

i) Consider first

$$A(x) = h^{-2}\delta^2 f(x_n, y_n). \tag{5.2}$$

We want to prove that, if

$$y_n = y(x_n) + h^2 e(x_n) + 0(h^4) \tag{5.3}$$

then,

$$\frac{d^{(4)} y(x)}{dx} = \frac{d^2 f(x, y(x))}{dx} = \frac{\delta^2 f(x_n, y_n)}{h^2} + 0(h^2). \tag{5.4}$$

If we were using $y(x_n)$ instead of y_n then (5..4) mould be trivially true, but as y_n only satisfies (5..3), some manipulations are needed. We have

$$\frac{d^2 f(x, y(x))}{dx^2} = f_{xx} + 2 f_{zy} y' + f_{yy} (y')^2 + f_y y'' \tag{5.5}$$

On the other hand,

(5..6) $\quad \delta^2 f(x_n, y_n) = f(x_{n-1}, y_{n-1}) - 2 f(x_n, y_n) + f(x_{n+1}, y_{n+1})$
and by developing in Taylor series we get

(5.7)

$$\begin{aligned}\delta^2 f(x_n, y_n) = {} & (\delta^2 y_n) f_y(x_n, y(x_n)) + h\,(y_{n+1} - y_{n-1}) + \\ & f_{xy}(x_n, y(x_n)) + [(y_{n-1} - y(x_n))^2 + (y_{n+1} - y(x_n))^2 - \\ & - 2(y_n - y(x_n))^2] + \frac{1}{2} f_{yy}(x_n, y(x_n)) + h^2 f_{xx}(x_n, y(x_n) + 0(h^4)\end{aligned}$$

The coefficient of f_{yy} can be expressed in a more convenient way. By using (5.3),

$$\begin{aligned}&(y_{n-1} - y(x_n))^2 + (y_{n+1} - y(x_n))^2 - 2(y_n - y(x_n))^2 = \\ &\qquad = (y(x_{n-1}) - y(x_n) + h^2 e(x_{n-1}))^2 + \\ &+ (y(x_{n+1}) - y(x_n) + h^2 e(x_{n+1}))^2 + 0(h^4) = \\ &\qquad = \left(-y'(x_n)\,h + \left[\frac{1}{2} y''(x_n) + e(x_{n-1})\right] h^2\right)^2 + \\ &+ \left(y'(x_n)\,h + \left[\frac{1}{2} y''(x_n) + e(x_{n+1})\right] h^2\right)^2 + 0(h^4)\end{aligned}$$

and the final expression is,

$$(5.8) \qquad (y_{n-1} - y(x_n))^2 + (y_{n+1} - y(x_n))^2 - 2(y_n - y(x_n))^2 = \\ = 2\,(y'(x_n))^2 h^2 + 0(h^4)$$

Then (5.7) and (5.8) imply,

$$\frac{\delta^2 f\,(x_n, y_n)}{h^2} = f_{xx}\,(x_n, y(x_n)) + \frac{\delta^2\, y_n}{h^2}\, f_y(x_n, y(x_n)) + 2\frac{y_{n+1} - y_{n-1}}{2h} \cdot \\ \cdot f_{xy}(x_n, y(x_n)) + (y'(x_n))^2\, f_{yy}(x_n, y(x_n)) + 0(h^2) = \\ = \frac{d^2 f}{dx^2}\,(x_n, y(x_n)) + 0(h^2)$$

which proves (5.4)

An inmediate advantage of using $\delta^2 f$ instead of $\delta^4 y$ is, that no external values are required to compute the difference at points close to the boundary, avoiding the use of special formulas and information unrelated with the problem.

Since the values $f(x_n, y_n)$ are already computed (from the last iteration in the solution of (2.2)) no extra work is necessary and there is always less computation in carrying the second differences compared with the fourth.

ii) In cases in which $f(x, y)$ is easily differentiated, it would be worth to use the approximation,

$$(5.9) \qquad A(x_n) = f_{xx}(x_n, y_n) + f_{xy}(x_n, y_n)\, \frac{y_{n+1} - y_{n-1}}{h} + \\ + f_{yy}(x_n, y_n)\, \frac{(y_{n+1} - y_{n-1})^2}{4h^2} + f_y(x_n, y_n)\, f(x_n, y_n)$$

For instance, if $f(x, y)$ is independent of x, (5.9) becomes

$$A(x_n) = f_{yy}(x_n, y_n)\, \frac{(y_{n-1} - y_{n+1})^2}{4h^2} + f_y(x_n, y_n)\, f(x_n, y_n)$$

If $f(x,y) = g(x)\, y + h(x)$ then,

$$A(x_n) = g''(x_n)\, y_n + g'(x_n)\, \frac{y_{n+1} - y_{n-1}}{h} + g^2\,(x_n)\, y_n + h'\,(x_n)$$

and so on.

The prof that (5.9) is an approximation to $y^{(4)}(x)$ of order at least h^2 goes in the same fashion as the proof for (5.2).

6. NUMERICAL RESULTS AND COMPARISON OF DIFFERENT METHODS.

We will now state two other finite difference procedures, the Numerov-Milne fourth order approximation, and a truncated version of the Fox difference correction. After that, we will compare them with the two methods described in the previous section and with a shooting type technique.

The Numerov-Milne fourth order method is,

(6.1) $$\mathrm{J}\mathrm{y} = -h^2\, \mathrm{B}\mathrm{f}(x,y) + \mathrm{a}$$

with $\beta_0 = \beta_2 = 1/12, \quad \beta_1 = 10/12.$

B can also be written as,

$$\mathrm{B} = \mathrm{I} - \frac{1}{12}\,\mathrm{J}.$$

The Fox difference correction with fixed fourth order length uses first, a second order approximation given by the solution of,

(6.2) $$Jy = -h^2 f(x, y) + a,$$

then one difference correction, in the form

(6.3) $$Je = -h^2\, F\,(x,y,e - \frac{1}{12}\, J^2\, y)$$

and finally.

(6.4) $$\mathrm{y} = \mathrm{y} + h^2\, \mathrm{e}$$

Thus, the use of fourth differences makes it necessary to compute external values for y. Fox suggests the use of equation (6.2) to extrapolate values out of the interval of integration, giving the two special formulas,

$$y_{-1} = 2\,\alpha - y_1 + h^2 f(a, \alpha)$$

(6.5)

$$y_{N+1} = 2\,\beta - y_{N-1} + h^2 \mathrm{f}\,(b, \beta)$$

Equations (6.1) and (6.2) through (6.5) will be referred to as Methods I and II, respectively. Methods III and IV will be the ones which stem from formulas (5.2) and (5.9).

The procedure used for these methods is similar to the one used for Method II, the change appearing in equation (6.3). For Method III we get instead of (6.3),

$$\mathrm{J\,e} = -h^2\,\mathrm{F}\,(x, \bar{\mathrm{y}})\,\mathrm{e} + \frac{1}{12}\,\mathrm{J\,f}\,(x, \bar{\mathrm{y}}) \tag{6.6}$$

Method IV expressed in components is,

(6.7)

$$- e_{n-1} + 2\,e_n - e_{n+1} = h^2 f_y(x_n\,\bar{y}_n)\,e_n - \frac{1}{12}\Big[\,h^2 f_{xx}\,(x_n, y_n) +$$

$$+ h\,f_{xy}\,(x_n, \bar{y}_n)\,(\bar{y}_{n+1} - \bar{y}_{n-1}) + \frac{1}{4}\,f_{yy}\,(x_n\,\bar{y}_n)\,(\bar{y}_{n+1} - \bar{y}_{n-1})^2$$

$$+ h^2 f_y\,(x_n, \bar{y}_n)\,f\,(x_n, \bar{y}_n)\,\Big]\,.$$

In spite of its complicated aspect, method IV turns out to be the fastest and the most accurate whenever the partiel derivatives of $f\,(x, y)$ are simple and can be calculated easily.

Now we want to point out a common feature of the methods using the correction difference. We recall that if Newton's method is used to solve (6.2) the formulas are (care has to be taken on the boundary points),

$$\mathrm{r}(\mathrm{y}^{(i)}) = \mathrm{J}\mathrm{y}^{(i)} + h^2\,\mathrm{f}(\mathrm{x}, \mathrm{y})^{(i)}) \tag{6.8}$$

$$\triangle\,\mathrm{y}^{(i)} = -\,(\mathrm{J} + h^2\,\mathrm{F}\,(\mathrm{y}^{(i)}))^{-1}\,\mathrm{r}\,(\mathrm{y}^{(i)}) \tag{6.9}$$

and

$$\mathrm{y}^{(i+1)} = \mathrm{y}^{(i)} + \triangle\mathrm{y}^{(i)}\,. \tag{6.10}$$

In solving either the linear systems (6.3), (6.6) or (6.7) we equations which resemble very much those above. In fact, the changes are: in the expressions for $r(y^{(i)})$; (6.10) becomes $y^{(i+1)} = y^{(i)} - h^2 \triangle y^{(i)}$ and only one iteration is required.

The $r(y)$ corresponding to (6.3), (6.6) and (6.7) are respectively,

$$r(y) = -\frac{1}{12h^2} J^2 \bar{y} \tag{6.11}$$

$$r(y) = -\frac{1}{12} J f(x, \bar{y}) \tag{6.12}$$

$$r(y) = -\frac{1}{12} A \tag{6.13}$$

In (6.13), A stands for the matrix obtained from the second term in the right-hand side of (6.7).

Thus, if the correction difference is combined with Newton's method in the earlier stages, practically the same code can be used in both parts. We have written an Extended Algol program for the B5000 at Stanford which took advantage of this situation. The program modifications for the different methods were very slight, and the procedure followed in the numerical comparisons has been to introduce these modifications in the most direct fashion.

Another important observation, from the time consuming point of view, is that the quantities $f(x, y)$ and $F(x, y)$ do not have to be computed again in order to perform difference correction since the values calculated for the last iteration of the Newton method are in general good enoug, and no noticeable improvement is observed when these values are recomputed.

We have chosen as our first example a problem which has a known analytical solution and is completely worked out in Collatz [1960] pp. 145-147. The method used there is a combination of shooting and interpolation which, at least in this fashion, does not seem to be very suitable for automatic computation.

By using the same step length, $h = 1/5$, we have computed pproximate solutions with the four methods described above.

The problem is,

$$y'' = \frac{3}{2} y^2; \quad y(0) = 4, \quad y(1) = 1 \tag{6.14}$$

with one solution equal to

(6.15) $$y(x) = \frac{4}{(1+x)^2}$$

In all the methods the first guess $y^{(0)}$ was constructed from a linear interpolation of the given data

$$y^{(0)}(x) = -3x + 4 .$$

In Table I the values of the five approximate solutions are given; and in Table II information about number of iterations, computing time, and deviation from the true solution is recorded. The subscripts stands for the numbering we have given to the different methods. Method V is the one used in Collatz and $y(x)$ is the exact solution (6.15).

TABLE I

x	$y(x)$	y_I	y_{II}	y_{III}	y_{IV}	y_V
0	4.00000	4.00000	4.00000	4.00000	4.00000	4.00000
0.2	2.77778	2.77680	2.77718	2.77719	2.77757	2.79464
0.4	2.04082	2.03995	2.04019	2.04019	2.04054	2.05787
0.6	1.56250	1.56191	1.56202	1.56202	1.56226	1.57519
0.8	1.23457	1.23427	1.23431	1.23431	1.23443	1.24138
1.0	1.00000	1.00000	1.00000	1.00000	1.00000	1.00003

TABLE II

	y_I	y_{II}	y_{III}	y_{IV}	y_V
Number of Interations in Newton Part.	4	3	3	3	—
$\Vert y(x) - y_{APR.}\Vert_2$	9.75×10^{-4}	6.29×10^{-4}	6.27×10^{-4}	2.74×10^{-4}	293×10^{-4}
Computation time in second (1)	1.70	1.63	1.62	1.63	—

(1) In the Burroughs B5000 at Stanford Computation Center.

It is observed that this is a problem in which method IV is fairly convenient. In fact, (6.13) becomes

$$r_n(\overline{y}) = -\frac{1}{12}\,(0.75\,(\overline{y}_{n-1} - \overline{y}_{n+1})^2 + h^2\,4.5\,\overline{y}_n{}^3)$$

Method V is included as a matter of reference, but no attempt is made in comparing it with the finite differences type procedures since they are completely different in principle.

Methods I through IV have been numbered in order of increasing speed and accuracy. There is no discussion about the accuracy in this example. One word to be said about the speed. The figures in the third row of Table II show that the computation time was practically the same in all four methods with a tiny seven hundreth of a second in favor of the difference correction. This situation will also be noted in the second problem presented at the end of this section. However, we can mention some reasons which lead us to believe that the ordering is also meaningful in so far as computational speed is concerned.

The solution by Newton's method of the system (6.1) is much more complicated than the solution of (6.2) which is basic for all the methods using the difference correction. Moreover, as was mentioned in Section IV, the requirements of precision in these latter methods are less than for the Numerov-Milne method. That implies, that in general less iterations can be expected for methods II, III, and IV than for method I. That is shown in the first row of Tables II and IV. Of course, one more iteration (the difference correction) has to be counted, but in general, as can be seen in formulas (6.11) (6.12) and (6.13), this iteration involves less computation than the one corresponding to the regular Newton formulas. That is more noticeable after recalling that f and F do not have to be recomputed for this correction.

A last remark is that all the linear systems involved in this discussion are tridiagonal, and a simplified Gauss-type elimination procedure can be used, saving both computation and storage (see, for instance, Henrici [1962] pp. 351-354, or D. T. Thurnau [1963]).

To finish with this section, we present another example which behaves in the same fashion as the first one.

$$y'' = -e^{-2y}; \qquad y(1) = 0, \qquad y(2) = ln(2).$$

The exact solution is $y(x) = ln$ (x).

The step length used was $h = 1/16$, and in Tables III and IV we give the numerical results corresponding to the nodal points $x = 1, 1.25, 1.5, 1.75$.
Since

$$f(x, y) = -e^{-2y}; \quad f_y(x, y) = 2\, e^{-2y}; \quad f_{yy}(x, y) = -2 f_y(x, y)$$

(6.13) becomes

$$r_n(\bar{y}) = -\frac{1}{6} f_y(x_n, \bar{y}_n)\, [h^2 f_y(x_n, \bar{y}_n) - (\bar{y}_{n+1} - \bar{y}_{n-1})^2]$$

TABLE III

x	$y(x)$	y_I	y_{II}	y_{III}	y_{IV}
1	0	0	0	0	0
1.25	0.223143551	0.223143676	0.223143656	0.223143656	0.223143525
1.50	0.405465108	0.405465223	0.405465209	0.405465209	0.405465088
1.75	0.559615788	0.559615853	0.559615847	0.559615847	0.559615778

TABLE IV

	y_I	y_{II}	y_{III}	y_{IV}
Number of Iterations in Newton Part.	4	3	3	3
$\lVert y(x) - y_{APR.} \rVert^2$	12.9×10^{-8}	10.9×10^{-8}	10.9×10^{-8}	2.7×10^{-8}
Computation time in seconds	4.24	4.17	4.20	4.13

We note again that methods II, III, and IV are about the same in speed and somehow faster than method I. Methods II and III gave practically the same results when h was fairly small. The increasing accuracy which we have when pass from method I to IV is really remarkable.

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