The iterative solution of non-linear ordinary differential equations in Chebyshev series

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The Newton iteration formula is applied to the solution of non-linear ordinary differential equations. For the first-order equation $y' = f(x, y)$ successive applications of Newton's rule yield the formula $y'_i = f(x, y_{i-1}) + (y_i - y_{i-1})f_y(x, y_{i-1})$. All functions which occur in the formula are represented by their Chebyshev series, and the analytic operations involved are performed by arithmetic operations on the coefficients of these series. This iterative method is of particular value when solving boundary-value problems since the more usual step-by-step methods are less powerful in these cases. Several examples are given to illustrate the effectiveness of the method.

1. Introduction

There has been much recent work on the application of Chebyshev series to the numerical solution of practical problems. Chebyshev series have been applied to quadrature (Clenshaw and Curtis, 1960), the solution of integral equations (Elliott, 1960 and 1963), ordinary linear differential equations (Lanczos, 1938, 1952 and 1957; Clenshaw, 1957) and parabolic partial differential equations (Elliott, 1961). Series methods for the solution of differential equations have particular advantages when applied to boundary-value problems, since the *type* of boundary condition is irrelevant to the numerical procedure.

In a recent paper (Clenshaw and Norton, 1963) a method was described for the solution of non-linear ordinary differential equations in Chebyshev series. Basically, this method, hereafter referred to as Method 1, consists in the application of Chebyshev series to Picard iteration. Non-linear operations on Chebyshev series are avoided; non-linear terms occurring in the equations are evaluated at the Chebyshev points ($x_r = \cos r\pi/N$, $r = 0, 1, \ldots, N$, for the range $-1 \leqslant x \leqslant +1$), and from these their Chebyshev series are computed.

For some boundary-value problems, however, Method 1 is divergent. In this paper a procedure, based on Newton iteration, is described (Section 3) which secures convergence for a larger class of problems and also increases the rate of convergence for problems which can be solved by Method 1. Two alternative methods of using Chebyshev series in Newton iteration are described in Sections 4, 5 and 6. There follow, in Section 7, some examples of the solution of first-order differential equations. The particular application to second-order differential equations is dealt with in Sections 8, 9 and 10.

2. The iterative solution of differential equations

Let us consider [as in Clenshaw and Norton, 1963] the solution of the differential equation of the first order

$$\frac{dy}{dx} = f(x, y), \qquad (1)$$

with the associated boundary condition

$$y(\xi) = \eta. \qquad (2)$$

In Picard iteration, a sequence of functions $y_i(x)$ ($i = 0, 1, 2, \ldots$) is generated from

$$y_i(x) = \eta + \int_{\xi}^{x} f(s, y_{i-1}(s))ds, \qquad (3)$$

starting with $y_0(x) = \eta$. The convergence of the sequence of iterates, $\{y_i(x)\}$, has been studied in detail [see, for example, Ince, 1956, Chapter 3]. It is clear that if the sequence converges to a limit for every value of x in a given range, that limit will be a solution of (1) satisfying the boundary condition (2).

When the boundary condition is of the form $\alpha y(-1) + \beta y(+1) = \gamma$, we may still generate a sequence of iterates, $\{y_i(x)\}$, by using the equations

$$\frac{dy_i}{dx} = f(x, y_{i-1}), \qquad (4)$$

$$\alpha y_i(-1) + \beta y_i(+1) = \gamma. \qquad (5)$$

For this general problem, however, necessary conditions for the convergence of the sequence of iterates are not known. We must, therefore, proceed with caution when solving boundary-value problems and not expect convergence in general.

An iteration formula more powerful than (4) can be derived for equation (1) in the following way. We assume $f(x, y)$ to be a function of y, regular in a region which includes the solution and our approximations to it, for every value of x in the range $-1 \leqslant x \leqslant +1$. We then define a sequence, $\{y_i\}$, of approximations to y, by considering the leading terms in the Taylor-series expansion for $f(x, y)$, in the form

$$y'_i = f(x, y_{i-1}) + (y_i - y_{i-1}) f_y(x, y_{i-1}). \qquad (6)$$

We call (6) the Newton iteration formula in view of its close conceptual connection with Newton's method for approximating a root of an equation.

For each cycle of the iteration, a particular solution $y_i = v(x)$ of the inhomogeneous linear equation (6) may

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be calculated, to which is to be added a multiple, $\mu u(x)$, of the solution, $u(x)$, of the homogeneous equation $u' - uf_y(x, y_{i-1}) = 0$.

The factor μ is chosen so that the resulting iterate $y_i(x) = v(x) + \mu u(x)$ satisfies the given boundary condition.

The use of formula (6) will clearly yield the solution of any linear differential equation in just one iteration, whereas the method of Picard iteration often fails to converge (for example, in the case $y'' + \lambda^2 y = 0$ in $-1 \leqslant x \leqslant +1$ with y given at $x = \pm 1$ and $\lambda > \pi/2$).

Kalaba (1959) establishes the convergence of the iterates $y_i(x)$ determined by equation (6) both for the initial-value problem of a single first-order equation and also when the method is extended to certain boundary-value problems of the form

$$y'' = F(x, y, y'); \quad y(0) = y(1) = 0.$$

His proofs require that the functions $f(x, y)$, $F(x, y, y')$ be strictly convex (or strictly concave) as functions of y and y, y' respectively. We shall not, however, impose these restrictions but present a numerical technique for obtaining the representative Chebyshev series when convergence holds.

3. Use of Chebyshev polynomials in Newton iteration

We now derive the relations between the coefficients in the Chebyshev series of the functions which are used in the Newton iteration formula (6). Let the functions be represented by the following series:

$$y_i(x) = \sum_{r=0}^{N}{}' A_r^{(i)} T_r(x), \tag{7}$$

$$y_i'(x) = \sum_{r=0}^{N-1}{}' A_r'^{(i)} T_r(x), \tag{8}$$

$$f(x, y_{i-1}) = \sum_{r=0}^{N}{}' b_r^{(i)} T_r(x) \tag{9}$$

and

$$f_y(x, y_{i-1}) = \sum_{r=0}^{s}{}' c_r^{(i)} T_r(x). \tag{10}$$

We use the notation Σ' to denote a sum in which the first term is to be halved. For convenience in writing we shall usually omit the index i and write a_r for $A_r^{(i-1)}$ in order to distinguish $A_r^{(i-1)}$ from $A_r^{(i)}$. Thus

$$y_{i-1}(x) = \sum_{r=0}^{N}{}' a_r T_r(x). \tag{11}$$

Substitution of expressions (7) to (11) in (6) involves the multiplication of the Chebyshev series for $(y_i - y_{i-1})$ by each term in the expansion (10). Thus the greater the number of terms in this expansion, the more cumbersome are the computational formulae; we therefore take s in (10) to be small. Quite often the use of only the first term, $\frac{1}{2}c_0$, is sufficient to yield a rapidly convergent process (as will be seen in the examples of Section 7).

The multiplication of the series for $(y_i - y_{i-1})$ by each term in (10) is carried out using the relation

$$T_m(x)T_n(x) = \frac{1}{2}[T_{m+n}(x) + T_{|m-n|}(x)]. \tag{12}$$

We may then equate the coefficients of $T_r(x)$ in the right and left members of (6) to obtain the formulae

$$A_r' = b_r + \frac{1}{2}c_0(A_r - a_r) + \frac{1}{2}c_1(A_{r+1} + A_{|r-1|} - a_{r+1}$$
$$- a_{|r-1|}) + \frac{1}{2}c_2(A_{r+2} + A_{|r-2|} - a_{r+2} - a_{|r-2|})$$
$$+ \dots, \quad r = 0, 1, \dots, N - 1. \tag{13}$$

The sets of coefficients $\{A_r\}$ and $\{A_r'\}$ are also related [see Clenshaw and Norton, 1963, Section 3] by the equations

$$2rA_r = A_{r-1}' - A_{r+1}', \quad r = 1, 2, \dots, N. \tag{14}$$

If on the right-hand side of (14) we substitute the expressions for A_{r-1}' and A_{r+1}' obtained from (13), we derive a set of N linear algebraic equations in the A_r. These equations may be written in the form

$$c_0(A_{r-1} - A_{r+1}) - 4rA_r = g_r, \quad r = 1, 2, \dots, N, \tag{15}$$

where

$$g_r = 2(b_{r+1} - b_{r-1}) + c_0(a_{r-1} - a_{r+1})$$
$$+ c_1(A_{r+2} - A_{|r-2|} - a_{r+2} + a_{|r-2|})$$
$$+ c_2(A_{r+3} + A_{r-1} - A_{r+1} - A_{|r-3|}$$
$$- a_{r+3} - a_{r-1} + a_{r+1} + a_{|r-3|}) + \dots. \tag{16}$$

Quantities such as a_r and A_r, $r > N$ which occur in equations (15) are assumed to be zero.

The iterative process can now be outlined as follows.

1. Given the coefficients a_r, $r = 0, 1, \dots, N$ in the Chebyshev series for $y_{i-1}(x)$, we evaluate $y_{i-1}(x_r)$ for $r = 0, 1, \dots, N$ at the points $x_r = \cos r\pi/N$ using the formula $y_{i-1}(x) = \frac{1}{2}(\alpha_0 - \alpha_2)$ where the sequence α_p for $p = N, N - 1, \dots, 0$ is determined recursively from $\alpha_p = 2x\alpha_{p+1} - \alpha_{p+2} + a_p$ with $\alpha_{N+2} = \alpha_{N+1} = 0$ (see Clenshaw, 1962, p. 9).

2. At the points x_r we compute the values $f(x_r, y_{i-1}(x_r))$ and $f_y(x_r, y_{i-1}(x_r))$ for $r = 0, 1, \dots, N$.

3. The coefficients b_r in expansion (9) (and similarly c_r in (10)) are now derived using the formulae

$$b_r = \sum_{s=0}^{N}{}' \beta_s T_s(x_r), \quad r = 0, 1, \dots, N - 1,$$

$$b_N = \frac{1}{2} \sum_{s=0}^{N}{}' \beta_s T_s(-1),$$

where

$$\beta_r = \frac{2}{N} f(x_r, y_{i-1}(x_r)), \quad r = 0, 1, \dots, N - 1$$

and $\beta_N = \frac{1}{N} f(-1, y_{i-1}(-1))$.

4. The equations (15) together with the boundary condition now form a set of $N + 1$ simultaneous equations in the $N + 1$ unknowns A_r, $r = 0, 1, \dots, N$.

The solution of these equations gives an improved approximation $y_i(x) = \sum\limits_{r=0}^{N}{}' A_r T_r(x)$ to the solution of the differential equation and this may be used in step 1 to start another iterative cycle. Remarks concerning the value of N which might be used at each stage of the iteration are to be found in Clenshaw and Norton (1963, Section 5).

The initial approximation, $y_0(x)$, to the solution is conveniently taken to be the simplest polynomial which satisfies the boundary conditions.

In step 4 the linear equations may be solved directly. In the next three Sections, however, we exploit the special form of the equations to obtain their solution more efficiently. A recursive method is described in Sections 4 and 5, and a method of successive approximation in Section 6.

4. Recursive solution of the linear equations

We consider the solution of equations (15) for the case in which c_r is neglected for $r > 0$; that is to say we approximate g_r by

$$g_r^* = 2(b_{r+1} - b_{r-1}) + c_0(a_{r-1} - a_{r+1}). \quad (17)$$

It may be noted that (15) and (17) are precisely the relations obtained for the coefficients in the Chebyshev series when $y_i(x)$ is a solution of the equation

$$y' - \tfrac{1}{2}c_0 y = g(x) \quad (18)$$

with $g(x) = f(x, y_{i-1}(x)) - \tfrac{1}{2}c_0 y_{i-1}(x)$.

The required solution of the set (15) is thus of the form

$$A_r = E_r + \mu I_r(\tfrac{1}{2}c_0), \quad r = 0, 1, \ldots, N+1, \quad (19)$$

where $\{E_r\}$ is any particular solution of (15) corresponding to a particular integral of (18), while I_r is the modified Bessel function which forms the complementary function of (15), corresponding to the complementary function

$$e^{\frac{1}{2}c_0 x} = 2\sum\limits_{r=0}^{\infty}{}' I_r(\tfrac{1}{2}c_0) T_r(x)$$

of equation (18). [The function $K_r(\tfrac{1}{2}c_0)$ also appears in a complementary function of (15), but since it increases with r for large r it clearly has a zero coefficient in any solution with a convergent Chebyshev series expansion. This is consistent with the absence of a second complementary function of (18).]

The solution E_r can be generated by recurrence, using the method of Clenshaw (1957). Starting with $E_{N+2} = E_{N+1} = 0$ we calculate $E_N, E_{N-1}, \ldots, E_0$ in succession from

$$c_0 E_{r-1} = c_0 E_{r+1} + 4r E_r + g_r^*. \quad (20)$$

Similarly, starting with $F_{N+1} = 0$, $F_N = 1$ and employing the corresponding homogeneous relation

$$c_0 F_{r-1} = c_0 F_{r+1} + 4r F_r \quad (21)$$

with $r = N, N-1, \ldots, 1$ we derive a sequence $\{F_r\}$ which is substantially a multiple of the sequence $\{I_r(\tfrac{1}{2}c_0)\}$. We may now construct a solution

$$A_r = E_r + \mu F_r, \quad r = 0, 1, \ldots, N, \quad (22)$$

where the factor μ is determined so that the function $y_i = \sum\limits_{r=0}^{N}{}' A_r T_r(x)$ satisfies the boundary condition. For example, if the boundary condition is $y(-1) + \alpha y(+1) = \beta$ we require that

$$\tfrac{1}{2}A_0 - A_1 + \ldots + (-1)^N A_N$$
$$+ \alpha(\tfrac{1}{2}A_0 + A_1 + \ldots + A_N) = \beta. \quad (23)$$

Thus the required value of μ is given by $E + \mu F = \beta$ where

$$E = \tfrac{1}{2}E_0 - E_1 + \ldots + (-)^N E_N$$
$$+ \alpha(\tfrac{1}{2}E_0 + E_1 + \ldots + E_N)$$

and

$$F = \tfrac{1}{2}F_0 - F_1 + \ldots + (-)^N F_N$$
$$+ \alpha(\tfrac{1}{2}F_0 + F_1 + \ldots + F_N).$$

We have so far represented $f_y(x, y_{i-1})$ by $\tfrac{1}{2}c_0$, an average value for the range $-1 \leqslant x \leqslant +1$. Higher accuracy in g_r might be achieved subsequently by inserting the value A_r obtained as above into the right of (16), while using a value of s greater than zero in (10). The new g_r may be used in place of g_r^* to produce better values of A_r. The resulting increase in complication might be expected to be worthwhile in that fewer iterations will be required to solve the differential equation. Numerical experiment shows, however, that the advantage gained is slight. Some results which exemplify this conclusion, in the case when $s = 2$, will be found in Section 7.

5. Recursive procedure when c_0 is small

When c_0 is small, there may be cancellation in using (22) to form A_r. This is a consequence of the fact that the complementary function $e^{\frac{1}{2}c_0 x}$ of (18) then has a Chebyshev series expansion which has a more rapid rate of convergence than that of the wanted solution, so that both E_r and F_r become largely multiples of $I_r(\tfrac{1}{2}c_0)$ as c_0 becomes small.

The following modification, due to G. F. Miller,† overcomes this difficulty. The sequence $\{F_r\}$ may be computed as before. In place of $\{E_r\}$, however, we compute for $p = N, N-1, \ldots, 1$ sequences $\{E_r^{(p)}\}$ $(r = p-1, p, \ldots, N+1)$ satisfying the relation (20) and the conditions $E_p^{(p)} = 0$, $E_{N+1}^{(p)} = 0$. Given the sequence $\{E_r^{(p)}\}$ we compute the quantity $E_{p-1}^{(p)}$ and hence the new sequence $\{E_r^{(p-1)}\}$ from the relations

$$\left.\begin{aligned} E_{p-1}^{(p)} &= E_{p+1}^{(p)} + \frac{1}{c_0} g_p^* \\[2mm] E_r^{(p-1)} &= E_r^{(p)} - \frac{E_{p-1}^{(p)}}{F_{p-1}} F_r, \quad r = p, p+1, \ldots, N \end{aligned}\right\}. \quad (24)$$

* We remark that a similar problem has been considered by Lago (1960); the method of solution he proposes is, however, less convenient for our purposes.

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(We note that the first of these relations is equivalent to (20) with $E_p^{(p)} = 0$.) Thus each sequence is obtained from its predecessor by subtracting a multiple of $\{F_r\}$. We finally obtain a solution $\{E_r^{(1)}\}$ with the desired property that it is not dominated by $\{F_r\}$.

The above procedure facilitates the use of this method when $0 < |c_0| < 2$. In the degenerate case $c_0 = 0$ we have $E_0 = A$, $E_r = -g_r^*/4r$ $(r \geqslant 1)$ where the arbitrary constant A is chosen so that the boundary condition is satisfied. The procedures described here are applicable to most problems. If, however, some term other than c_0 dominates the expansion (10) it is possible to derive a more suitable recurrence equation from (15) by rearrangement.

6. Iterative solution of the linear equations

Equations (15) may also be solved by an iterative procedure. That is, at each stage of the main iteration we may solve iteratively the set of linear algebraic equations for A_r, $r = 0, 1, \ldots, N$. Such a procedure involves computing successive approximations $A_{r,j}$ to A_r, given by

$$A_{r,j} = \frac{1}{4r} h_{r,j}, \quad j = 1, 2, \ldots \tag{25}$$

where

$$
\begin{aligned}
h_{r,j} = {} & 2(b_{r-1} - b_{r+1}) \\
& + c_0(A_{r-1,j-1} - A_{r+1,j-1} - a_{r-1} + a_{r+1}) \\
& + c_1(A_{|r-2|,j-1} - A_{r+2,j-1} - a_{|r-2|} + a_{r+2}) \\
& + c_2(A_{|r-3|,j-1} - A_{r-1,j-1} + A_{r+1,j-1} \\
& \quad - A_{r+3,j-1} - a_{|r-3|} + a_{r-1} - a_{r+1} \\
& \hspace{4cm} + a_{r+3}) + \ldots.
\end{aligned}
$$

As an initial estimate of A_r it is convenient to take $A_{r,0} = a_r$. Equation (25) then gives for $j = 1$

$$A_{r,1} = \frac{1}{2r}(b_{r-1} - b_{r+1}),$$

and the set of values $\{A_{r,1}\}$ is identical with the set which would be obtained by one step of Picard iteration starting from the approximation $y_{i-1}(x)$. Thereafter the successive sets of values $\{A_{r,j}\}$, $j = 1, 2, \ldots$, give improved approximations to the solution of the differential equation.

A limitation of this method is that successive approximations $\{A_{r,j}\}$, $j = 1, 2, \ldots$, diverge if the values c_r are too large. A crude estimate of acceptable upper limits for the c_r can be obtained by estimating the effect on the $A_{r,j}$ of small errors in the $A_{r,j-1}$. In the case when the boundary condition consists of a given value for y at $x = -1$ or at $x = +1$, for example, we derive the limits $|c_r| < 4/5$ for $r = 0, 1, 2$ in the case when $s = 2$. Practical examples suggest that these limits err on the side of safety; indeed, values of c_r in excess of 2 have been found tolerable in some cases (see Examples 1 and 2 in Section 7).

A limitation which this procedure shares with Method 1 is that it cannot be used without modification

Table 1

Solution of $y' = y^2$, $y(-1) = 0 \cdot 4$

r	$10^{10}a_r$	r	$10^{10}a_r$
0	1 78885 43820	13	65902
1	68328 15730	14	25172
2	26099 03370	15	9615
3	9968 94380	16	3673
4	3807 79770	17	1403
5	1454 44930	18	536
6	555 55020	19	205
7	212 20129	20	78
8	81 05368	21	30
9	30 95975	22	11
10	11 82557	23	4
11	4 51697	24	2
12	1 72533	25	1

to solve problems with the periodic boundary condition $y(-1) = y(+1)$.

It may be noted that the methods described here and in Section 4 are mathematically equivalent when the same approximation to $f_y(x, y_{i-1})$ is used at each stage.

7. Examples

The main purpose of the following examples is to compare the numbers of iterations which are necessary to obtain solutions to 10 decimal places when using Picard and Newton iteration. For simplicity, in each example the same number of terms was used for every cycle of the iteration; the number was chosen to yield 12 decimal places in the solution in order to allow for rounding errors. The computations were carried out on the ACE computer of the National Physical Laboratory.

Example 1

The problem

$$
\left.
\begin{aligned}
y' &= y^2 \\
y(-1) &= 0 \cdot 4
\end{aligned}
\right\}
$$

has the solution

$$y = \frac{2}{3 - 2x}, \quad -1 \leqslant x \leqslant +1.$$

The coefficients in the infinite Chebyshev expansion of this solution are given by

$$a_r = \frac{4}{\sqrt{5}}\left(\frac{3 - \sqrt{5}}{2}\right)^r.$$

The initial approximation used in this problem was $y_0(x) = 0 \cdot 4$ and the value used for N was 30. The solution given in Table 1 (correct to 5×10^{-11}) was

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obtained by Picard iteration in 20 steps. Using Newton iteration, with $s = 0$ in (10), twelve iterations were needed. When the successive correction procedure described at the end of Section 4 was used, with $s = 2$, 10 iterations were needed; the numbers of successive corrections required at each stage being 1, 9, 9, 8, 6, 5, 7, 2, 3, 4.

Since $\partial f/\partial y = 2y$ we see from Table 1 that the coefficients $c_0^{(i)}$, $c_1^{(i)}$ and $c_2^{(i)}$ tend to the values $2a_0 = 3 \cdot 577\ldots$, $2a_1 = 1 \cdot 366\ldots$ and $2a_2 = 0 \cdot 521\ldots$, respectively. The tentative analysis indicated in Section 6 notwithstanding, the procedure indicated by (25) converges in this case, and only 8 iterations were necessary. The numbers of successive approximations required at each stage were 14, 17, 16, 13, 11, 7, 6, 2.

Example 2

The problem

$$\left.\begin{array}{l} y' = x - y^2 \\ y(0) = -0 \cdot 72901\ 11329\ 47\ldots \end{array}\right\}$$

has the formal solution

$$y = \frac{A_i'(x)}{A_i(x)}$$

where $A_i(x)$ is the Airy integral, given by

$$A_i(x) = \frac{1}{\pi}\int_0^\infty \cos(\tfrac{1}{3}t^3 + xt)\,dt.$$

With $N = 18$ and $y_0(x) = -0 \cdot 72901\ldots$, the Chebyshev coefficients given in Table 2 were obtained. With Picard iteration 16 iterations were necessary to obtain this solution. When Newton iteration was used with $s = 0$, 11 iterations were necessary. With $s = 2$, 8 iterations were needed when the algebraic equations were solved recursively, and 6 when the algebraic equations were solved by iteration.

Example 3

As an example of a problem for which $c_0^{(i)} = 0$ we take

$$\left.\begin{array}{l} y' = \sin y \\ y(-1) = \cos^{-1}(\tanh 1) \end{array}\right\}.$$

The solution $y(x)$ satisfies the equation $\cos y = -\tanh x$. Thus $\partial f/\partial y$, which is equal to $\cos y$, is an odd function $(-\tanh x)$ of x and all terms of even order in its Chebyshev series are zero. In particular, $c_0 = 0$. With Method 1, 10 iterations were needed to attain the coefficients in Table 3. Newton iteration with $s = 1$ was applied and gave the solution in 7 iterations.

Example 4

A problem with periodic boundary conditions is exemplified by

$$\left.\begin{array}{l} y' = 1 - y^{1/2} + \cos \pi x, \quad -1 \leqslant x \leqslant +1, \\ y(-1) = y(+1). \end{array}\right\}$$

Table 2

Solution of $y' = x - y^2$, $y(0) = -0 \cdot 729\ldots$

r	$10^{10}a_r$	r	$10^{10}a_r$
0	$-$ 1 33182 01337	8	$+$ 61673
1	$-$ 56577 45689	9	$-$ 13822
2	$+$ 6555 80575	10	$+$ 3101
3	$-$ 1231 16778	11	$-$ 696
4	$+$ 257 48695	12	$+$ 156
5	$-$ 55 97968	13	$-$ 35
6	$+$ 12 37501	14	$+$ 8
7	$-$ 2 75722	15	$-$ 2

Table 3

Solution of $y' = \sin y$, $y(-1) = +0 \cdot 705\ldots$

r	$10^{10}a_r$	r	$10^{10}a_r$
0	$+$ 3 14159 26536	9	$+$ 67117
1	$+$ 89586 72584	10	0
2	0	11	$-$ 4660
3	$-$ 3167 09343	12	0
4	0	13	$+$ 335
5	$+$ 166 85090	14	0
6	0	15	$-$ 25
7	$-$ 10 16267	16	0
8	0	17	$+$ 2

This problem has a unique solution. Newton iteration, using recursive solution of the algebraic equations is readily applicable to this problem. Starting with $y_0(x) = 1$ and $s = 0$ the values given in Table 4 were obtained after 6 iterations. With $s = 2$, 7 iterations were necessary. This lack of improvement when $s = 2$ is due to c_3 being the most dominant term, after c_0, in the Chebyshev series for $\partial f/\partial y$. In fact, with $s = 3$, only 4 iterations were necessary.

8. Second-order equations

Differential equations of order higher than the first may be expressed as a set of first-order equations, provided only that the derivative of highest order is expressible explicitly. Thus no new techniques are required. The frequent occurrence of second-order equations in practical problems, however, indicates the desirability of more direct methods of attack for such problems. The extension of Method 1 for the equation

$$y'' = f(x, y, y') \tag{26}$$

has been given by Clenshaw and Norton (1963).

From the first-order terms of the Taylor series for $f(x, y, y')$, in some neighbourhood of $y = y_{i-1}(x)$, we

Table 4

Solution of $y' = 1 - y^{1/2} + \cos \pi x$, $y(-1) = y(+1)$

r	$10^{10}a_r$	r	$10^{10}a_r$
0 +	1 99458 82313	13 +	13328
1 +	17707 96542	14 −	349
2 −	4830 96257	15 −	2374
3 −	20694 41133	16 +	1094
4 +	1478 90267	17 +	14
5 +	3167 72534	18 −	236
6 −	121 73954	19 +	101
7 −	185 14891	20 +	7
8 −	1 53820	21 −	25
9 +	4 03430	22 +	10
10 +	1 79605	23 +	1
11 −	27527	24 −	3
12 −	26764	25 +	1

may derive the Newton iteration formula

$$y_i'' - g(x)y_i' - h(x)y_i = f(x, y_{i-1}, y_{i-1}')$$
$$- g(x)y_{i-1}' - h(x)y_{i-1}, \quad (27)$$

where $h(x) = f_y(x, y_{i-1}, y_{i-1}')$ and $g(x) = f_{y'}(x, y_{i-1}, y_{i-1}')$, which is directly analogous to formula (6).

In this Section we shall give a numerical procedure similar to that described in Section 4. For simplicity, only the first (constant) term in each of the Chebyshev expansions of f_y and $f_{y'}$ will be considered. That is, we shall assume that

$$h(x) = \tfrac{1}{2}c_0^{(i)}, \quad g(x) = \tfrac{1}{2}c_0'^{(i)}.$$

Let the functions occurring in (27) be represented by the following series:

$$y_i(x) = \sum_{r=0}^{N}{}' A_r^{(i)}T_r(x),$$

$$y_i'(x) = \sum_{r=0}^{N}{}' A_r'^{(i)}T_r(x),$$

$$y_i''x = \sum_{r=0}^{N}{}' A_r''^{(i)}T_r(x)$$

and

$$f(x, y_{i-1}, y_{i-1}') = \sum_{r=0}^{N}{}' b_r^{(i)}T_r(x).$$

As in Section 3, we omit the index i and denote the coefficients $\{A_r^{(i-1)}\}$, $\{A_r'^{(i-1)}\}$ by $\{a_r\}$ and $\{a_r'\}$, respectively. It is again assumed that N is large enough to ensure that the series represent the functions to sufficient accuracy. Substituting these expressions in (27) and equating coefficients of $T_r(x)$ we obtain

$$A_r'' - \tfrac{1}{2}c_0'A_r' - \tfrac{1}{2}c_0A_r = d_r, \quad r = 0, 1, \ldots, N \quad (28)$$

where $d_r = b_r - \tfrac{1}{2}c_0'a_r' - \tfrac{1}{2}c_0a_r$.

From (28) we have

$$(A_{r-1}'' - A_{r+1}'') - \tfrac{1}{2}c_0'(A_{r-1}' - A_{r+1}')$$
$$- \tfrac{1}{2}c_0(A_{r-1} - A_{r+1}) = d_{r-1} - d_{r+1}.$$

Using (14), i.e. $2rA_r = A_{r-1}' - A_{r+1}'$, and the corresponding expression $2rA_r' = A_{r-1}'' - A_{r+1}''$, we derive

$$2rA_r' - c_0'rA_r - \tfrac{1}{2}c_0(A_{r-1} - A_{r+1}) = d_{r-1} - d_{r+1}. \quad (29)$$

Equations (29) and (14) may be rewritten as the following system of recurrence equations

$$\left.\begin{array}{l} c_0A_{r-1} = c_0A_{r+1} + 2r(2A_r' - c_0'A_r) + 2(d_{r+1} - d_{r-1}) \\ A_{r-1}' = A_{r+1}' + 2rA_r \end{array}\right\} \quad (30)$$

for $r = N, N-1, \ldots, 1$. Every solution of this system may be expressed as the sum of one particular solution E_r, E_r' $(r = 0, 1, \ldots, N)$ and a linear combination of four independent solutions of the corresponding homogeneous system

$$\left.\begin{array}{l} c_0B_{r-1} = c_0B_{r+1} + 2r(2B_r' - c_0'B_r) \\ B_{r-1}' = B_{r+1}' + 2rB_r. \end{array}\right\} \quad (31)$$

By our method of solution we automatically exclude two of these solutions, which tend to infinity with r. Therefore we need to construct *two* solutions of (31), F_r, F_r' and G_r, G_r' say, which tend to zero as r tends to infinity.

We then determine the constants μ and ν in the expression

$$A_r = E_r + \mu F_r + \nu G_r, \quad (32)$$

to ensure that the iterate $y_i(x) = \sum_{r=0}^{N}{}' A_rT_r(x)$ satisfies the prescribed boundary conditions.

In order to illustrate the method, we describe the above process, using $N = 4$, for the equation $y'' = y^2$, with the boundary conditions $y(-1) = 0$, $y(+1) = 1$. We take $y_0(x) = \tfrac{1}{2}(1 + x) = \tfrac{1}{2} + \tfrac{1}{2}T_1(x)$ as our initial approximation to the solution, this being the simplest polynomial which satisfies the boundary conditions. Then

$$f(x, y_0, y_0') = y_0^2 = \tfrac{1}{2}(\tfrac{3}{4}) + \tfrac{1}{2}T_1(x) + \tfrac{1}{8}T_2(x),$$
$$f_{y'}(x, y_0, y_0') \equiv 0$$

and $\quad f_y(x, y_0, y_0') = 2y_0 = \tfrac{1}{2}(2) + T_1(x).$

Hence $c_0 = 2$, $c_0' = 0$, $d_0 = -\tfrac{1}{4}$, $d_1 = 0$ and $d_2 = \tfrac{1}{8}$.

The recurrence equations (30) become

$$\left.\begin{array}{l} A_{r-1} = A_{r+1} + 2rA_r' + d_{r+1} - d_{r-1} \\ A_{r-1}' = A_{r+1}' + 2rA_r \end{array}\right\}$$

and, letting $E_{N+1} = E_{N+1}' = 0$, $E_N = E_N' = 1$ we obtain for $N = 4$, the values in Table 5. Similarly, equations (31) become

$$\left.\begin{array}{l} B_{r-1} = B_{r+1} + 2rB_r' \\ B_{r-1}' = B_{r+1}' + 2rB_r \end{array}\right\}$$

and with $F_5 = F_5' = G_5 = G_5' = 0$, $F_4 = F_4' = G_4 = 1$.

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Table 5

Solution of $y'' = y^2$, $y(-1) = 0$, $y(+1) = 1$

First iteration

r	d_r	E_r	E'_r	F_r	F'_r	G_r	G'_r	A_r
0	−0·25	456·25	457	457	457	457	−457	0·891
1	0	204	203·5	204	204	−204	204	0·481
2	0·125	48·875	49	49	49	49	− 49	0·051
3	0	8	8	8	8	− 8	8	0·019
4	0	1	1	1	1	1	− 1	0·004

Second iteration

r	$y_1\left(\cos\dfrac{r\pi}{4}\right)$	$y_1^2\left(\cos\dfrac{r\pi}{4}\right)$	b_r	d_r	E_r	E'_r	F_r	F'_r	G_r	G'_r	A_r	SOLUTION CORRECT TO 4D
0	1·000	1·000	0·630	−0·164	564·690	563·630	565·662	565·662	565·662	−565·662	0·892	0·8910
1	0·768	0·590	0·454	0·025	254·474	227·000	255·391	227·520	−255·391	227·520	0·484	0·4830
2	0·398	0·158	0·171	0·126	54·750	54·682	54·880	54·880	54·880	− 54·880	0·051	0·0513
3	0·114	0·013	0·046	0·029	8·947	8	8·980	8	− 8·980	8	0·016	0·0165
4	0·000	0·000	0·014	0·010	1	1	1	1	1	− 1	0·003	0·0031
5												0·0005
6												0·0001

and $G'_4 = -1$ we obtain the values of F_r, F'_r, G_r, G'_r given in Table 5. We may note that the equation satisfied by y_1 is $y''_1 - y_1 = -\frac{1}{4} + \frac{1}{4}x^2$.

The Chebyshev coefficients F_r, G_r are obviously multiples of those of the complementary functions e^x and e^{-x}, respectively, and E_r is identical with F_r except for the addition of the particular integral

$$y_1 = -\tfrac{1}{4} - \tfrac{1}{4}x^2 = \tfrac{1}{2}(-\tfrac{3}{4}) - \tfrac{1}{8}T_2(x).$$

The boundary conditions $y(-1) = 0$, $y(+1) = 1$ imply that

$$\tfrac{1}{2}A_0 + A_2 + A_4 = \tfrac{1}{2},$$
$$A_1 + A_3 = \tfrac{1}{2}.$$

We therefore compute the quantities

$$\tfrac{1}{2}E_0 + E_2 + E_4 = 278, \quad \tfrac{1}{2}F_0 + F_2 + F_4 = 278\cdot5,$$
$$\tfrac{1}{2}G_0 + G_2 + G_4 = 278\cdot5$$

$$E_1 + E_3 = 212, \quad F_1 + F_3 = 212, \quad G_1 + G_3 = -212$$

and from the equations

$$278 + \mu278\cdot5 + \nu278\cdot5 = 0\cdot5$$
$$212 + \mu212 - \nu212 = 0\cdot5$$

we find that $\mu = -0\cdot997025$, $\nu = +0\cdot000616$. Then the values of A_r given by

$$A_r = E_r + \mu F_r + \nu G_r, \quad r = 0, 1, \ldots, 4,$$

satisfy the requirements imposed by the boundary conditions.

From the coefficients A_r the values of $y_1(x)$ can be computed at the points $x_r = \cos(r\pi/4)$, hence the values of $y_1^2(x)$, the coefficients b_r in the Chebyshev series representing $y_1^2(x)$ and finally the numbers d_r ($r = 0, 1, \ldots, 4$).

For the second iteration $c_0 = 1\cdot782$, and the recur-

rence formulae are

$$A_{r-1} = A_{r+1} + 2\cdot245rA'_r + 1\cdot122(d_{r+1} - d_{r-1})\Big\}$$
$$A'_{r-1} = A'_{r+1} + 2rA_r.$$

The values obtained during the second iteration are given in Table 5 and also the solution correct to four decimals.

9. Second-order equations when c_0 is small

As in the case of first-order equations considered in Section 5, there may be cancellation consequent upon the use of (32) to obtain A_r when c_0 is small. Let us suppose that straightforward application of the recurrence relations (31) for $r = N, N - 1, \ldots, 1$ starting with $F_N = F'_N = 1$ and $F_{N+1} = F'_{N+1} = 0$, yields sequences $\{F_r\}$, $\{F'_r\}$. To obtain a second solution $\{G_r\}$, $\{G'_r\}$ which is essentially distinct from $\{F_r\}$, $\{F'_r\}$ we compute sequences $\{G_r^{(p)}\}$, $\{G_r'^{(p)}\}$ $(r = p - 1, p, \ldots, N)$ for $p = N, N - 1, \ldots, 1$ from the relations

$$G_{N+1}^{(N)} = 0, \quad G_N^{(N)} = 0, \quad G_N'^{(N)} = 1, \quad G_{N+1}'^{(N)} = 0,$$
$$c_0 G_{p-1}^{(p)} = c_0 G_{p+1}^{(p)} + 4rG_p^{(p)}, \quad G_{p-1}'^{(p)} = G_{p+1}'^{(p)},$$
$$\left.\begin{array}{l} G_r^{(p-1)} = G_r^{(p)} - \gamma_p F_r \\ G_r'^{(p-1)} = G_r'^{(p)} - \gamma_p F'_r \end{array}\right\} \quad r = p - 1, p, \ldots, N$$

where $\gamma_p = G_{p-1}^{(p)}/F_{p-1}$ is chosen so that $G_{p-1}^{(p-1)} = 0$. Finally we take $G_r = G_r^{(1)}$, $G'_r = G_r'^{(1)}$.

To obtain a solution $\{E_r\}$, $\{E'_r\}$ of the inhomogeneous system (30) which is not dominated by $\{F_r\}$, $\{F'_r\}$ (or possibly by $\{G_r\}$, $\{G'_r\}$) we calculate sequences $\{E_r^{(p)}\}$, $\{E_r'^{(p)}\}$ $(r = p - 1, p, \ldots, N)$ for $p = N, N - 1, \ldots, 1$ concurrently with the sequences $\{G_r^{(p)}\}$, $\{G_r'^{(p)}\}$ from the relations

$$E_{N+1}^{(N)} = E_N^{(N)} = E_{N+1}'^{(N)} = E_N'^{(N)} = 0$$
$$c_0 E_{p-1}^{(p)} = c_0 E_{p+1}^{(p)} + 2(d_{r+1} - d_{r-1})$$

Table 6

Recursive procedure when c_0 is small

r	d_r	F_r	F'_r	$G_r^{(4)}$	$G'^{(4)}_r$	$G_r^{(3)}$	$G'^{(3)}_r$	$E_r^{(3)}$	$E'^{(3)}_r$
0	$-0\cdot25$	457	457						
1	0	204	204						
2	$0\cdot125$	49	49			-49	0	$-0\cdot125$	0
3	0	8	8	8	0	0	-8	0	0
4	0	1	1	0	1	-1	0	0	0

r	$G_r^{(2)}$	$G'^{(2)}_r$	$E_r^{(2)}$	$E'^{(2)}_r$	$G_r^{(1)}$	$G'^{(1)}_r$	$E_r^{(1)}$	$E'^{(1)}_r$
0					-457	0	$0\cdot370$	0
1	204	0	0	$0\cdot020$	0	-204	0	0
2	0	49	0	0	-49	0	$-0\cdot005$	0
3	8	0	0	$0\cdot020$	0	-8	0	$0\cdot019$
4	0	1	$0\cdot003$	0	-1	0	$0\cdot003$	0

$$E'^{(p)}_{p-1} = E'^{(p)}_{p+1}$$

$$\left.\begin{array}{l} E_r^{(p-1)} = E_r^{(p)} - \alpha_p F_r - \beta_p G_r^{(p-1)} \\ E'^{(p-1)}_r = E'^{(p)}_r - \alpha_p F'_r - \beta_p G'^{(p-1)}_r \end{array}\right\} \quad r = p, p+1, \ldots, N$$

where α_p and β_p are determined so that

$$E_{p-1}^{(p-1)} = E'^{(p-1)}_{p-1} = 0.$$

Since $G_{p-1}^{(p-1)} = 0$ we have

$$\alpha_p = E_{p-1}^{(p)}/F_{p-1}$$

$$\beta_p = \frac{E'^{(p)}_{p-1} - \alpha_p F'_{p-1}}{G'^{(p-1)}_{p-1}}.$$

Finally the solution with the desired property is given by $E_r = E_r^{(1)}$, $E'_r = E'^{(1)}_r$.

This process is exemplified in Table 6 where the sequences are given for the first iteration in the example $y'' = y^2$, which was presented in the last Section.

In the degenerate case, $c_0^{(i)} = 0$, the system (30) becomes

$$\left.\begin{array}{l} A'_{r-1} = A'_{r+1} + 2rA_r \\ c_0'A_{r-1} = 2A'_{r-1} + \dfrac{1}{r-1}(d_r - d_{r-2}) \end{array}\right\}$$

for $r = N, N-1, \ldots, 2$. Only one solution of the corresponding homogeneous system is here required to obtain the general solution. The boundary conditions are satisfied by calculation of A_0 and of the arbitrary parameter in the general solution.

When, in addition, $c_0' = 0$ the system (30) becomes

$$\left.\begin{array}{l} A'_r = \dfrac{1}{2r}(d_{r-1} - d_{r+1}) \\ A_r = \dfrac{1}{2r}(A'_{r-1} - A'_{r+1}) \end{array}\right\}$$

which is merely another form of the equations given by Clenshaw and Norton (1963) (in Section 6) when extending Method 1.

10. Examples

1. As an example of a second-order differential equation we consider van der Pol's equation

$$\frac{d^2y}{dt^2} + (y^2 - 1)\frac{dy}{dt} + y = 0$$

with the boundary conditions $y(-\frac{1}{2}) = 0$, $y(+\frac{1}{2}) = 1$. Writing $t = \frac{1}{2}x$ and using primes, as before, to denote derivatives with respect to x we have $y'' = \frac{1}{2}(1 - y^2)y' - \frac{1}{4}y$, with $y(-1) = 0$, $y(+1) = 1$.

The values, to 10 decimals, of the coefficients which represent the solution $y(x)$ are given in Table 7. With the present method these values were obtained after eight iterations. Using the obvious extension of Method 1 described by Clenshaw and Norton (1963), 11 iterations were necessary.

Table 7

**Solution of $y'' = \frac{1}{2}(1 - y^2)y' - \frac{1}{4}y$,
$y(-1) = 0$, $y(+1) = 1$**

r	$10^{10}a_r$	r	$10^{10}a_r$
0	$+$ 96831 51979	8	$-$ 7368
1	$+$ 50955 14886	9	$-$ 2786
2	$+$ 1727 88627	10	$-$ 154
3	$-$ 959 25858	11	$+$ 70
4	$-$ 148 30708	12	$+$ 15
5	$+$ 3 59122	13	0
6	$+$ 4 73599	14	$-$ 1
7	$+$ 54566	15	0

Also used was a process of successive approximation, similar to that of Section 6, at each stage of the iteration to take account of three terms in the expansions of f_y or $f_{y'}$, or both. The results are summarized in Table 8. The consequent reduction in the number of iterations does not appear to justify the extra complication of the method.

Table 8

COEFFICIENTS CONSIDERED	NUMBER OF ITERATIONS
None	11
c_0 c_0'	8
c_0, c_1, c_2 c_0'	8
c_0 c_0', c_1', c_2'	6
c_0, c_1, c_2 c_0', c_1', c_2'	5

2. A problem which arose in connection with the analysis of sea-waves involved finding periodic solutions of the differential equation

$$yy'' + Ay'^2 + B(y - 20 - 1/12 \sin \pi x) = 0$$

with $A = 1 \cdot 003736$ and $B = 176 \cdot 44545$. The result was required to three decimals and was obtained to this accuracy after four iterations starting with $y_0(x) = 20$. The solution to four decimals is given in Table 9.

Table 9

Solution of

$$yy'' + A(y')^2 + B\left(y - 20 - \frac{1}{12} \sin \pi x\right) = 0$$

r	$10^4 a_r$	r	$10^4 a_r$
0	+ 400034	6	− 44
1	− 4002	7	+ 47
2	+ 46	8	+ 12
3	+ 4690	9	− 1
4	+ 50	10	− 2
5	− 734	11	0

11. Comparison with Runge–Kutta method of solution

It is of interest to compare the application of the present method with that of a standard fourth-order Runge-Kutta program. Accordingly the comparison

was made in the case of two first-order equations, the first a simple initial-value problem and the second a less simple boundary-value problem.

The Runge-Kutta program gave the solution to the first problem of Section 7, $y' = y^2$, $y(-1) = 0 \cdot 4$ in the range $-1 \leqslant x \leqslant +1$, to 10 decimal places at an interval of 2^{-8} in x. This implies a total of about 2,560 multiplications. Newton iteration in Chebyshev series requires a total of about 20,000 multiplications in the 12 cycles which secure the desired accuracy. [This figure might be halved if N is allowed to vary during the computation as in Section 5 of Clenshaw and Norton (1963), but this device is not considered here.]

In Example 4 of Section 7, we have to find a 10-decimal solution of

$$y' = 1 - y^{\frac{1}{2}} + \cos \pi x, \quad y(-1) = y(+1)$$

in the range $-1 \leqslant x \leqslant +1$. A single trial step-by-step solution here using the Runge-Kutta program with an interval in x of 2^{-7} requires about 4,000 operations of multiplication and division, and several such trial solutions may be needed before the boundary condition is satisfied. Starting with $y(-1) = 1$ and solving the variational equation at the same time, four trial solutions were needed and a total of some 20,000 operations. In contrast, the Newton iteration procedure gives the solution directly in about 10,000 operations.

12. Conclusion

It seems likely that the method of Newton iteration using Chebyshev series will often be useful in the solution of boundary-value problems, particularly with non-linear differential equations. The method is more widely applicable than the simpler one described earlier by Clenshaw and Norton (1963) and can form the basis of a computer program which may be as easily operated.

For initial-value problems the method is likely to compare poorly with the standard Runge–Kutta methods. In some cases, however, the form of the solution may be considered to be an advantage.

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Correspondence

To the Editor,
The Computer Journal,

Sir,

Hardware Representation of Algorithmic Languages

I write in support of those correspondents to *The Computer Journal* who have urged the need for the hardware used in tape preparation to be tailored to the needs of the user. This is in no way to deny that, so long as cost and availability of hardware impose limitations, it is useful to devise hardware representations which mitigate these limitations, as is done for example in the Royal Radar Establishment's 5-hole code for ALGOL 60 described by Mr. P. Taylor on page 335 of your January 1964 issue.

In the long run, however, these limitations must be overcome rather than circumvented. On the same page, Dr. D. Barron asks why current tape preparation equipment is not more suitable and economical. Particularly with regard to cost, part of the answer lies in commercial reasons which it might be invidious to debate but which we can influence as buyers. The unsuitability of present equipment arises basically from the fact that it was never intended for computer use, but has been adapted from other applications.

Teleprinters were devised for remote working by means of a single electrical circuit. In computer applications, the distance to be spanned is generally much less and multi-wire working is preferable. The serial coder and de-coder, which are central to the working of the machine in telegraphy, have therefore to be removed or nullified for computer use. This leads neither to convenience nor economy.

The teleprinter shares with electric typewriters, whether associated with punched paper tape or not, the defect of an insufficient character set. A character set which is adequate for its intended purpose of business communication is quite inadequate for mathematics, as anyone knows who has published a paper and has had to fill in much of the mathematics by hand on the typescript. While it is not impossible to represent almost any algorithmic language with any

character set, reasonable transparency of interpretation and ease of punching need at least the 88 type slugs potentially available on current electrical typewriters, even when non-escaping keys or similar tricks are used in order to increase the effective number of available characters. A considerable loss in transparency or convenience results from providing a double-case full point or from wasting both cases of one key on an erase symbol.

The rotating-head typewriter gives some improvement, in as much as the character set can be altered by exchanging the type head. A fully available set of 128 or 256 characters would be very much better, however, and this probably implies a non-mechanical method of printing. It would require 7- or 8-hole tape, in conformity with Dr. Barron's remarks.

The scale of money and effort needed to develop tape preparation equipment that is really suited to the needs of the user is small in comparison with that required to design and construct a medium-sized computer. If a computer manufacturer were to undertake this task, it would be surprising if the resultant increase in computer usage failed to recompense him for the investment. While it is undesirable to impose conformity at too early a stage, the Computer Society could help catalysing co-operation in these developments.

In a forthcoming issue of the *Automatic Programming Information Bulletin*, I urge the need for compilers to give the user the option of declaring his input and output hardware representations (including composite symbols) during input. Any manufacturer who in this way makes his computer directly compatible with the hardware representations of *all* potential users will evidently place himself at an advantage.

Yours faithfully,

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17 March 1964.