The solution of nonlinear ordinary differential equations in Chebyshev series

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The paper describes a simple iterative method for obtaining the solution of an ordinary differential equation in the form of a Chebyshev series. Nonlinear terms which occur in the equation are dealt with by evaluating their components at the Chebyshev points ($\cos r\pi/N$), performing the nonlinear operations and then deriving the representative Chebyshev series for the nonlinear term from its values at the Chebyshev points.

1. Introduction

In an earlier paper (Clenshaw, 1957) one of us has shown how an ordinary linear differential equation may be solved numerically in Chebyshev series. Where readily applicable, the method has considerable advantages over finite-difference methods, particularly for boundary-value problems. The method is such that by its very nature the *type* of boundary condition is irrelevant to the numerical procedure, so that boundary-value problems are solved with no more difficulty than initial-value problems.

The main drawback in practice is that the class of problems to which the method can be applied directly is limited by the requirement that the coefficients occurring in the differential equation must be polynomial functions of the independent variable. Although it is true that a much wider class of problems may be tackled by resorting to polynomial approximation of non-polynomial coefficients, such a procedure often raises its own difficulties. For when the polynomial coefficients are of high degree, the method involves the use of recurrence relations of high order, and is therefore cumbersome in operation.

It is natural, therefore, to consider other methods capable of exploiting the advantages of Chebyshev series expansions, while avoiding the restrictions inherent in the method mentioned above. One possibility, which we discuss in this paper, is to adopt the principle of Picard iteration [see Ince (1953), Chapter 3], while representing functions of the independent variable in Chebyshev series. This procedure enables us to attack not only linear differential equations with non-polynomial coefficients, but also nonlinear differential equations.

In the next section we outline the basic iterative procedure. Some properties of Chebyshev polynomials are discussed in Section 3, while Section 4 contains a description of a simple method of solution in which Chebyshev series are employed in the iterative procedure of Section 2. In Section 5 we consider the problem of determining the degree of Chebyshev series which is to be used at each stage of the computation. A simple extension of the method to second-order equations is given in Section 6.

2. Picard iteration

For simplicity we discuss the solution of the differential equation of the first order

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

with the associated boundary condition

$$y(\xi) = \eta. \tag{2}$$

It is easy to see that any differential equation which expresses the derivative of highest order explicitly in terms of the lower-order derivatives and the independent variable can be replaced by a system of equations, each of the form (1) [see Ince (1953) §3.3], but where f now represents a function of *all* the dependent variables. This form is thus of fundamental importance.

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

$$y_i = \eta + \int_0^x f(x, y_{i-1})dx, \tag{3}$$

starting with $y_0 = \eta$. It is clear that if this 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). It has been shown [see, for example, Ince (1953), Chapter 3] that if $f(x, y)$ and $\partial f/\partial y$ are bounded and f is of integrable modulus in a region of the (x, y) plane containing the point (ξ, η), then the sequence (3) does indeed converge to a solution in a neighbourhood of $x = \xi$.

Unfortunately, this convergence property is of limited value in the general problem. For, although the property remains valid for *systems* of equations of the form (1) in the case of initial-value problems, it is not applicable to the very case in which we are primarily interested, namely that of boundary-value problems. We shall, therefore, proceed to apply the iterative procedure with caution, and not expect convergence in general without some modification of the procedure.

3. Properties of Chebyshev polynomials

We henceforth assume without loss of generality that the finite range of variable in which we are interested has been transformed to $-1 \leqslant x \leqslant 1$. The Chebyshev polynomial of degree n appropriate to this range is defined by

$$T_n(x) = \cos(n \cos^{-1} x). \quad (4)$$

Accounts of the properties of these polynomials, and of their applications to problems of numerical analysis, may be found in Clenshaw (1962), Lanczos (1957) and National Bureau of Standards (1952). We now briefly discuss the particular properties which are of value in the solution of differential equations; they are all considered in greater detail in Clenshaw (1962).

It is known from the theory of Fourier series that any function which is continuous and of bounded variation in the range $-1 \leqslant x \leqslant 1$ possesses a unique convergent expansion of the form

$$f(x) = \tfrac{1}{2}c_0 + c_1T_1(x) + c_2T_2(x) + \ldots = \sum_{r=0}^{\infty}{}' c_rT_r(x),$$

say. (5)

If the series (5) is truncated at the term $c_nT_n(x)$, we have a polynomial approximation to $f(x)$ of degree n. It is found that in many cases of practical interest this approximation differs little from the "best" polynomial approximation of that degree, defined as the polynomial whose greatest deviation from $f(x)$ in the range $-1 \leqslant x \leqslant 1$ is as small as possible. In such cases the Chebyshev series provides a convenient and economical form of representation for the function.

The coefficients c_r for an arbitrary function $f(x)$ are determined to a specified accuracy by a summation formula.

For if $$f(x) = \sum_{s=0}^{N}{}'' \bar{c}_rT_r(x)$$

where $\sum''$ denotes a sum whose first and last terms are halved

(e.g. $\sum_{s=0}^{N}{}'' u_s = \tfrac{1}{2}u_0 + u_1 + u_2 + \ldots + u_{N-1} + \tfrac{1}{2}u_N$),

then

$$\bar{c}_r = \frac{2}{N}\sum_{s=0}^{N}{}'' f\left(\cos\frac{\pi s}{N}\right)\cos\frac{\pi rs}{N} \quad (r = 0, 1, 2, \ldots, N). \quad (6)$$

If N is now chosen to be so large that for $r \geqslant N$ the coefficients c_r in (5) are negligible, we may write with similar accuracy

$$c_r = \bar{c}_r(r = 0, 1, 2, \ldots, N-1),\ c_N = \tfrac{1}{2}\bar{c}_N. \quad (7)$$

The approximation of degree $n(\leqslant N)$, which we denote by

$$f_n(x) = \sum_{r=0}^{n}{}' c_rT_r(x), \quad (8)$$

may be evaluated by a recurrence procedure. It can be shown (Clenshaw, 1962) that if we form successively $b_n, b_{n-1}, b_{n-2}, \ldots, b_0$ from the relation

$$b_r = 2xb_{r+1} - b_{r+2} + c_r, \quad (9)$$

with $b_{n+1} = b_{n+2} = 0$, then we have $f_n(x) = \tfrac{1}{2}(b_0 - b_2)$.

It may be observed that a computer subroutine for evaluating $f_n(x)$ from the coefficients c_r in (8) may also be used to calculate the coefficients $\bar{c}_r$ from (6), given the function values $f(x_s) = f\left(\cos\frac{\pi s}{N}\right)$. For if we write $C_s = \frac{2}{N}f(x_s)$ for $s = 0, 1, 2, \ldots, N-1$, and $C_N = \frac{1}{N}f(-1)$, equation (6) becomes

$$\bar{c}_r = \sum_{s=0}^{N}{}' C_sT_s(x_r), \quad (10)$$

which is clearly of the same form as (8).

A Chebyshev series may be integrated readily. If we write

$$y = \sum_{r=0}^{\infty}{}' a_rT_r(x), \qquad \frac{dy}{dx} = \sum_{r=0}^{\infty}{}' a_r'T_r(x), \quad (11)$$

then we have

$$2ra_r = a_{r-1}' - a_{r+1}'. \quad (12)$$

This equation does not, of course, give a_0, which is a constant of integration.

To summarize this Section, we note that the coefficients in the Chebyshev series expansion of an arbitrary function $f(x)$ may be found from the summation formula (6). Truncation of this series furnishes a polynomial approximation $f_n(x)$ which may be evaluated for any argument value by recurrence using (9), and also integrated simply with the aid of (12). Use will be made of these properties in applying Chebyshev expansion techniques in conjunction with Picard iteration.

4. Use of Chebyshev series in Picard iteration

We now consider the details involved in carrying out the iterative procedure described in Section 2, while representing the functions y_i and their derivatives by polynomial approximations in the form of Chebyshev series. Let $y_{i-1}(x)$ be represented by a Chebyshev series of degree N:

$$y_{i-1}(x) = \sum_{r=0}^{N}{}' a_rT_r(x).$$

We have now to calculate the Chebyshev series for $f(x, y_{i-1})$, given an algorithm for computing the value of $f(x, y)$ for any (x, y) pair in the region of interest.

Since we no longer suppose $f(x, y)$ to be a linear function of y or a polynomial function of x, we must use a method of more general applicability than that of Clenshaw (1957). The summation formula (6) suggests such a method; it shows that a function which is adequately represented by $N + 1$ terms of its Chebyshev series may be equally well represented by its numerical values at $N + 1$ special points. The latter mode of representation has the advantage that nonlinear operations which are difficult to apply to the Chebyshev series may be readily applied to the function values.

The procedure to be adopted is therefore as follows. The Chebyshev series for y_{i-1} is evaluated at the points $x_s = \cos\frac{\pi s}{N}$ for $s = 0, 1, 2, \ldots, N$. The values of $f[x_s, y_{i-1}(x_s)]$ can then be calculated at each of these $N + 1$ points and equation (6) used to obtain the coefficients A_r' in the series

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

The integration required in the subsequent calculation of the Chebyshev series of y_i from (3) is then readily performed using (12). Thus the coefficients A_r $(r > 0)$ in the expansion

$$y_i(x) = \sum_{r=0}^{N+1}{}' A_r T_r(x),$$

are obtained from the relations

$$2rA_r = A_{r-1}' - A_{r+1}',\ r = 1, 2, 3, \ldots, N,$$
$$2(N+1)A_{N+1} = A_N',$$

and A_0 is determined from the boundary condition. For example, if the condition is $y(-1) = \eta$, we have

$$A_0 = 2[\eta + A_1 - A_2 + A_3 - \ldots + (-)^N A_{N+1}].$$

This sequence of operations represents one cycle. The process may be repeated until each member of the current set of coefficients differs from the corresponding member of the previous set by less than a prescribed amount, this amount being a measure of the accuracy required in the solution.

To illustrate the procedure we consider the simple example

$$y' + y = 0,\ y(0) = 1.$$

We take $N = 5$, and writing $y_i(x) = \sum_{r=0}^{5}{}' a_r^{(i)} T_r(x)$ we obtain the values given in Table 1, which also gives for comparison the leading coefficients a_r in the infinite Chebyshev series for e^{-x}.

Here the values in each column are given by the relations

$$2ra_r^{(i)} = -a_{r-1}^{(i-1)} + a_{r+1}^{(i-1)} \quad (0 < r \leqslant 5),$$
$$a_r^{(i)} = 0 \quad (r > 5),$$

and $$a_0^{(i)} = 2(1 + a_2^{(i)} - a_4^{(i)});$$

the latter condition arising from the boundary condition, $y(0) = 1$.

It is clear that for $i \leqslant N$ the Chebyshev series for $y_i(x)$ is merely the truncated Taylor series for e^{-x}, rearranged appropriately. This is a special feature of this example; we shall not expect the i^{th} iterate to be a simple truncation of the Taylor series in the *general* case. When $i > N$, however, this behaviour no longer persists, and it is of interest to continue the iterative procedure until the coefficients have settled down to a given accuracy, say 6 decimal places. This occurs at $i = 12$; the coefficients $a_r^{(12)}$ are accordingly given in Table 1.

Since $y_5(x)$ is a rearrangement of the truncated Taylor series for e^{-x}, it is clear that its maximum error occurs at $x = -1$ and is given by

$$e - \sum_{r=0}^{5}{}' (-)^r a_r^{(5)} = e - 2\cdot71\dot{6} = 0\cdot00162.$$

In contrast, comparison of the coefficients $a_r^{(12)}$ with a_r shows that the error of $y_{12}(x)$ can nowhere exceed

$$\sum_{r=0}^{5}{}' |a_r^{(12)} - a_r| + \sum_{r=6}^{\infty} |a_r| = 0\cdot00017. \qquad (13)$$

Thus continuation of the iterative process from $i = 5$ to $i = 12$ gives a significant gain in accuracy, even though the degree of the approximation has not been increased.

A less trivial example is afforded by the problem

$$y' = y^2, \qquad y(-1) = \tfrac{2}{5}.$$

Since the equation is nonlinear, the successive iterates will no longer bear any simple relation to the Taylor series for the solution, which is known to be $(\frac{3}{2} - x)^{-1}$. The iterations were carried out on the N.P.L. ACE

Table 1

Approximations to e^x

r	$a_r^{(0)}$	$a_r^{(1)}$	$a_r^{(2)}$	$a_r^{(3)}$	$a_r^{(4)}$	$a_r^{(5)}$	$a_r^{(12)}$	a_r
0	+2	+2	$+\frac{5}{2}$	$+\frac{5}{2}$	$+\frac{81}{32}$	$+\frac{81}{32} = +2\cdot531250$	$+2\cdot532020$	$+2\cdot532132$
1	0	−1	−1	$-\frac{9}{8}$	$-\frac{9}{8}$	$-\frac{217}{192} = -1\cdot130208$	$-1\cdot130268$	$-1\cdot130318$
2	0	0	$+\frac{1}{4}$	$+\frac{1}{4}$	$+\frac{13}{48}$	$+\frac{13}{48} = +0\cdot270833$	$+0\cdot271483$	$+0\cdot271495$
3	0	0	0	$-\frac{1}{24}$	$-\frac{1}{24}$	$-\frac{17}{384} = -0\cdot044271$	$-0\cdot044335$	$-0\cdot044337$
4	0	0	0	0	$+\frac{1}{192}$	$+\frac{1}{192} = +0\cdot005208$	$+0\cdot005473$	$+0\cdot005474$
5	0	0	0	0	0	$-\frac{1}{1920} = -0\cdot000521$	$-0\cdot000547$	$-0\cdot000543$
6								$+0\cdot000045$
7								$-0\cdot000003$

computer, with $N = 30$. The coefficients showed no change in the 11th decimal place after 22 iterations, and they are given to this accuracy in Table 2. It can be seen that they are correct to within a unit of the last figure, by comparison with the exact expression for the coefficients in the infinite Chebyshev expansion, given by

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

An upper bound for the error in $y(x)$ for any x in the range $-1 \leqslant x \leqslant 1$ can be readily estimated in a manner similar to that used above in (13). The error of $y_i(x)$ can nowhere exceed

$$\sum_{r=0}^{N}{}' |a_r^{(i)} - a_r| + \sum_{r=N+1}^{\infty} |a_r|,$$

where a_r is the coefficient in the infinite Chebyshev expansion. Although a_r is generally unknown, the second sum in this expression can be estimated by observation of the rate of convergence of the $a_r^{(i)}$, while the first may be regarded simply as the sum of a number of quantities which contain one-signed rounding errors. In our second example, for instance, we might estimate the truncation error as being $0 \cdot 6 \times 10^{-11}$, while the sum of the rounding errors should not exceed 14×10^{-11}, and probably does not exceed 4×10^{-11}.

Table 2

Solution of $y' = y^2$, $y(-1) = \frac{2}{5}$

r	a_r	r	$10^{11}a_r$
0	1·78885 43820 0	14	25172 2
1	0·68328 15730 0	15	9614 9
2	0·26099 03370 0	16	3672 6
3	0·09968 94380 0	17	1402 8
4	0·03807 79770 0	18	535 8
5	0·01454 44929 9	19	204 7
6	0·00555 55019 7	20	78 2
7	0·00212 20129 3	21	29 9
8	0·00081 05368 1	22	11 4
9	0·00030 95975 1	23	4 4
10	0·00011 82557 3	24	1 7
11	0·00004 51696 7	25	6
12	0·00001 72532 8	26	2
13	0·00000 65901 7	27	1

5. Choice of N

Most of the arithmetic involved in the method described in Section 4 occurs in the calculation of the Chebyshev series for $f(x, y_{i-1})$ from the series for y_{i-1}. If the same degree of approximation N is used for both functions, then about $2N^2$ multiplications are required in each cycle, in addition to the arithmetic necessary to compute each value of $f(x, y)$. The minimum value of N which is necessary to represent both y and $f(x, y)$ to the desired accuracy will not, in general, be known in advance. Although no harm would result from the use of a value larger than necessary, this would clearly be uneconomic. Indeed, during the early iterations, when the approximation is poor, it may be desirable to use a value of N smaller than that ultimately required to achieve the full accuracy.

One possibility is to start with a moderate or small value, say $N = 4$, and then introduce further coefficients only when their inclusion appears necessary for further improvement of the solution. In order to program this method for a computer, we need a fully automatic and reliable criterion for deciding when to increase N.

The criterion may be based on a comparison of the magnitude of the later coefficients in the series for $y_i(x)$, with the difference between $y_{i-1}(x)$ and $y_i(x)$. This difference is in turn reflected in the change in the early (most significant) coefficients in the series for $y_i(x)$ from one cycle to the next. Accordingly, we have adopted the criterion that if, for a suitably chosen integer p ($\geqslant 0$),

$$|A_0 - a_0| + |A_1 - a_1| < |A_{N-p}| + |A_{N-p-1}|, \qquad (14)$$

and provided A_{N-1} and A_N are not both smaller than the permitted error (in which case the problem is solved), then we increase the value of N by 2. In (14) we have used (as in Section 4) a_r and A_r to represent the coefficients in the Chebyshev series for $y_{i-1}(x)$ and $y_i(x)$ respectively. Several examples have been tried with various values of p, and $p = 2$ seems the most satisfactory.

An alternative to (14) is obtained by replacing its right-hand side by $k(|A_N| + |A_{N-1}|)$. It is difficult to determine a value of k suitable for all problems, however; solutions with rapidly convergent Chebyshev series seem to demand a large value of k, while less well-behaved solutions may need a smaller value.

The inclusion of two terms rather than one in both members of the inequality (14) is designed to reduce the risk of its "freak" satisfaction which might otherwise arise if, for example, the alternate coefficients in the series are small or zero. A similar circumstance might *still* arise of course if *two* zero (or very small) coefficients are followed by larger coefficients. However, this unlikely occurrence would usually lead only to an occasional loss in efficiency, and very rarely to an erroneous result.

6. 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 technique is required. The frequent occurrence of second-order equations in practical problems, however, indicates the desirability of a more direct method attack for such problems. The obvious extension of (3) for the equation

$$y'' = f(x, y, y') \qquad (15)$$

is obtained by integrating

$$y_i'' = f(x, y_{i-1}, y'_{i-1}). \qquad (16)$$

Table 3

Solution of van der Pol's equation

r	a_r
0	+2·06806 63183 9
1	+1·02398 06778 3
2	−0·03279 45404 3
3	−0·02485 57498 6
4	−0·00136 68544 3
5	+0·00090 10786 3
6	+0·00013 65318 3
7	−0·00002 64079 5
8	−0·00000 87217 2
9	+ 3786 5
10	+ 4436 0
11	+ 255 6
12	− 186 3
13	− 30 7
14	+ 6 0
15	+ 2 1
16	− 1
17	− 1

From the Chebyshev series for y_{i-1} and y'_{i-1}, their values at the points $x_s = \cos \frac{s\pi}{N}$ may be computed, and hence the values of $f(x_s, y_{i-1}(x_s), y'_{i-1}(x_s))$. With the aid of the summation formula (6), we can then compute the coefficients A''_r in

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

Then using the relations

$$2rA'_r = A''_{r-1} - A''_{r+1} \text{ and } 2rA_r = A'_{r-1} - A'_{r+1} \quad (17)$$

we can calculate the coefficients A'_r and A_r in the expansions

$$y'_i = \sum_{r=0}^{n+1}{}' A'_r T_r(x) \text{ and } y_i = \sum_{r=0}^{n+2}{}' A_r T_r(x). \quad (18)$$

The coefficients A'_0, A_0 and A_1 cannot be found from (17); they are determined with the aid of the boundary conditions.

As an example we consider van der Pol's equation

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

with the boundary conditions

$$y(-\tfrac{1}{4}) = 0, \qquad y(+\tfrac{1}{4}) = 2.$$

Writing $t = \frac{1}{4}x$ and using primes to denote derivatives with respect to x we have

$$y'' = \tfrac{1}{4}(1 - y^2)y' - \tfrac{1}{16}y,$$

with

$$y(-1) = 0, \qquad y(+1) = 2.$$

The boundary conditions yield for A_0 and A_1 the expressions

$$A_0 = 2 - 2(A_2 + A_4 + A_6 + \ldots)$$
$$A_1 = 1 - (A_3 + A_5 + A_7 + \ldots).$$

We suppose that the coefficients are required to 11 decimal places; we find that 11 iterations are sufficient to achieve this accuracy, and the result is given in Table 3. In accordance with the procedure of Section 4, we may estimate the truncation error of this finite series to be less than 10^{-11}, and note that the error in $y(x)$ due to rounding errors should not exceed 9×10^{-11}, and probably does not exceed 3×10^{-11}.

7. Conclusions

The iterative method described in this paper can be used to obtain the numerical solution in Chebyshev series of a class of differential equations. The class includes many nonlinear problems to which the earlier methods using Chebyshev series (see Clenshaw, 1957, Lanczos, 1957) are not applicable. For many problems, however, the iterative procedure as herein described will fail to converge. As a simple example, the problem

$$y'' + \lambda^2 y = 0; \qquad y(-1) = 0, \quad y(+1) = 1$$

can be solved by the present method only when $\lambda < \frac{1}{2}\pi$.

We suggest that this essentially simple approach may serve as the basis for more powerful methods designed to solve nonlinear boundary-value problems. In a subsequent paper, techniques will be described which are designed to secure convergence in a wide class of problems for which the present method diverges, and also to reduce the number of iterations required in other cases.

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