APPLICATIONS OF CHEBYSHEV POLYNOMIALS IN NUMERICAL ANALYSIS.

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INTRODUCTION.

In this thesis, two applications of Chebyshev polynomials to the numerical solution of problems have been given. The thesis can be split into three almost independent parts. In Chapter 1, a brief review of the most important properties of Chebyshev polynomials is given. This is followed by a description of Clenshaw's method for the numerical solution of ordinary linear differential equations by the expansion of the unknown function and its derivatives directly in terms of their Chebyshev series. This work is the starting point of the whole thesis and it is appropriate to mention here my acknowledgements to Mr. C.W. Clenshaw who first introduced me to his method when we worked together in the Mathematics Division of the National Physical Laboratory, England. The work in this thesis is, however, entirely my own both in conception and development. To my knowledge, none of this work has been duplicated elsewhere.

In Chapters 2, 3 and 4 we consider the application of Chebyshev polynomials to the solution of the one-dimensional heat equation,

$$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial x^2}$$

In Chapters 2 and 3, we consider the range of x to be finite, and are able to compare the numerically found solutions with the analytic solutions in a couple of particular cases. These indicate that the method is a powerful one, yielding accurate numerical solutions for a comparatively small amount of computation.

In Chapter 4, we attempt to apply the method to the same equation, where the range of x is infinite. The independent variable x is first transformed to a new independent variable $\xi = \tanh x$. The algebraisation of the resulting equation is then straightforward. The numerical solution of these equations in a particular case, however, indicate that the resultant Chebyshev series expansions of θ are very slowly convergent. This casts considerable doubt on the utility of the method, and consequently it is considered to be a failure. It is nevertheless included in this thesis, as at first glance it appears to be a possible means of solving an essentially difficult problem.

In Chapter 5, a generalisation is made of Clenshaw's method to the solution of ordinary linear differential equations in terms of any of the ultraspherical polynomials. One of the objects of this exercise was to investigate whether the computation in Clenshaw's method might be reduced by using for example, Legendre polynomials. The answer is most emphatically, no; the Chebyshev polynomials being by far the simplest to use. The analysis does, however, give a fairly rapid means of finding the expansion of functions satisfying simple linear differential equations, in terms of Legendre polynomials. This is used in Chapter 6.

Chapter 6 is concerned with the second of our two problems, namely the numerical solution of non-singular linear integral equations of the Fredholm type. Again, the unknown function is expanded in a series of Chebyshev polynomials, and substitution of this series into the equation gives relations between the coefficients in the expansion which can be solved numerically. The cases of separable and non-separable kernels are investigated in detail. A comparison is also made with Crout's method of using Lagrangian type polynomial expansions for the unknown function. In the example considered, the Chebyshev series expansion to the same degree, gives a much more accurate solution than Crout's. Finally, we consider expansions in terms of Legendre polynomials, and this is illustrated by an example. The computations in these last two Chapters were done on desk machines.

Throughout this work, we notice that in cases where Chebyshev polynomials can be used, a considerable amount of precision can be obtained in the final result for a comparatively small amount of computing. The methods are not by any means as versatile as the more usual finite-difference methods. The Chebyshev series techniques used here depend, for their success, on a ready algebraisation of the particular problem. This is not always straightforward by any means. Consequently the method should not be used indiscriminately; a careful evaluation of the particular problem under consideration is always an essential preliminary. The methods should be considered as a useful supplement to the more standard techniques.

In this thesis we have not attempted to discuss the properties of expansions of functions in any set of orthogonal polynomials. The well known properties of Chebyshev expansions have been stated in Chapter 1. No attempt either has been made to find the minimax approximation to an arbitrary function, using the Chebyshev series as a first approximation. The view has been taken throughout, that the calculation of the coefficients in a Chebyshev (or Legendre) expansion is a sufficient end in itself. The calculation of the minimax approximation to a function defined as the solution of some differential equation with associated boundary conditions, should provide a useful topic for future research.

Of the publications arising out of this thesis; the contents of Chapters 2 and 3 were presented in a very abbreviated form at the First Australian Conference on Automatic Computing and Data Processing held in Sydney from May 24-27, 1960 in a paper entitled "The Numerical Solution of the Heat Equation using Chebyshev Series". A synopsis is given in the Proceedings of that Conference. Two other papers entitled "The Expansion of Functions in Ultraspherical Polynomials" and "The Numerical Solution of Integral

Equations using Chebyshev Polynomials", based on Chapters 5 and 6 respectively, have been accepted for publication in the Journal of the Australian Mathematical Society.

Finally, there remains the pleasant task of thanking those people who have assisted me with this work. Thanks are due to Dr. J. Bennett and Miss J. Elliott of the SILLIAC Laboratory for help with the computations of Chapter 3; and to Mr. R.G. Smart and Miss J. Campbell of the UTECOM Laboratory for those of Chapter 4. I would like to thank Professor R.B. Potts for many helpful suggestions, his willingness to listen patiently at all times to a multitude of ridiculous ideas, and for the readiness with which he has read and criticised all the written work of this thesis. Finally, my thanks are due to my wife Lesley who in spite of daily receding further from the typewriter did such an excellent job of the typing, which was not always transferred to the reproduced copies.

CHAPTER 1

PROPERTIES OF THE CHEBYSHEV POLYNOMIALS $T_n(x)$

1.1 Definitions.

The Chebyshev polynomial $T_n(x)$ of the first kind and of degree n is defined for $-1 \leq x \leq 1$ by,

(1.1.1) $$T_n(x) = \cos n\theta \quad \text{where} \quad x = \cos\theta.$$

These polynomials are just one member of the set of ultra-spherical (or Gegenbauer) polynomials. The ultra-spherical polynomial $P_n^{(\lambda)}(x)$ of degree n and order λ is defined by

(1.1.2) $$P_n^{(\lambda)}(x) = \frac{\Gamma(n+2\lambda)\Gamma(\lambda+\frac{1}{2})(-1)^n}{\Gamma(2\lambda)\Gamma(n+\lambda+\frac{1}{2})2^n\, n!}(1-x^2)^{-\lambda+\frac{1}{2}}\frac{d^n}{dx^n}\left[(1-x^2)^{n+\lambda-\frac{1}{2}}\right],$$

for n = 0, 1, 2, - - - . The $T_n(x)$ polynomials correspond to λ = 0 although the standardisation constant is different from that in equation (1.1.2).

In fact,

(1.1.3) $$T_n(x) = \frac{n}{2}\lim_{\lambda\to 0}\frac{1}{\lambda}P_n^{(\lambda)}(x).$$

The other most commonly used ultra-spherical polynomials are (1) the Legendre polynomials $P_n(x)$, corresponding to $\lambda = \frac{1}{2}$; (2) the Chebyshev polynomials $U_n(x)$ of the second kind, corresponding to λ = 1 and (3) the polynomials x^n which are obtained in the limit as $\lambda \to \infty$. For (1) and (2), the polynomials are obtained by the direct substitution of the appropriate value of λ in equation (1.1.2). For a given value of λ, the polynomials $P_n^{(\lambda)}(x)$ for n = 0, 1, 2, - - - - form a complete orthogonal set of functions in $-1 \leq x \leq 1$, the orthogonality being with respect to the weight function

$$w(x) = (1-x^2)^{\lambda - 1/2}$$

An alternative definition for $U_n(x)$ is given by,

(1.1.4) $$U_n(x) = \frac{\sin(n+1)\theta}{\sin\theta} \quad \text{where} \quad x = \cos\theta.$$

We shall also require the definition of the "shifted" Chebyshev polynomial $T_n^*(x)$ which is defined for $0 \leq x \leq 1$ by,

(1.1.5) $$T_n^*(x) = \cos n\theta \quad \text{where} \quad 2x-1 = \cos\theta$$

The relation between $T_n(x)$ and $T_n^*(x)$ is given by,

(1.1.6) $$T_n^*(x) = T_n(2x-1) = T_{2n}(\sqrt{x}).$$

1.2 Properties of $T_n(x)$.

There are two important properties of the $T_n(x)$ polynomials which we shall note here.

An arbitrary analytic function $f(x)$ can be expanded in an infinite series of the ultra-spherical polynomials $P_n^{(\lambda)}(x)$ by the relations,

(1.2.1) $$f(x) = \sum_{n=0}^{\infty} a_n^{(\lambda)} P_n^{(\lambda)}(x)$$

$$\text{where} \quad a_n^{(\lambda)} = \frac{\Gamma(2\lambda)(n+\lambda)\,n!\,\Gamma(\lambda)}{\sqrt{\pi}\,.\,\Gamma(n+2\lambda)\,.\,\Gamma(\lambda+\frac{1}{2})} \int_{-1}^{+1} (1-x^2)^{\lambda-\frac{1}{2}} P_n^{(\lambda)}(x)\,.\,f(x)\,dx$$

Lanczos (ref. 1), has shown that of all expansions for different $P_n^{(\lambda)}(x)$, that corresponding to $\lambda = 0$ (i.e. $T_n(x)$

polynomials) gives the most rapid convergence of the coefficients $a_n^{(\lambda)}$. On the other hand, the expansion corresponding to $\lambda = \infty$ (the Taylor series expansion about x = 0) gives the least rapid convergence of the coefficients.

Bernstein (ref. 2) has defined the polynomial $p_N(x)$ of degree N, of "best fit" to f(x), in the range $-1 \leq x \leq 1$ to be that polynomial for which

$$\max_{-1 \leq x \leq 1} \left| f(x) - p_N(x) \right|$$

is least. Furthermore he shows that the quantity

$$f(x) - p_N(x)$$

obtains its greatest numerical value at least (N + 2) times in $-1 \leq x \leq 1$, and changes sign successively at these points. Consider the expansion of f(x) in terms of the $T_n(x)$ polynomials, i.e.

$$f(x) = \frac{1}{2} a_0 + \sum_{n=1}^{N} a_n T_n(x) \tag{1.2.2}$$

(The coefficient ½ is included for later convenience).

Then the remainder $R_N(x)$ is given by,

$$R_N(x) = f(x) - \left[\frac{1}{2} a_0 + \sum_{n=1}^{N} a_n T_n(x) \right] = \sum_{n=N+1}^{\infty} a_n T_n(x). \tag{1.2.3}$$

Suppose $R_N(x)$ can be closely approximated by the single term $a_{N+1} T_{N+1}(x)$. The polynomial $T_{N+1}(x)$ is such that it attains its maximum value ± 1 at (N + 2) points in $-1 \leq x \leq 1$ i.e. including the end points. Thus if f(x) were a polynomial of degree (N + 1), the expansion (1.2.2) would give exactly the polynomial of best fit of degree N.

In general f(x) is not, of course, a polynomial of degree (N + 1), but the rapid convergence of the coefficients a_n frequently allows the remainder $R_N(x)$ to be closely approximated by the term $a_{N+1} T_{N+1}(x)$. Hence, for many functions f(x), we find the expansion (1.2.2) to be a close approximation to the polynomial of best fit to f(x).

These two properties together make the polynomials $T_n(x)$, very useful to the numerical analyst. In the following section, and in Chapters 2, 3, 4 and 6 we shall be concerned mostly with expansions in terms of the $T_n(x)$ and $T_n^*(x)$ polynomials. In Chapter 5, we shall discuss the general expansion in terms of the ultra-spherical polynomials $P_n^{(\lambda)}(x)$.

There is one more result concerning the expansion of an arbitrary function f(x) in terms of the $T_n(x)$ polynomials which we shall quote here.

If
$$f(x) = \tfrac{1}{2} a_0 + \sum_{n=1}^{\infty} a_n T_n(x)$$

then

$$a_n = \frac{2}{\pi} \int_{-1}^{+1} \frac{f(x)\, T_n(x)}{\sqrt{1 - x^2}}\, dx$$

(1.2.4)

$$= \frac{2}{\pi} \int_{0}^{\pi} f(\cos\theta) \cos n\theta \, d\theta .$$

1.3 Solution of differential equations in terms of $T_n(x)$.

Clenshaw (ref. 3) has shown how an ordinary linear differential equation with associated boundary conditions can be solved directly in terms of a series of Chebyshev polynomials $T_n(x)$. In this Section, we shall describe

Clenshaw's method in some detail; and in the next we shall consider a fairly trivial example to which the solution can be found analytically, and which will be of considerable interest in Chapter 3.

Suppose we have an m th. order linear differential equation in the range $-1 \leqslant x \leqslant 1$, given by,

(1.3.1) $$p_m(x)\frac{d^m y}{dx^m} + p_{m-1}(x)\frac{d^{m-1}y}{dx^{m-1}} + \cdots + p_0(x)y = q(x)$$

where $q(x), p_0(x), p_1(x), \cdots p_m(x)$ are given functions of x only. Together with this equation there will be m boundary conditions, and in cases where both the differential equation and boundary conditions are homogeneous, a further normalising condition. Unlike the methods of numerical solution of differential equations by finite differences, it is immaterial whether the boundary conditions form an initial or a boundary value problem. If it is known that y is continuous in the closed interval $-1 \leqslant x \leqslant 1$, then we can write,

(1.3.2) $$y(x) = \tfrac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n T_n(x).$$

The sth. derivative of y can be written formally as,

(1.3.3) $$y^{(s)}(x) = \tfrac{1}{2}a_0^{(s)} + \sum_{n=1}^{\infty} a_n^{(s)} T_n(x) \quad , \quad s = 1, 2, \cdots, m$$

(For a full discussion on the validity of these expansions, see Chapter 5, Section 2).

From the relation,

(1.3.4) $$2\frac{dT_n(x)}{dx} = \frac{1}{(n+1)}T_{n+1}(x) - \frac{1}{(n-1)}T_{n-1}(x)$$

it can be shown that,

(1.3.5) $$2n a_n^{(s)} = a_{n-1}^{(s+1)} - a_{n+1}^{(s+1)}$$

This is a relation between the coefficients in the Chebyshev expansion of $y^{(s)}(x)$ and $y^{(s+1)}(x)$.

Also, from

(1.3.6) $$2x T_n(x) = T_{n+1}(x) + T_{n-1}(x) \quad ;$$

if $C_n(y)$ denotes the coefficient of $T_n(x)$ in the expansion of y, then

(1.3.7) $$C_n(xy) = \frac{1}{2}(a_{n-1} + a_{n+1}).$$

Continued application of this equation gives the relation between the coefficients in the expansion of $x^r y$ and y, for all r = 1, 2, - - - - as,

(1.3.8) $$C_n(x^r y) = \frac{1}{2^r}\sum_{j=0}^{r}\binom{r}{j} a_{|n-r+2j|}$$

If the coefficients $p_0(x), p_1(x), \ldots\ldots, p_m(x)$ in equation (1.3.1) are polynomials in x, then equation (1.3.8) gives us fairly rapidly the n th. coefficient in the Chebyshev expansion of $p_r(x)\frac{d^r y}{dx^r}$ in terms of $a_n^{(r)}$ for r = 0, 1, - - -, m. In cases where $p_r(x)$ are not polynomials in x, they can be replaced by suitable polynomial approximations. By using equation (1.3.8), and equating coefficients of $T_n(x)$ on each side of equation (1.3.1) for all n, we obtain a system of linear equations for the unknown coefficients $a_n^{(s)}$ for s = 0, 1, - - -, m and all n. The use of equation (1.3.5) frequently enables us to remove the coefficients $a_n^{(s)}$ corresponding to the largest values of S. These equations and those obtained from the boundary conditions can be solved numerically either by a recurrence or an iterative method, which have been described in detail by Clenshaw and will be referred to again in Chapter 5.

It is worthwhile to note here the simple forms taken by the Chebyshev series at the points x = 0, ± 1 :

$$\text{(1.3.9)} \quad \begin{cases} y(0) = \frac{1}{2}a_0 - a_2 + a_4 - a_6 + a_8 - a_{10} + \cdots\cdots \\ y(-1) = \frac{1}{2}a_0 - a_1 + a_2 - a_3 + a_4 - a_5 + \cdots\cdots \\ y(1) = \frac{1}{2}a_0 + a_1 + a_2 + a_3 + a_4 + a_5 + \cdots\cdots \end{cases}$$

These results are useful since boundary conditions are frequently specified at either the end points or the mid-point of the range.

Similar results can be found for expansions in terms of the shifted Chebyshev polynomials $T_n^*(x)$, valid for $0 \leq x \leq 1$. If,

$$y^{(s)}(x) = \frac{1}{2}A_0^{(s)} + \sum_{n=1}^{\infty} A_n^{(s)} T_n^*(x)$$

for s = 0, 1, 2, - - - -, then the results corresponding to equations (1.3.5), (1.3.8) and (1.3.9) are given by

$$\text{(1.3.5A)} \qquad 4n A_n^{(s)} = A_{n-1}^{(s+1)} - A_{n+1}^{(s+1)}$$

$$\text{(1.3.8A)} \qquad C_n^*(x^r y) = \frac{1}{2^{2r}} \sum_{j=0}^{2r} \binom{2r}{j} A_{|n-r+j|}$$

where $C_n^*(f)$ denotes the coefficient of $T_n^*(x)$ in the Chebyshev expansion of f, and

$$(1.3.9A)\quad \begin{cases} y(0) = \frac{1}{2}A_0 - A_1 + A_2 - A_3 + A_4 - A_5 + \cdots\cdots \\ y(\frac{1}{2}) = \frac{1}{2}A_0 - A_2 + A_4 - A_6 + A_8 - A_{10} + \cdots\cdots \\ y(1) = \frac{1}{2}A_0 + A_1 + A_2 + A_3 + A_4 + A_5 + \cdots\cdots \end{cases}$$

1.4 An example using Clenshaw's method.

We shall illustrate the method by finding the Chebyshev expansion of the function $y = \cos(r + \frac{1}{2})\pi x$ in $-1 \leqslant x \leqslant 1$, for integer values of r. This function satisfies the differential equation

$$(1.4.1)\qquad \frac{d^2y}{dx^2} + (r + \tfrac{1}{2})^2\pi^2 y = 0$$

with the conditions y (0) = 1, $y'(0) = 0$.

As in Section (1.3), we assume that

$$y^{(s)}(x) = \frac{1}{2}a_0^{(s)} + \sum_{n=1}^{\infty} a_n^{(s)} T_n(x), \text{ for } s = 0, 1, 2.$$

(When refering to the function values we omit the superscript (0) and for the first and second derivatives, use a superscripted dash and double dash respectively). Equating the coefficients of $T_n(x)$ to zero for all n in equation (1.4.1) we have

$$(1.4.2)\qquad a_n'' + (r + \tfrac{1}{2})^2\pi^2 a_n = 0 \text{ for all } n = 0, 1, 2, \cdots\cdots$$

We shall solve these equations by the recurrence method, using equation (1.3.5) in the forms

$$(1.4.3)\quad a'_{n-1} = a'_{n+1} + 2na_n, \quad a''_{n-1} = a''_{n+1} + 2na_n.$$

In Table 1.1, we give the numerical solution to 6D for the case r = 0. We start the computation with $a_{10} = 1$, $a_{11} = a_{12} = \ldots\ldots = 0$, $a'_{10} = a'_{11} = \ldots\ldots = 0$, and $a''_{10} = a''_{11} = \ldots = 0$. Since the function is even in $-1 \leq x \leq 1$, we have immediately that a_n and a''_n are zero when n is odd and a'_n is zero when n is even. With the given initial values we use equation (1.4.3) to give a'_9 and a''_8 in turn. Equation (1.4.2) is used in the form

$$a_n = -0{\cdot}40528\ 47346\ a''_n$$

to give a_8, from which we compute a'_7 and a''_6 using again equation (1.4.3), and then a_6. The process is continued until we reach a_0.

n	a_n	a'_n	a''_n	normalised a_n	theoretical a_n
0	−205 58772	0	+507 26736	+0.944 002	+0.944 002
1	0	+387 81288	0	0	0
2	+108 76156	0	−268 35840	−0.499 403	−0.499 403
3	0	−47 23336	0	0	0
4	−6 09620	0	+15 04176	+0.027 992	+0.027 992
5	0	+1 53624	0	0	0
6	+ 12995	0	− 32064	−0.000 597	−0.000 597
7	0	− 2316	0	0	0
8	− 146	0	+ 360	+0.000 007	+0.000 007
9	0	+ 20	0	0	0
10	+ 1	0	0	0	0

$\cos \frac{1}{2}\pi x = 0{\cdot}472\ 001 \quad -0{\cdot}499\ 403\, T_2(x) + 0{\cdot}027\ 992\, T_4(x) - 0{\cdot}000\ 597\, T_6(x) + 0{\cdot}0^5 7\, T_8(x).$

Table 1.1

Having computed all a_n, a'_n, a''_n by the method described above, the solution has to be normalised in order to give $y(0) = 1$. This is done by multiplying the a_n computed by $-1/2177\ 8329$, the denominator being the value of $\frac{1}{2}a_0 + \sum_{n=1}^{5}(-1)^n a_{2n}$ of the computed a_n. The required value of the coefficients in the Chebyshev expansion of $\cos\frac{1}{2}\pi x$ are given in the column headed "normalised a_n". For other values of r, a similar computation can be carried out.

The Chebyshev expansion of this simple function can also be found analytically. This is shown in the next Section, where we also derive the properties of an important matrix $\underset{\sim}{\Gamma}$ which will appear later, in Chapter 3.

1.5 The matrix $\underset{\sim}{\Gamma}$.

In the previous section we described how Clenshaw's method can be used to find numerically the coefficients in the Chebyshev expansion of $\cos(r+\frac{1}{2})\pi x$, and illustrated the method in the case of r = 0.

From equation (1.2.4), we have that the coefficients are given directly by

(1.5.1) $$a_n = \frac{2}{\pi}\int_{-1}^{+1}\frac{\cos(r+\frac{1}{2})\pi x . T_n(x)}{\sqrt{1-x^2}}\,dx$$

Obviously when n is odd, a_n is zero since the integrand is then an odd function of x. In the case of n even ($= 2m$, say) the integral in equation (1.5.1) is closely related to the Bessel function $J_{2m}(x)$ of the first kind and of order $2m$.

The Bessel function $J_{2m}(x)$ can be defined by (see, for example, ref. 4)

(1.5.2) $$J_{2m}(x) = \frac{1}{\pi}\int_0^{\pi}\cos(x\sin\theta - 2m\theta)\,d\theta$$

Writing $\theta = \phi + \frac{\pi}{2}$, and expanding the integrand we have,

$$J_{2m}(x) = \frac{2(-1)^m}{\pi}\int_0^{\pi/2} \cos(x\cos\phi).\cos 2m\phi . d\phi,$$

the second integral being zero. If we further write

$t = \cos\phi$, then

$$J_{2m}(x) = \frac{(-1)^m}{\pi}\int_{-1}^{+1} \frac{\cos(xt)\,T_{2m}(t)}{\sqrt{1-t^2}}\,dt.$$

Hence we have immediately that

$$a_{2m} = 2(-1)^m J_{2m}\left[(r+\tfrac{1}{2})\pi\right] \tag{1.5.3}$$

for m = 0, 1, 2, - - - - and all r.

The comparison of the theoretical value with the numerically calculated value for r = 0 is given in Table 1.1 The results are in exact agreement to 6D.

Let us look now in more detail at equations (1.4.2). If we apply the results of equation (1.3.5) twice to this equation, we find the following relation between the coefficients a_{2m} $(n = 2m)$

$$a_{2m} + (r+\tfrac{1}{2})^2\pi^2\left[\frac{a_{2m-2}}{8m(2m-1)} - \frac{a_{2m}}{2(4m^2-1)} + \frac{a_{2m+2}}{8m(2m+1)}\right] = 0 \tag{1.5.4}$$

valid for m = 1, 2, - - - - -. For the purposes of this Section, we will not use the boundary conditions as given in equation (1.4.1), but will use the fact that $\cos(r+\frac{1}{2})\pi x$ is zero when x = 1, so that,

$$\tfrac{1}{2}a_0 + \sum_{m=1}^{\infty} a_{2m} = 0 \tag{1.5.5}$$

If, from equation (1.5.5), we subtract equations (1.5.4) for all values of m, we find

$$\tfrac{1}{2}a_0 - \frac{(r+\frac{1}{2})^2\pi^2}{4}\left[\tfrac{1}{2}a_0 - \tfrac{7}{12}a_2 + \sum_{m=2}^{\infty}\frac{3}{(m^2-1)(4m^2-1)}a_{2m}\right] = 0. \tag{1.5.6}$$

On further rearrangement of equations (1.5.4) and (1.5.6) we find the following system of equations

$$
(1.5.7)\quad \begin{cases} -a_0 + \frac{7}{6} a_2 - \sum_{m=2}^{\infty} \frac{24}{(4m^2-4)(4m^2-1)} a_{2m} = -\frac{16}{(2r+1)^2\pi^2} a_0 \\ \frac{1}{2m(2m-1)} a_{2m-2} - \frac{2}{(4m^2-1)} a_{2m} + \frac{1}{2m(2m+1)} a_{2m+2} \\ \text{for } m = 1, 2, \ldots \qquad = -\frac{16}{(2r+1)^2\pi^2} a_{2m} \end{cases}
$$

Equations (1.5.7) can be written in the matrix form

$$
(1.5.8)\qquad \underset{\sim}{P}\,\underset{\sim}{a} = -\frac{16}{(2r+1)^2\pi^2}\,\underset{\sim}{a}
$$

where $\underset{\sim}{a}$ is the column vector $\{a_0, a_2, \ldots\}$ and $\underset{\sim}{P}$ is the matrix (p_{ij}) $i = 0, 1, 2, \ldots$, $j = 0, 1, 2, \ldots$ given by

$$
(1.5.9)\quad \begin{cases} p_{00} = -1,\ p_{01} = \frac{7}{6},\ p_{0j} = \frac{-24}{(4j^2-4)(4j^2-1)} \text{ for } j = 2, 3, 4, \ldots \\ p_{i0} = \ldots = p_{i,i-2} = 0,\ p_{i,i-1} = \frac{1}{2i(2i-1)},\ p_{i,i} = -\frac{2}{(4i^2-1)} \\ \text{for all } i \geq 1 \qquad p_{i,i+1} = \frac{1}{2i(2i+1)},\ p_{i,i+2} = \ldots = 0 \end{cases}
$$

From equation (1.5.8) we have that the latent roots of the infinite matrix $\underset{\sim}{P}$ are given by

$$
\lambda_r = -\frac{16}{(2r+1)^2\pi^2} \quad \text{for } r = 0, 1, 2, \ldots
$$

These results for the matrix $\underset{\sim}{P}$ will be used in Chapter 3, where we shall compare its analytic properties with the numerical solution of the one-dimensional heat equation in a particular case.

CHAPTER 2

THE ONE-DIMENSIONAL HEAT EQUATION.

2.1 Statement of the problem.

The major part of this thesis is concerned with the application of Chebyshev polynomials to the solution of linear partial differential equations of the parabolic type. In this Chapter we shall consider the numerical solution of the equation,

$$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial x^2}, \tag{2.1.1}$$

for $t \geqslant 0$, where we assume that the range of x has been adjusted to $-1 \leqslant x \leqslant 1$. This equation is the well known heat (or diffusion) equation in one (space) dimension. In these contexts the variable t represents the time, x some space co-ordinate, and $\theta(x,t)$ the temperature (or concentration). We shall frequently refer to these variables with such physical interpretation in mind.

Along the boundaries $x = \pm 1$, we specify general linear boundary conditions of the form,

$$\left\{ \begin{array}{l} \lambda_1 \theta + \mu_1 \dfrac{\partial \theta}{\partial x} = \phi_1(t) \quad \text{along } x = +1 \\ \text{and } \lambda_{-1} \theta + \mu_{-1} \dfrac{\partial \theta}{\partial x} = \phi_{-1}(t) \quad \text{along } x = -1, \end{array} \right. \tag{2.1.2}$$

where $\phi_1(t)$, $\phi_{-1}(t)$ are given functions of the time t, and λ_1, μ_1, λ_{-1}, μ_{-1} are constants. Together with these boundary conditions, there will be an initial condition of the form,

$$\theta = f(x) \quad \text{for } -1 \leqslant x \leqslant 1, \quad t = 0. \tag{2.1.3}$$

We shall assume that the Chebyshev expansion of $f(x)$ is known.

In Chapter 4, we shall again consider equation (2.1.1) in the case where the range of x is infinite. In order to use Chebyshev polynomials, the space variable has first to be transformed to a new variable ξ, say, such that $-1 \leq \xi \leq 1$. The most suitable form of transformation is found to be

$$\xi = \tanh x$$

The partial differential equation is then of the form

$$\frac{\partial \theta}{\partial t} = p_2(\xi)\frac{\partial^2\theta}{\partial \xi^2} + p_1(\xi)\frac{\partial \theta}{\partial \xi} + p_0(\xi)\theta \tag{2.1.4}$$

where p_0, p_1 and p_2 are polynomials in ξ. This is the most general form of the equation which can be solved by the method of Chebyshev polynomials.

In the case of equation (2.1.1), however, we can compare our numerical solutions with known analytic solutions, and this enables us to make a detailed analysis of the method. For the infinite range, we are not so fortunately placed, and can only use the results of the finite range to guide the method of numerical solution.

2.2 Brief Review of Finite Difference methods of Solution.

The usual way of finding numerical solutions of equations (2.1.1), (2.1.2) and (2.1.3), is to replace both derivatives by some finite difference approximations, and to solve the resulting system of difference equations numerically using some form of digital computer. It has been found that there are stability problems, arising from the behaviour of the rounding-off error, which depend upon the form in which the difference approximations to the derivatives are made. Richtmeyer (reference 5) gives a full discussion of these problems.

Consider the (x,t) plane covered with a mesh of width $\delta x, \delta t$. Any point (x, t) in the plane can then be represented by a number pair (m, n) where

$$x = m.\delta x \quad , \quad t = n.\delta t,$$

and we shall write $\theta(m\delta x, n\delta t)$ as $\theta_{m,n}$. Richardson, in his pioneer work on the subject, replaced the partial differential equation at the point (x,t) by the partial difference equation,

$$\frac{\theta_{m,n+1} - \theta_{m,n-1}}{2\delta t} = \frac{\theta_{m-1,n} - 2\theta_{m,n} + \theta_{m+1,n}}{(\delta x)^2} \tag{2.2.1}$$

There is a truncation error in this equation, but this is originally taken to be zero. The only unknown quantity in equation (2.2.1) is $\theta_{m,n+1}$ which can be expressed in terms of the remaining known functions. Such a form is said to be "explicit". It can be shown, however, that in the repeated application of equation (2.2.1), the round-off errors will dominate the required solution for all values of

$$r = \frac{\delta t}{(\delta x)^2} > 0$$

Thus, the above finite-difference representation of the partial differential equation is useless for computing purposes. (Richardson was unaware of this since he only performed the integration up to a small value of t, and the round-off errors were still small at this stage. (Equation (2.2.1) is of the second order in the t-direction, whereas equation (2.1.1) is only of the first order. It is now realised that replacing a differential equation by a higher order difference equation frequently leads to spurious solutions being introduced, which may swamp the required solution).

Another explicit system of difference equations can be found by replacing $\frac{\partial \theta}{\partial t}$ by $\frac{\theta_{m,n+1} - \theta_{m,n}}{\delta t}$, to give,

(2.2.2) $\theta_{m,n+1} = \theta_{m,n} + r(\theta_{m-1,n} - 2\theta_{m,n} + \theta_{m+1,n})$

The numerical solution of these equations remains stable provided $r \leq 1/2$. This means that δt and δx cannot be chosen independently and, for example, with a fixed r, if we halve δx then we must take a quarter of δt. In many cases, this means that we must take a large number of steps over a small interval δt, in order to keep the truncation error within specified limits.

An alternative method of approach is to use an "implicit" representation of the partial differential equation where the difference equation now contains more than one unknown value of θ at $t = (n+1)\delta t$. For example, if we replace the derivatives by differences at the point $(x, t + \frac{1}{2}\delta t)$ we find a system of equations

(2.2.3) $\theta_{m,n+1} - \theta_{m,n} = \frac{r}{2}\left[\begin{array}{l}\theta_{m-1,n+1} - 2\theta_{m,n+1} + \theta_{m+1,n+1} \\ + \theta_{m-1,n} - 2\theta_{m,n} + \theta_{m+1,n}\end{array}\right]$

These equations are stable for all $r \geq 0$, however, over each step δt we must now solve a system of simultaneous equations. The values of δx and δt can now be chosen independently of each other (compatible with the allowable truncation error). The amount of computation over each step δt is now greater than for equation (2.2.2), but we can generally take a larger value for δt than before.

Many other implicit forms of equations can be used, and these are fully discussed in reference 5. We shall say no more about them here.

2.3 The method of Hartree and Womersley.

A rather different method for the solution of equation (2.1.1) has been given by Hartree and Womersley (reference 6). They replace only the time derivative by a finite-difference approximation, and consider the resulting system of ordinary differential equations. Considering now only the t-direction subdivided into intervals of width δt, we can replace equation (2.1.1) at the point $t_0 + \frac{1}{2}\delta t$ by,

$$(2.3.1) \qquad \frac{\theta_1 - \theta_0}{\delta t} = \frac{1}{2}\left[\frac{d^2\theta_0}{dx^2} + \frac{d^2\theta_1}{dx^2}\right] + O(\delta t)^2$$

The subscripts $0, 1$ denote values at the times t_0 and $t_0 + \delta t$, respectively. Once again neglecting the truncation error, equation (2.3.1) represents a two-point boundary value problem (from the boundary conditions at $x = \pm 1$), where θ_0 is known and θ_1 is the function to be found. Having determined $\theta_1(x)$, this becomes the new $\theta_0(x)$ over the next interval δt. In this way the integration can proceed in the t-direction, and the truncation error depends only upon the value of δt. Hartree and Womersley proposed solving equation (2.3.1) by means of an analogue computer, and in particular a differential analyser.

There is one important fact which must be noted. In solving equation (2.3.1) it is assumed that the truncation error is small enough to be neglected in a first approximation. This will only be the case provided that the function $\theta(x,t)$ has no singularities and in particular that there is no singularity initially. The initial function $f(x)$ must therefore satisfy the boundary conditions along $x = \pm 1$. If this is not the case, the initial singularity must be removed in some way.

2.4 The Method of Chebyshev Polynomials.

In the method to be described here we solve a slightly modified form of equation (2.3.1), using Clenshaw's method of direct expansion in Chebyshev polynomials. We choose as the dependent variable not $\theta_1(x)$ but the function

$$g(x) = \theta_1(x) - \theta_0(x)$$

Neglecting the truncation error, the equation for $g(x)$ is given by

(2.4.1) $$\frac{d^2 g}{dx^2} - 2kg = -2\frac{d^2\theta_0}{dx^2} \quad \text{for } -1 \leq x \leq 1$$

where $k = 1/\delta t$. We write,

(2.4.2) $$\begin{cases} g(x) = \frac{1}{2}a_0 + \sum_{n=1}^{N} a_n T_n(x) \\ \theta_0(x) = \frac{1}{2}b_0 + \sum_{n=1}^{N} b_n T_n(x), \end{cases}$$

with similar expressions for the first and second derivatives except that they are polynomials of degree (N-1) and (N-2) respectively. On substituting expansions (2.4.2) into equation (2.4.1) and equating coefficients of $T_n(x)$, we obtain,

(2.4.3) $$2k\,a_n = a_n'' + 2b_n'' \text{ for } n = 0, 1, 2, \dots, N-2.$$

Applying equation (1.3.5) once, gives

(2.4.4) $$a_n' + 2b_n' = \frac{k}{n}\left(a_{n-1} - a_{n+1}\right) \text{ for } n = 1, 2, \dots, N-1.$$

Using equation (1.3.5) again, we find the following relation between the a_n and b_n coefficients,

(2.4.5) $$\frac{k}{4n(n-1)}\,a_{n-2} - \left[\frac{1}{2} + \frac{k}{2(n^2-1)}\right]a_n + \frac{k}{4n(n+1)}\,a_{n+2} = b_n$$

for n = 2, 3, - -, N provided we take $a_{N+1} = a_{N+2} = 0$.

These equations are of a fairly simple form. To find those corresponding to n = 0 and 1, we must investigate the boundary conditions along x = ±1.

2.5 The Boundary Conditions along x = ±1.

We shall first consider how the boundary condition along x = 1 can be expressed in terms of a_n and b_n. The corresponding condition along x = -1 will then be quoted without proof, since its derivation is similar to that along x = 1.

From the boundary conditions at $t = t_1$, and $t = t_0$, on subtracting we find

(2.5.1) $$\lambda_1 g + \mu_1 \frac{dg}{dx} = \phi_1(t_1) - \phi_1(t_0) \text{ for } x = 1.$$

Rewriting this in terms of a_n, a'_n and using equation (1.3.9) we have,

$$(2.5.2)\quad \lambda_1\left[\tfrac{1}{2}a_0 + \sum_{n=1}^{N} a_n\right] + \mu_1\left[\tfrac{1}{2}a'_0 + \sum_{n=1}^{N-1} a'_n\right] = \phi_1(t_1) - \phi_1(t_0)$$

From this equation we want to eliminate the a'_n. Now from the boundary condition at $t = t_0$, we have,

$$(2.5.3)\quad \lambda_1\left[\tfrac{1}{2}b_0 + \sum_{n=1}^{N} b_n\right] + \mu_1\left[\tfrac{1}{2}b'_0 + \sum_{n=1}^{N-1} b'_n\right] = \phi_1(t_0).$$

On adding twice equation (2.5.3) to equation (2.5.2) we get

$$(2.5.4)\quad \left\{\begin{aligned} &\lambda_1\left[\tfrac{1}{2}(a_0 + 2b_0) + \sum_{n=1}^{N}(a_n + 2b_n)\right] + \mu_1\left[\tfrac{1}{2}(a'_0 + 2b'_0) + \sum_{n=1}^{N-1}(a'_n + 2b'_n)\right] \\ &\qquad = \phi_1(t_1) + \phi_1(t_0). \end{aligned}\right.$$

From equations (2.4.5) and (2.4.4) we find, after some algebraic reduction,

$$(2.5.5)\quad \left\{\begin{aligned} \sum_{n=1}^{N}(a_n + 2b_n) = {}& a_1 + 2b_1 + k\Big\{\tfrac{1}{4}a_0 + \tfrac{1}{12}a_1 - \tfrac{7}{24}a_2 - \tfrac{1}{10}a_3 \\ &+ \sum_{n=4}^{N-2}\frac{6}{(n^2-4)(n^2-1)}a_n - \frac{(N-6)}{2N(N-2)(N-3)}a_{N-1} - \frac{(N-5)}{2(N-2)(N^2-1)}a_N\Big\} \end{aligned}\right.$$

and

$$(2.5.6)\quad \sum_{n=1}^{N-1}(a'_n + 2b'_n) = k\left\{a_0 + \tfrac{1}{2}a_1 - \sum_{n=2}^{N-2}\frac{2}{n^2-1}a_n - \frac{a_{N-1}}{N-2} - \frac{a_N}{N-1}\right\},$$

respectively. It now remains to find an expression for $(a'_0 + 2b'_0)$ in terms of a_n and b_n. Again, using equation (1.3.5) with n = 1, and equation (2.4.4) with n = 2, we find,

$$(2.5.7)\quad a'_0 + 2b'_0 = \frac{k}{2}(a_1 - a_3) + 2(a_1 + 2b_1)$$

Summing up, the boundary condition along x = 1 gives the following relation between the a_n and b_n :-

$$(2.5.8)\begin{cases} -a_0\left[\lambda_1\left(\frac{1}{2}+\frac{k}{4}\right)+k\mu_1\right]-a_1\left[\lambda_1\left(1+\frac{k}{12}\right)+\mu_1\left(1+\frac{3k}{4}\right)\right] \\ +a_2\left[\frac{7k}{24}\lambda_1+\frac{2k}{3}\mu_1\right]+a_3\left[\frac{k}{10}\lambda_1+\frac{k}{2}\mu_1\right] \\ -6k\lambda_1\sum_{n=4}^{N-2}\frac{1}{(n^2-4)(n^2-1)}a_n+2k\mu_1\sum_{n=4}^{N-2}\frac{1}{(n^2-1)}a_n \\ +a_{N-1}\left[\frac{(N-6)k\lambda_1}{2N(N-2)(N-3)}+\frac{k\mu_1}{(N-2)}\right] \\ +a_N\left[\frac{(N-5)k\lambda_1}{2(N-2)(N^2-1)}+\frac{k\mu_1}{(N-1)}\right] \\ =\lambda_1 b_0+2(\lambda_1+\mu_1)b_1-\phi_1(t_1)-\phi_1(t_0) \end{cases}$$

This equation is not very elegant. We notice, however, that all the unknown a_n appear on the left hand side, with all known quantities on the right hand side.

A similar expression is found for the boundary condition along x = -1, and is given by

$$(2.5.9)\begin{cases} -a_0\left[\lambda_{-1}\left(\frac{1}{2}+\frac{k}{4}\right)-k\mu_{-1}\right]-a_1\left[-\lambda_{-1}\left(1+\frac{k}{12}\right)+\mu_{-1}\left(1+\frac{3k}{4}\right)\right] \\ +a_2\left[\frac{7k}{24}\lambda_{-1}-\frac{2k}{3}\mu_{-1}\right]+a_3\left[-\frac{k}{10}\lambda_{-1}+\frac{k}{2}\mu_{-1}\right] \\ -6k\lambda_{-1}\sum_{n=4}^{N-2}\frac{(-1)^n}{(n^2-4)(n^2-1)}a_n-2k\mu_{-1}\sum_{n=4}^{N-2}\frac{(-1)^n}{(n^2-1)}a_n \\ +a_{N-1}\left[\frac{(-1)^{N-1}(N-6)k\lambda_{-1}}{2N(N-2)(N-3)}-\frac{(-1)^{N-1}k\mu_{-1}}{(N-2)}\right] \\ +a_N\left[\frac{(-1)^N(N-5)k\lambda_{-1}}{2(N-2)(N^2-1)}-\frac{(-1)^N k\mu_{-1}}{(N-1)}\right] \\ =\lambda_{-1}b_0+2(-\lambda_{-1}+\mu_{-1})b_1-\phi_{-1}(t_1)-\phi_{-1}(t_0) \end{cases}$$

2.6 Method of Solution.

Equations (2.4.5), (2.5.8) and (2.5.9) completely define the problem. On the left hand sides of the equations we have the unknown coefficients a_n, on the right hand sides all the quantities are known. Before representing these equations in matrix form, we further manipulate equations (2.5.8) and (2.5.9) to give two equations on the right hand sides of which we have quantities of the form $b_0^* = b_0 + \psi_0(t_0, t_1)$ and $b_1^* = b_1 + \psi_1(t_0, t_1)$ respectively. The quantities ψ_0 and ψ_1 are linear combinations of the functions $\phi_1(t_0), \phi_1(t_1), \phi_{-1}(t_0), \phi_{-1}(t_1)$ obtained from the above manipulation. The two new equations which we consider as replacing equations (2.5.8) and (2.5.9) are so messy algebraically that no attempt will be made to write them down here. When considering a particular problem within this general scheme, the elimination is generally straightforward.

The resulting system of modified equations can be written in the matrix form as

$$\underset{\sim}{M}_N(k)\, \underset{\sim}{a} = \underset{\sim}{b}^* \tag{2.6.1}$$

where $\underset{\sim}{a}$ is the column vector $\{a_0, a_1, \text{-----}\, a_N\}$, $\underset{\sim}{b}^*$ is the column vector $\{b_0^*, b_1^*, b_2^*, \ldots, b_N^*\}$ where $b_n^* = b_n$ for $n \geqslant 2$, and $\underset{\sim}{M}_N(k)$ is the square matrix of order $(N+1)$ of the coefficients in the equation. Its general form is

$$
M_N(k) = \begin{pmatrix}
\times & \times & \times & \times & \times & \cdots & \cdots & \times \\
\times & \times & \times & \times & \times & \cdots & \cdots & \times \\
\times & 0 & \times & 0 & \times & & & \\
 & \times & 0 & \times & 0 & \times & \text{zeros} & \\
 & & \cdot & & \ddots & & & \\
\text{zeros} & & & & & \ddots & & \\
 & & & & \times & 0 & \times & 0 \\
 & & & & & \times & 0 & \times
\end{pmatrix}
$$

The proposed procedure for computation is as follows.

Suppose we have reached the value $t = n.\delta t$. The Chebyshev expansion of θ for this value of t is known, and we define the column vector $\underset{\sim}{b}^{(n)}$ to be the vector of the coefficients i.e.

$$\underset{\sim}{b}^{(n)} = \{ b_0, b_1, b_2, \ldots, b_N \}$$

Let $\underset{\sim}{\psi}^{(n)}$ denote the column vector

$$\underset{\sim}{\psi}^{(n)} = \{ \psi_0(n\delta t, (n+1)\delta t), \psi_1(n\delta t, (n+1)\delta t), 0, \ldots 0 \}$$

We define the column vector $\underset{\sim}{b}^{*(n)}$ by

$$\underset{\sim}{b}^{*(n)} = \underset{\sim}{b}^{(n)} + \underset{\sim}{\psi}^{(n)}$$

Finally the column vector $\underset{\sim}{a}$ of the Chebyshev coefficients of $g(x)$ gives,

$$\underset{\sim}{a} = \underset{\sim}{b}^{(n+1)} - \underset{\sim}{b}^{(n)}.$$

We solve the complete system of equations by,

$$\underset{\sim}{b}^{(n+1)} = \underset{\sim}{T}_N(k)\, \underset{\sim}{b}^{*(n)} - \underset{\sim}{\psi}^{(n)} \tag{2.6.2}$$

where, from equation (2.6.1) we have that $\underset{\sim}{T}_N(k)$ is a square matrix of order $(N+1)$ given by

$$\underset{\sim}{T}_N(k) = \underset{\sim}{I}_N + \underset{\sim}{M}_N^{-1}(k)$$

$\underset{\sim}{I}_N$ being the unit matrix of order $(N+1)$. We use equation

(2.6.2) successively starting at $n = 0$, to give $\underset{\sim}{b}^{(1)}$, $\underset{\sim}{b}^{(2)}$, $\underset{\sim}{b}^{(3)}$ etc. in turn i.e. the Chebyshev expansion of the function $\theta(x, t)$ for $t = \delta t, 2\delta t, 3\delta t$ etc.

In using equation (2.4.1) we have assumed the truncation error to be zero. To minimise the effect of this error, we perform 2 integrations over the entire range of t required, one at interval, δt, the other at interval $\delta t/2$. After these integrations, the coefficients are combined at corresponding values of t using h^2- extrapolation. Full details of this will be given in the next Chapter where we consider the integration in two cases whose analytic solutions can be expressed in terms of elementary functions. We shall also discuss more fully the computational procedure and presentation of results. Finally, we shall discuss the advantages and disadvantages of the method and compare it with the finite difference methods outlined in Section (2.2).

CHAPTER 3.

THE COOLING AND RADIATION PROBLEMS.

3.1 The Symmetric Cooling Problem.

We shall now consider in some detail the numerical solution of the "cooling" problem, which is symmetric about $x = 0$. The boundary conditions are now given simply by

$$\theta = 0 \quad \text{for} \quad x = \pm 1 \;, \quad \text{all} \quad t > 0.$$

We shall take the case where the initial temperature is parabolic i.e.

$$\theta(x,0) = 1 - x^2 = \tfrac{1}{2}T_0 - \tfrac{1}{2}T_2 \quad \text{for} \quad -1 \leq x \leq 1.$$

The analytic solution of this problem is given by (see, for example, reference 7),

$$\theta(x,t) = \frac{32}{\pi^3}\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)^3}\exp\left[-\frac{(2n+1)^2\pi^2 t}{4}\right]\cos\left(n+\tfrac{1}{2}\right)\pi x. \tag{3.1.1}$$

Since we are considering only the symmetric case we will have $a_n = 0$ whenever n is odd. Writing $n = 2r$ with $N = 2R$ and substituting $\lambda_1 = 1$, $\mu_1 = 0$, $\phi_1(t) \equiv 0$ in equation (2.5.8), we find,

$$\left\{ -\left(\frac{1}{2}+\frac{k}{4}\right)a_0 + \frac{7k}{24}a_2 - 6k\sum_{r=2}^{R-1}\frac{1}{(4r^2-4)(4r^2-1)}a_{2r} + \frac{(2R-5)k}{4(R-1)(4R^2-1)}a_{2R} = b_0 \right. \tag{3.1.2}$$

Equation (2.5.9) gives exactly the same relation, and equation (2.4.5) becomes

$$\frac{k}{8r(2r-1)}a_{2r-2} - \left[\frac{1}{2}+\frac{k}{2(4r^2-1)}\right]a_{2r} + \frac{k}{8r(2r+1)}a_{2r+2} = b_{2r} \tag{3.1.3}$$

for $r = 1, 2, \ldots, R$ taking $a_{2R+2} = 0$.

Equations (3.1.2) and (3.1.3) are in the form suggested in Section (2.6) as most suitable for computation, and we write them in the form

$$(3.1.4) \qquad \underset{\sim}{M}_R(k)\,\underset{\sim}{a} = \underset{\sim}{b}.$$

$\underset{\sim}{a}$ and $\underset{\sim}{b}$ are the column vectors $\{a_0, a_2, \ldots\ldots, a_{2R}\}$ and $\{b_0, b_2, \ldots\ldots, b_{2R}\}$ respectively. $\underset{\sim}{M}_R(k)$ is a square matrix of order $(R+1)$, whose coefficients depend upon the parameter k. We can write

$$(3.1.5) \qquad \underset{\sim}{M}_R(k) = -\frac{1}{2}\underset{\sim}{I}_R + \frac{k}{4}\underset{\sim}{P}_R$$

where $\underset{\sim}{I}_R$ is the unit matrix of order $(R+1)$, and $\underset{\sim}{P}_R$ is a square matrix of order $(R+1)$ whose elements p'_{ij}; $i,j = 0,1,\ldots,R$ are independent of k, defined by

$$(3.1.6) \begin{cases} p'_{00} = -1,\ p'_{01} = \frac{7}{6},\ p'_{0j} = \dfrac{-24}{(4j^2-4)(4j^2-1)},\ p'_{0R} = \dfrac{2R-5}{(R-1)(4R^2-1)} \\ \qquad \text{for } j = 2,3,\ldots R-1. \\ p'_{i0} = \ldots = p'_{i,i-2} = 0,\ p'_{i,i-1} = \dfrac{1}{2i(2i-1)},\ p'_{i,i} = \dfrac{-2}{(4i^2-1)} \\ \qquad p'_{i,i+1} = \dfrac{1}{2i(2i+1)},\ p'_{i,i+2} = \ldots = p'_{i,R} = 0 \\ \text{for } i = 1,2,\ldots,R-1 \text{ and} \\ p'_{R0} = \ldots = p'_{R,R-2} = 0,\ p'_{R,R-1} = \dfrac{1}{2R(2R-1)},\ p'_{R,R} = \dfrac{-2}{4R^2-1} \end{cases}$$

The matrix $\underset{\sim}{P}_R$ is closely related to the infinite matrix $\underset{\sim}{P}$ discussed in Section (1.5); in fact $\underset{\sim}{P}_R$ is the principal sub-matrix of order $(R+1)$ of $\underset{\sim}{P}$ except for a change in the last element of the first row.

3.2 The matrices $\underset{\sim}{P}_R$ and $\underset{\sim}{P}$.

Before investigating the numerical solution of equation (3.1.4), let us look in more detail at the properties of the matrices $\underset{\sim}{P}_R$ and $\underset{\sim}{P}$. Suppose we had assumed that the Chebyshev expansions for $g(x)$ and $\theta_0(x)$ contained an infinite number of terms. Proceeding in a similar way to that described in Sections (2.4) and (2.5) for the symmetric cooling problem, the resulting infinity of equations can be represented in matrix form as

$$(3.2.1) \quad \begin{cases} \underset{\sim}{M}(k)\, \underset{\sim}{a} = \underset{\sim}{b} \\ \text{where } \underset{\sim}{M}(k) = -\frac{1}{2}\underset{\sim}{I} + \frac{k}{4}\underset{\sim}{P} \end{cases}$$

$\underset{\sim}{a}$, $\underset{\sim}{b}$ are now infinite column vectors $\{a_0, a_2, \ldots\}$, $\{b_0, b_2, \ldots\}$ respectively, and the matrix $\underset{\sim}{P}$ is exactly that defined in Section (1.5). In this "ideal" case we can find the latent roots and vectors of the infinite matrix $\underset{\sim}{M}(k)$, from the known results for the matrix $\underset{\sim}{P}$. What effect does the truncation of the series after $(R+1)$ terms have on these latent roots and vectors? The latent roots of $\underset{\sim}{P}_R$ have been computed on SILLIAC (the computer at the University of Sydney) for $R = 10$, and are compared with the first $(R+1)$ latent roots of $\underset{\sim}{P}$ in Table (3.1).

In the computation of the latent roots of $\underset{\sim}{P}_R$, the data was given to $8D$. Since the matrix $\underset{\sim}{P}_R$ is unsymmetric the latent roots were computed by first forming the characteristic equation, and then finding the roots of this polynomial, a process which may lead to considerable error in the roots of smallest modulus, so that too much significance should not be placed on these roots. In the solution

r	$\lambda_r = -\frac{16}{(2r+1)^2\pi^2}$	latent roots of $\underset{\sim}{P}_{10}$
0	-1.6211 3894	-1.6211 3894
1	-0.1801 2655	-0.1801 2654
2	-0.0648 4556	-0.0648 4556
3	-0.0330 8447	-0.0330 8451
4	-0.0200 1406	-0.0200 1214
5	-0.0133 9784	-0.0134 1043
6	-0.0095 9254	-0.0093 1712
7	-0.0072 0506	-0.0062 5123
8	-0.0056 0948	-0.0030 2379
9	-0.0044 9069	-0.0011 7067
10	-0.0036 7605	-0.0000 0002

Comparison of first eleven latent roots of $\underset{\sim}{P}$ with those of $\underset{\sim}{P}_{10}$

Table (3.1)

of equations (3.2.1), it is shown in Section (3.4) that we are interested only in the latent roots of $\underset{\sim}{P}_R$ with largest moduli. It can be seen from Table 3.1 that these roots agree extremely well with those of the infinite matrix $\underset{\sim}{P}$.

Due to the amount of computing involved, the latent vectors of $\underset{\sim}{P}_R$ have not been compared directly with the known latent vectors of $\underset{\sim}{P}$. However, in Section (3.3), there is an excellent check found of the computed values with the analytic values of the coefficients in the Chebyshev expansion of $\theta(x, t)$ for particular values of t. This shows that the latent vectors of $\underset{\sim}{P}_R$ must agree fairly well with the latent vectors of $\underset{\sim}{P}$.

3.3 Numerical Solution of the Cooling Problem.

Equations (3.1.4) have been solved by the method outlined in Section (2.6). If $\underset{\sim}{b}^{(n)}$ denotes the vector of Chebyshev coefficients at the time $t = n.\delta t$, then,

$$\underset{\sim}{b}^{(n+1)} = \underset{\sim}{T}_R(k)\, \underset{\sim}{b}^{(n)}$$

(3.3.1) $$\text{where } \underset{\sim}{T}_R(k) = \underset{\sim}{I}_R + M_R^{-1}(k), \text{ with } \underset{\sim}{b}^{(0)} = \{1, -\tfrac{1}{2}, 0, \ldots, 0\}$$

Choosing suitable values of k and R, we first invert $\underset{\sim}{M}_R(k)$ and form the matrix $\underset{\sim}{T}_R(k)$. The integration proceeds by repeated post-multiplication of the matrix $\underset{\sim}{T}_R(k)$ by the column vectors $\underset{\sim}{b}^{(0)}$, $\underset{\sim}{b}^{(1)}$, $\underset{\sim}{b}^{(2)}$ etc. to give $\underset{\sim}{b}^{(1)}$, $\underset{\sim}{b}^{(2)}$, $\underset{\sim}{b}^{(3)}$, - - - - - respectively.

In this example, we have chosen $R = 10$ and have performed two integrations with $k = 200$ and 400 i.e. with $\delta t = 1/200$ and $1/400$ respectively. We shall examine in detail the results for a fairly small value of t $(t = 0 \cdot 2)$, and a fairly large value, $(t = 1)$. The computed values of the coefficients b_{2r} are given in the first two columns of Tables (3.2) and (3.3).

r	$k = 200$	$k = 400$	extrapolated	theoretical
0	+0.5950 1652	+0.5950 2014	+0.5950 2135	+0.5950 2134
1	−0.3145 2283	−0.3145 2387	−0.3145 2422	−0.3145 2420
2	+0.0173 0460	+0.0173 0354	+0.0173 0319	+0.0173 0317
3	−0.0002 8380	−0.0002 8349	−0.0002 8339	−0.0002 8340
4	−0.0000 0692	−0.0000 0696	−0.0000 0697	−0.0000 0697
5	+0.0000 0075	+0.0000 0075	+0.0000 0075	+0.0000 0078
6	−0.0000 0004	−0.0000 0004	−0.0000 0004	−0.0000 0004
7	$-0.\ 0^{8}2$	$+0.\ 0^{8}1$	0	0

The coefficients b_{2r} at $t = 0.2$

Table 3.2

r	$k = 200$	$k = 400$	extrapolated	theoretical
0	+0.0826 1925	+0.0826 2119	+0.0826 2184	+0.0826 2182
1	−0.0437 0785	−0.0437 0888	−0.0437 0922	−0.0437 0922
2	+0.0024 4987	+0.0024 4993	+0.0024 4995	+0.0024 4995
3	−0.0000 5222	−0.0000 5222	−0.0000 5222	−0.0000 5222
4	+0.0000 0059	+0.0000 0059	+0.0000 0059	+0.0000 0059
5	$-0.\ 0^{8}4$	$-0.\ 0^{8}4$	0	0

The coefficients b_{2r} at $t = 1.0$

Table 3.3

The coefficients which are not shown, are zero to 8D.

In these computations the coefficients of $\underset{\sim}{M}_R(k)$ were given to $8D$, so that the results for $k = 200, 400$ will contain some round-off error in the least significant place. Following the usual practice when integrating parabolic type partial differential equations, the truncation error can be reduced by combining the results obtained from these two integrations by means of "h^2-extrapolation". If $\underset{\sim}{b}(k)$ represents the vector at a certain time t obtained from an integration in steps of δt, and $\underset{\sim}{b}(2k)$ represents those values from an integration in steps of $\delta t/2$, the extrapolated value $\underset{\sim}{b}(\infty)$ is given by

$$(3.3.2) \qquad \underset{\sim}{b}(\infty) = \frac{1}{3}\left[4\,\underset{\sim}{b}(2k) - \underset{\sim}{b}(k)\right]$$

This extrapolation is performed after each integration has been completed i.e. using the "deferred approach to the limit." The extrapolated values of b_{2r} obtained in this way at $t = 0\cdot 2$ and $1\cdot 0$, are shown in column 3 of Tables 3.2 and 3.3 respectively.

Finally, the theoretical values of b_{2r} can be found in this case. From equation (3.1.1) we have

$$(3.3.3) \quad b_{2r} = \frac{32}{\pi^3}\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)^3}\exp\left[-\frac{(2n+1)^2\pi^2 t}{4}\right]C_{2r}\left[\cos(n+\tfrac{1}{2})\pi x\right],$$

where $C_{2r}\left[\cos(n+\frac{1}{2})\pi x\right]$ denotes the Chebyshev coefficient of $T_{2r}(x)$ in the expansion of $\cos(n+\frac{1}{2})\pi x$. In Section (1.5), we found,

$$(3.3.4) \quad C_{2r}\left[\cos(n+\tfrac{1}{2})\pi x\right] = 2(-1)^r J_{2r}\left[(n+\tfrac{1}{2})\pi\right].$$

The theoretical values obtained from equations (3.3.3) and (3.3.4) are shown in column 4 of Tables 3.2 and 3.3. The agreement of the extrapolated values with the theoretical values is seen, in both cases, to be excellent. The only discrepancies occur in the least significant digit. These results indicate that the latent vectors of $\underset{\sim}{P}_R$ must approximate closely, those of the matrix $\underset{\sim}{P}$.

3.4 Justification for h^2-extrapolation.

For large values of t, it can be shown that h^2-extrapolation over one step δt, reduces the truncation error from $O(\delta t)^3$ to $O(\delta t)^5$. From equation (3.1.1) when t is large enough so that the value of $\theta(x,t)$ can be represented by the first term only, then

$$(3.4.1) \qquad \theta(x, t+\delta t) = e^{-\frac{\pi^2 \delta t}{4}} \cdot \theta(x,t)$$

From equation (3.3.1), if $\mu_n(k)$ is a latent root of $\underset{\sim}{T}_R(k)$ corresponding to a latent root λ_n of $\underset{\sim}{P}_R$, then

$$(3.4.2) \quad \mu_n(k) = 1 + \frac{1}{-\frac{1}{2} + \frac{k}{4}\lambda_n} = \frac{k\lambda_n + 2}{k\lambda_n - 2}.$$

Since λ_n are all negative, the largest latent root $\mu_n(k)$ corresponds to the latent root λ_n of largest modulus. This root is $\lambda_0 = -16/\pi^2$, and the largest latent root $\mu_n(k)$ is therefore given by,

$$(3.4.3) \quad \mu_0(k) = \frac{1 - \frac{\pi^2 \delta t}{8}}{1 + \frac{\pi^2 \delta t}{8}} = 1 - \frac{\pi^2 \delta t}{4} + \frac{\pi^4 (\delta t)^2}{32} - \frac{\pi^6 (\delta t)^3}{256} + O(\delta t)^4$$

Again, from equation (3.3.1), for large enough n, then

(3.4.4) $$\underset{\sim}{b}^{(n+1)}(k) = \underset{\sim}{T}_R(k)\,\underset{\sim}{b}^{(n)} \simeq \mu_0(k)\,\underset{\sim}{b}^{(n)}.$$

On comparing this equation with equation (3.4.1) we see that the largest latent root of $T_R(k)$ must approximate $\exp\left(-\frac{\pi^2\delta t}{4}\right)$; but,

(3.4.5) $$e^{-\frac{\pi^2\delta t}{4}} = 1 - \frac{\pi^2\delta t}{4} + \frac{\pi^4(\delta t)^2}{32} - \frac{\pi^6(\delta t)^3}{384} + \frac{\pi^8(\delta t)^4}{6144} - \frac{\pi^{10}(\delta t)^5}{122\,880} + O(\delta t)^6$$

If we compare this expansion with that for $\mu_0(k)$, we see that there is an error of $O(\delta t)^3$ in each step δt.

Suppose now that we halve the interval of integration, and again integrate from $t = n.\delta t$ to $t = (n+1)\delta t$. If the largest latent root of $\underset{\sim}{T}_R(2k)$ is $\mu_0(2k)$, then on performing the integration over two steps of length $\delta t/2$, we have,

$$\underset{\sim}{b}^{(n+1)}(2k) = \mu_0^2(2k)\,\underset{\sim}{b}^{(n)}$$

Combining the two vectors $\underset{\sim}{b}^{(n+1)}(2k)$ and $\underset{\sim}{b}^{(n+1)}(k)$ by equation (3.3.2), for h^2-extrapolation, we have,

(3.4.6) $$\left\{\begin{aligned} \underset{\sim}{b}^{(n+1)}(\infty) &= \tfrac{1}{3}\left[4\mu_0^2(2k) - \mu_0(k)\right]\underset{\sim}{b}^{(n)} \\ &= \mu(\infty)\,\underset{\sim}{b}^{(n)} \quad (\text{say}) \end{aligned}\right.$$

Expanding $\mu(\infty)$ in terms of δt, we obtain

(3.4.7) $$\mu(\infty) = 1 - \frac{\pi^2\delta t}{4} + \frac{\pi^4(\delta t)^2}{32} - \frac{\pi^6(\delta t)^3}{384} + \frac{\pi^8(\delta t)^4}{6144} - \frac{\pi^{10}(\delta t)^5}{196\,608} + O(\delta t)^6$$

Thus, on comparing this expansion with that of $\exp(-\pi^2\delta t/4)$, we see that over one step δt, the error is now $O(\delta t)^5$ as compared with $O(\delta t)^3$ obtained previously.

This analysis gives a partial justification for h^2-extrapolation, although not for using the deferred approach to the limit.

3.5 Presentation of Results.

While we are still dealing with a comparatively simple problem, let us consider means of presenting the results of the integration for tabulation purposes. It is proposed that for each value of t, the function $\theta(x,t)$ be represented by the extrapolated Chebyshev coefficients (with one minor modification). The merits of such a scheme are discussed below.

In Table 3.4, we give the coefficients for $t = 0{\cdot}100(0{\cdot}005)0{\cdot}120$ of the cooling problem, extrapolated from the two integrations with $k = 200$ and 400. In place of b_0 as computed, we give instead $\frac{1}{2} b_0$.

r	$t = 0{\cdot}100$	$t = 0{\cdot}105$	$t = 0{\cdot}110$	$t = 0{\cdot}115$	$t = 0{\cdot}120$
0	+0.381 721	+0.376 938	+0.372 224	+0.367 577	+0.362 997
1	-0.401 492	-0.396 683	-0.391 921	-0.387 207	-0.382 541
2	+0.019 496	+0.019 543	+0.019 559	+0.019 548	+0.019 513
3	+0.000 360	+0.000 279	+0.000 207	+0.000 143	+0.000 086
4	-0.000 091	-0.000 082	-0.000 074	-0.000 066	-0.000 059
5	+0.000 005	+0.000 005	+0.000 005	+0.000 004	+0.000 004
6	0	0	0	0	0

The coefficients b_{2r} where $\theta(x,t) = \sum_{r=0}^{R} b_{2r} T_{2r}(x)$

Table 3.4

Consider the following points :-

(1) For a given tabulated value of t, to find $\theta(x,t)$ for any x in $-1 \leq x \leq 1$, the Chebyshev series can be evaluated by an ingenious method due to Clenshaw (reference 8).

If $f(x) = \sum_{n=0}^{N} b_n T_n(x)$ then

$$f(x) = d_0 - x d_1$$

where d_0, d_1, are found from the sequence

(3.5.1) $$d_n - 2x d_{n+1} + d_{n+2} = b_n$$

with $d_{N+1} = d_{N+2} = 0$. The error due to round-off found by computing $f(x)$ in this way is shown to be the same as that which would be obtained in summing the series directly. Thus by the use of equation (3.5.1), no interpolation is necessary in the x-direction as would be the case if function values were tabulated directly.

(2) For each value of t considered in Table 3.4, the function is given for all x by just 6 coefficients. In tabulating the function values, we would probably present $\theta(x,t)$ at intervals of say 0.05 in x i.e. 11 values would be required for each t. So, from the point of view of the compiler, space is saved. Also, if it is required to use the values of $\theta(x,t)$ for given values of t in some further computation involving an electronic computer, it is much easier to give the function in terms of its Chebyshev coefficients together with a sub-routine to sum the

Chebyshev series using equation (3.5.1), than to store discrete function values and a sub-routine for their interpolation.

(3) If $\theta(x,t)$ is not required to as many decimal places as tabulated, the series may be suitably truncated. Suppose, for example, we want $\theta(x,t)$ for some value of x at $t = 0{\cdot}1$ to $3D$ only. Then, neglecting all coefficients which are zero to $3D$, we need only use the first 3 terms in the expansion instead of the 6 as given. Since $|T_n(x)| \leq 1$ for all x in $-1 \leq x \leq 1$ and all n, the neglected coefficients cannot contribute more than their absolute value to the sum.

In evaluating $\theta(x,t)$ for non-tabular values of t, we can either interpolate on the function values evaluated for the required x at adjacent tabulated values of t, or interpolate directly on the Chebyshev coefficients and sum the resulting series. The coefficients given in Table 3.4 are quadratically interpolable in the t-direction, so that in this case, direct interpolation on the coefficients appears to be the more convenient method. To facilitate the interpolation, the second differences could also be tabulated.

3.6 The Radiation Problem.

In order to consider a case where the boundary condition contains a derivative, we have analysed the "radiation" problem in some detail. We shall consider the symmetric case, where the boundary condition is given by

(3.6.1) $$\theta + \frac{\partial \theta}{\partial x} = 0 \quad \text{along } x = 1$$

An initial temperature,

(3.6.2) $$\theta(x,0) = 3 - x^2 = \frac{5}{2} T_0(x) - \frac{1}{2} T_2(x),$$

has been taken which again gives us a problem with no singularity initially. The analytic solution is given by (see reference 7),

(3.6.3) $$\theta(x,t) = 4 \sum_{n=0}^{\infty} e^{-\alpha_n^2 t} \cdot \frac{\cos \alpha_n x}{\alpha_n^2 (\alpha_n^2 + 2) \cos \alpha_n}$$

where α_n are the roots of

(3.6.4) $$\alpha \tan \alpha = 1$$

The analysis of this problem is similar to that for the cooling problem. Consequently we shall only quote the essential results, keeping proofs and discussion to a minimum. From the boundary condition equation (2.5.8) on putting $n = 2r$, $N = 2R$ and $\lambda_1 = \mu_1 = 1$ and $\phi_1(t) \equiv 0$ we find,

(3.6.5) $$\left\{ \begin{array}{l} -\left(\frac{1}{2} + \frac{5k}{4}\right) a_0 + \frac{23}{24} k a_2 + k \sum_{r=2}^{R-1} \frac{8r^2 - 14}{(4r^2-1)(4r^2-4)} a_{2r} \\ \qquad + \frac{(8R^2 - 2R - 9)k}{(4R^2-1)(4R-4)} a_{2R} = b_0 \end{array} \right.$$

Equation (2.4.5) becomes,

(3.6.6) $$\frac{k}{8r(2r-1)} a_{2r-2} - \left[\frac{1}{2} + \frac{k}{2(4r^2-1)}\right] a_{2r} + \frac{k}{8r(2r+1)} a_{2r+2} = b_{2r}$$

for $r = 1, 2, \ldots, R$, taking $a_{2R+2} = 0$. These $(R+1)$ equations can be combined into the matrix form,

(3.6.7) $$\underset{\sim}{M}_R(k)\, \underset{\sim}{a} = \underset{\sim}{b}$$

where we now write

(3.6.8) $$\underset{\sim}{M}_R(k) = -\frac{1}{2}\underset{\sim}{I}_R + \frac{k}{4}\underset{\sim}{Q}_R$$

The matrix $\underset{\sim}{Q}_R$ is similar to $\underset{\sim}{P}_R$ except for different elements along the first row. It is closely related to an infinite matrix $\underset{\sim}{Q}$ which can be obtained by a method analogous to that for $\underset{\sim}{P}$, by considering the Chebyshev expansion of the function $y = \cos\alpha x$ in $-1 \leq x \leq 1$, such that,

(3.6.9) $$y + \frac{dy}{dx} = 0 \quad \text{along } x = 1.$$

This function satisfies the equation

(3.6.10) $$\frac{d^2y}{dx^2} + \alpha^2 y = 0$$

Assuming,

$$y = \frac{1}{2}a_0 + \sum_{r=1}^{\infty} a_{2r} T_{2r}(x)$$

we find in turn

(3.6.11) $$a''_{2r} + \alpha^2 a_{2r} = 0 \quad \text{for } r = 0, 1, 2, \ldots\ldots$$

(3.6.12) $$2(2r-1)\,a'_{2r-1} + \alpha^2(a_{2r-2} - a_{2r}) = 0 \quad \text{for } r = 1, 2, \ldots\ldots$$

and

(3.6.13) $$\frac{a_{2r-2}}{2r(2r-1)} - \frac{2a_{2r}}{(4r^2-1)} + \frac{a_{2r+2}}{2r(2r+1)} = -\frac{4}{\alpha^2}a_{2r}$$

for $r = 1, 2, \ldots\ldots$. The boundary condition, equation (3.6.9) gives

$$\frac{1}{2}a_0 + \sum_{r=1}^{\infty} a_{2r} + \sum_{r=1}^{\infty} a'_{2r-1} = 0$$

Using equation (3.6.12), the terms in a'_{2r-1} can be eliminated from this equation to give

(3.6.14) $$\frac{1}{2}a_0 + \sum_{r=1}^{\infty} a_{2r} - \alpha^2\left\{\frac{1}{2}a_0 - \sum_{r=1}^{\infty}\frac{1}{(4r^2-1)}a_{2r}\right\} = 0$$

If each of equations (3.6.13) is subtracted from equation (3.6.14), we find,

$$(3.6.15) \quad -5a_0 + \frac{23}{6} a_2 + \sum_{r=2}^{\infty} \frac{8r^2-14}{(r^2-1)(4r^2-1)} a_{2r} = -\frac{4}{\alpha^2} a_0$$

Equations (3.6.15) and (3.6.13) can be written as

$$(3.6.16) \qquad \underset{\sim}{Q}\,\underset{\sim}{a} = -\frac{4}{\alpha^2}\,\underset{\sim}{a}$$

where the matrix $\underset{\sim}{Q}$ has elements q_{ij} for $i, j = 0, 1, 2, \ldots$ defined by

$$(3.6.17) \quad \begin{cases} q_{00} = -5, \; q_{01} = \dfrac{23}{6}, \; q_{0j} = \dfrac{8j^2-14}{(j^2-1)(4j^2-1)} \text{ for } j = 2, 3, \ldots \\ q_{ij} = p_{ij} \text{ for } i, j \geq 1 \end{cases}$$

(see equation (1.5.9)). Since the function $y = \cos \alpha x$ satisfies the boundary condition (3.6.9) only for those values α_n satisfying equation (3.6.4), we have that the latent roots of $\underset{\sim}{Q}$ are given by $-4/\alpha_n^2$ for $n = 0, 1, 2, \ldots$ The coefficients of the Chebyshev expansion of $\cos \alpha_n x$ can be shown from Section (1.5) to be

$$a_{2r} = 2(-1)^r J_{2r}(\alpha_n) \text{ for } r = 0, 1, 2, \ldots$$

Thus we know the latent roots and corresponding latent vectors of $\underset{\sim}{Q}$.

A comparison of the first six latent roots of $\underset{\sim}{Q}$, and the latent roots of $\underset{\sim}{Q}_R$ for $R = 10$ is given in Table 3.5

n	$-4/\alpha_n^2$	latent roots Q_{10}
0	-5.404 134	-5.404 133
1	-0.340 865	-0.340 865
2	-0.096 528	-0.096 528
3	-0.044 049	-0.044 049
4	-0.025 015	-0.025 014
5	-0.016 081	-0.016 102
6		-0.011 034
7		-0.007 892
8		-0.004 313
9		-0.002 141
10		-0.000 309

Table 3.5

Only the first six values of λ_n have been computed. The comparison between these roots and those of $\underset{\sim}{Q}_{10}$ is excellent.

Solving equation (3.6.7) in the form

$$\underset{\sim}{b}^{(n+1)} = \underset{\sim}{T}_R(k)\, \underset{\sim}{b}^{(n)}$$

where

$$\underset{\sim}{T}_R(k) = \underset{\sim}{I}_R + \underset{\sim}{M}_R^{-1}(k)$$

the following results were obtained for $k = 200$ at $t = 0{\cdot}1,\ 0{\cdot}2$ and $1{\cdot}0$, and are compared with the theoretical values.

	$t = 0.1$		$t = 0.2$		$t = 1.0$	
r	$k = 200$	theoretical	$k = 200$	theoretical	$k = 200$	theoretical.
0	+4.630 179	+4.630 179	+4.296 174	+4.296 175	+2.375 388	+2.375 389
1	-0.480 835	-0.480 832	-0.451 175	-0.451 174	-0.250 842	-0.250 842
2	+0.004 655	+0.004 654	+0.006 216	+0.006 216	+0.003 966	+0.003 966
3	+0.000 296	+0.000 295	+0.000 068	+0.000 068	-0.000 025	-0.000 025
4	-0.000 015	-0.000 015	-0.000 006	-0.000 006	0	0
5	0	0	0	0	0	0

The coefficients b_{2r}

$$\theta(x,t) = \frac{1}{2} b_0 + \sum_{r=1}^{R} b_{2r} T_{2r}(x)$$

Table 3.6

These results, without h^2-extrapolation, show excellent agreement with the theoretical values, to $6D$.

Since we know the latent roots of $\underset{\sim}{Q}$, the effect of h^2-extrapolation can be investigated as in Section 3.4, to show that the truncation error over a single step δt is again reduced from $O(\delta t)^3$ to $O(\delta t)^5$. The remarks on presentation of results are applicable here also.

3.7 Conclusion.

In this Chapter we have considered in some detail the numerical solution of the parabolic-type heat equation in two particular cases. We have seen that the computation involves just two basic operations, the inversion of a matrix, and the multiplication of a matrix by a column vector. The effect of h^2-extrapolation has been shown to decrease the truncation error.

Let us now compare the advantages and disadvantages of this method with the finite-difference methods reviewed in Section 2.2.

(1) Once the matrix $\underset{\sim}{M}_R$ has been computed and inverted, the amount of computation involved in the integration is considerably less than in both the explicit and implicit finite difference methods. It is suggested that in cases where R can be taken small enough, the entire operation is a practicable proposition for desk machine computation.

(2) When an electronic computer is available, the programming is almost trivial, since all established machines have library programmes for the inversion and multiplication of matrices. The programming involved in the implicit finite difference method is certainly not trivial although it is straightforward.

(3) There are no stability problems to be considered as compared with the explicit finite difference method. The truncation error depends only upon one parameter, δt.

(4) In the tabulation of $\theta(x,t)$ as discussed in Section 3.5, we dispense with interpolation in the x-direction and need only consider interpolation in the t-direction. The finite difference methods, where function values are tabulated for discrete values of x and t, involve the user in two-dimensional interpolation. For the compiler, space can generally be saved by giving the Chebyshev coefficients instead of function values at discrete points.

(5) One disadvantage of the method is that R is not known a priori. A judicious guess for R must be made from consideration, for example, of the number of terms in the Chebyshev expansion of the initial function. If R is chosen too large, more work than necessary will have been done;

if R is taken too small, the calculations will have to be repeated. In the two examples considered above, R has been chosen too large for results to $6D$, so that more computing than necessary has been done.

(6) The method of Chebyshev series is not (in its present form) as versatile as finite difference methods which can for example, be used for non-linear equations. The amount of algebraization needed before computing is commenced is greater than in finite difference methods. It is also not at all certain that such a simple computational procedure can always be used.

In the case of the general linear equation given by equation (2.1.4), it is suggested that when the resultant ordinary differential equation has no singular points in $-1 \leqslant x \leqslant 1$, the direct method of computation used in this Chapter will always be possible. In the next Chapter, we shall consider an example where the ordinary differential equation has singularities at the end points of the range. An iterative method of solution is described in this case.

CHAPTER 4

THE ONE-DIMENSIONAL HEAT EQUATION, INFINITE RANGE.

4.1 Statement of the Problem.

In this Chapter we again consider the equation

$$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial x^2}, \tag{4.1.1}$$

where now the range of x is infinite i.e. $-\infty \leq x \leq \infty$. We shall consider only one fairly restricted set of boundary conditions, where

$$\lim_{x \to \pm\infty} \theta(x,t) = 0 \quad \text{for all } t \geq 0, \tag{4.1.2}$$

$$\text{and} \quad \theta(x,0) = f(x), \text{ given.}$$

As in the previous Chapters, the initial temperature must satisfy the boundary condition, so that,

$$\lim_{x \to \pm\infty} f(x) = 0.$$

There are four possible methods for the numerical solution of equations (4.1.1) and (4.1.2) :-

(1) Carslaw and Jaeger (reference 7) show that the analytic solution is given by

$$\theta(x,t) = \frac{1}{2\sqrt{\pi t}} \int_{-\infty}^{\infty} f(\eta) \exp\left[-\frac{(x-\eta)^2}{4t}\right] d\eta. \tag{4.1.3}$$

This integral may be evaluated numerically using Gauss-Hermitian quadrature. However, if $\theta(x,t)$ is required for a large number of values of x and t, this is perhaps not the best method of approach. For the spot-checking of values of $\theta(x,t)$ obtained by other, more direct, methods equation (4.1.3) is very useful.

(2) To the required accuracy, the function $\theta(x,t)$ may be zero for $|x| > X$, say. The range of x is then essentially $-X \leq x \leq X$. We may then use the finite-difference methods outlined in Chapter 2 for the numerical integration of equation (4.1.1). Alternatively, on defining a new space variable $\xi = \frac{x}{X}$, so that $-1 \leq \xi \leq 1$ we can use the Chebyshev series method of Chapters 2 and 3. The number of integrations needed to reach a given value of t is now proportional to X^2 as well as δt. If X is too large the method might not be very practicable.

(3) Hartree (reference 9) has described a finite-difference method of solution. As in reference (6), he replaces the partial differential equation by a system of ordinary differential equations. Suppose the integration has reached $t = t_0$, and we want to integrate over one step δt. At time $t_0 + \frac{1}{2}\delta t$ we can write

$$\left(\frac{\partial\theta}{\partial t}\right)_{x,t_0+\frac{1}{2}\delta t} = \frac{\theta(x,t_0+\delta t) - \theta(x,t_0)}{\delta t} + O(\delta t)^2$$

and
$$\left(\frac{\partial^2\theta}{\partial x^2}\right)_{x,t_0+\frac{1}{2}\delta t} = \frac{1}{2}\left[\left(\frac{\partial^2\theta}{\partial x^2}\right)_{x,t_0+\delta t} + \left(\frac{\partial^2\theta}{\partial x^2}\right)_{x,t_0}\right] + O(\delta t)^2.$$

Neglecting the truncation error, the partial differential equation (4.1.1) is replaced by

(4.1.4) $$\frac{d^2 w}{dx^2} - 2kw = -4k\theta_0$$

where $\omega(x) = \theta_1(x) + \theta_0(x)$, $k = 1/\delta t$ and the subscripts 0 and 1 denote values at the times t_0 and $t_0 + \delta t$ respectively. Together with the boundary conditions at $x = \pm\infty$, equation (4.1.4) constitutes a two point boundary value problem. An indiscriminate use of finite-difference methods will give serious build up of error in the numerical solution of equation (4.1.4). Hartree shows how this integration can be performed so that the round-off errors can always be kept under control. Having determined $\omega(x)$, we can compute $\theta_1(x)$ which is taken as the new $\theta_0(x)$ in the integration over the next time interval δt . The integration can thus proceed in the t-direction.

(4) In this Chapter we attempt to solve equation (4.1.4) by the method of Chebyshev series. In order to express ω and θ_0 in terms of Chebyshev series we must define a new independent variable $\xi = \xi(x)$ such that $-1 \leq \xi \leq 1$ The resulting differential equation can then be integrated by expanding all the dependent variables in series of $T_n(\xi)$ Thus, in theory, we can determine ω , hence θ_1 , and the integration can proceed in the t-direction. This is the general outline of the method to be discussed in this Chapter. Although by the choice of ξ given in Section (4.2), the algebraisation of the problem is comparatively simple, the solution of the resulting equations indicates that the Chebyshev series for θ are very slowly convergent. This necessitates

using a large number of terms in the series for θ at each value t. The evaluation of $\theta(x, t)$ for any particular value of x is then very tedious, thus defeating the purpose of the method. The breakdown of the method will be discussed more fully in Section (4.4), after a numerical solution of the equations for a particular case has been found in the next Section.

4.2 Reduction of the Equations.

Firstly we must choose a suitable new independent variable ξ. Obviously we must choose ξ such that the range $-\infty \leqslant x \leqslant \infty$ corresponds to $-1 \leqslant \xi \leqslant 1$. Furthermore, we want ξ such that if we write

(4.2.1) $$w = \frac{1}{2} a_0 + \sum_{n=1}^{N} a_n T_n(\xi),$$

then the coefficients in the Chebyshev expansions of $\frac{dw}{dx}$ and $\frac{d^2w}{dx^2}$ can be expressed fairly simply in terms of the coefficients a_n. In a numerical solution of the Orr-Sommerfeld equation, Clenshaw and the author (reference 10) found that the transformation

(4.2.2) $$\xi = \tanh x$$

satisfied both these requirements. If $C_n(y)$ denotes the coefficient of $T_n(\xi)$ in the Chebyshev expansion of y, and if we write

(4.2.3) $$\frac{d^s w}{d\xi^s} = \frac{1}{2} a_0^{(s)} + \sum_{n=1}^{N-s} a_n^{(s)} T_n(\xi)$$

for $s = 1, 2$, then

$$C_n\left(\frac{dw}{dx}\right) = C_n\left[(1-\xi^2)\,\frac{dw}{d\xi}\right]$$
$$= \frac{1}{2}\left[(n+1)\,a_{n+1} - (n-1)\,a_{n-1}\right]$$

on using equations (1.3.7) and (1.3.5). Similarly, we find,

$$(4.2.4)\quad C_n\left(\frac{d^2w}{dx^2}\right) = \frac{1}{4}\left[(n+1)(n+2)\,a_{n+2} - 2n^2 a_n + (n-1)(n-2)\,a_{n-2}\right]$$

These forms for $C_n\left(\frac{dw}{dx}\right)$ and $C_n\left(\frac{d^2w}{dx^2}\right)$ are fairly simple, and the author has been unable to find a "better" transformation in this respect.

Writing,

$$(4.2.5)\qquad \theta_0(x) = \frac{1}{2}\,b_0 + \sum_{n=1}^{N} b_n\,T_n(\xi)\,,$$

substituting these expansions into equation (4.1.4), and equating coefficients of $T_n(\xi)$ we find,

$$(4.2.6)\quad -\frac{(n-1)(n-2)}{16k}\,a_{n-2} + \left[\frac{1}{2} + \frac{n^2}{8k}\right]a_n - \frac{(n+1)(n+2)}{16k}\,a_{n+2} = b_n$$

valid for $n = 0, 1, 2, \ldots, N$. These are $(N+1)$ equations for the $(N+1)$ unknowns a_n, provided we take $a_{N+1} = a_{N+2} = 0$. There is therefore no need for any extra equations given by the boundary conditions.

To investigate this more fully, let us look at the differential equation with ξ as the independent variable. Applying the transformation given by equation (4.2.2) to equation (4.1.4) we obtain,

$$(4.2.7)\quad (1-\xi^2)^2\,\frac{d^2w}{d\xi^2} - 2\xi(1-\xi^2)\,\frac{dw}{d\xi} - 2kw = -4k\theta_0$$

This equation has regular singularities at $\xi = \pm 1$, but there is only <u>one</u> solution which is regular at both points. Thus there is only one solution for $-1 \leq \xi \leq 1$ possessing a convergent Chebyshev series, and this solution is determined uniquely by the differential equation. (In Chapter 2, equation (2.4.1) possessed two solutions having convergent Chebyshev series and the boundary conditions had to be used to determine which combination of these two solutions was required). Returning to equation (4.2.7), we have specified that the functions θ_0 , θ_1 must vanish at $\xi = \pm 1$. In the "ideal" case where an infinite number of terms are taken in the Chebyshev expansions of θ_0 and ω , it is easy to show that these conditions are automatically satisfied. From equations (4.2.6), if to half the equation for $n = 0$ we add each of the equations corresponding to $n = 1, 2,$ ------- we find,

(4.2.8) $$\frac{1}{2}\left[\frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n\right] = \frac{1}{2}b_0 + \sum_{n=1}^{\infty} b_n$$

Thus $\theta_1 = \theta_0 = 0$ at $\xi = 1$ without any extra condition being needed. A similar analysis holds for $\xi = -1$ if again to equation (4.2.6) corresponding to $n = 0$ we add $(-1)^n$ times the equations for $n = 1, 2,$ ----.

When considering a finite number of terms in the expansion of ω and θ_0 , the boundary condition is not satisfied exactly at $\xi = \pm 1$. Even though we start with $\theta_0 = 0$ at $\xi = \pm 1$, θ_1 will not vanish at $\xi = \pm 1$. In the step by step integration an error is therefore introduced at each step. To overcome this, the equations corresponding to $n = N-1, N$ are modified so that θ_1 is equal to zero at $\xi = \pm 1$. This is considered in greater detail in the next Section, where a numerical solution is evaluated.

4.3 Numerical Solution of the Equations.

In this Section we consider in detail the numerical solution of equations (4.1.1) and (4.1.2) where

(4.3.1) $\theta(x,0) = \operatorname{sech}^2 x = 1 - \xi^2 = \frac{1}{2} - \frac{1}{2} T_2(\xi)$.

In this case the solution is even, so that in equations (4.2.6), $a_n = b_n = 0$ when n is odd. Writing $n = 2r$ and $N = 2R$ these equations become

(4.3.2)
$$\left\{\begin{aligned} &\tfrac{1}{2} a_0 - \tfrac{1}{4k} a_2 = b_0 \\ &-\frac{(2r-1)(2r-2)}{16k} a_{2r-2} + \left(\frac{1}{2} + \frac{r^2}{2k}\right) a_{2r} - \frac{(2r+2)(2r+1)}{16k} a_{2r+2} \\ &\qquad = b_{2r} \end{aligned}\right.$$

for $r = 1, 2, ---, R$ with $a_{2R+2} = 0$. In order that $\frac{1}{2} a_0 + \sum_{r=1}^{R} a_{2r}$ should be zero at each step in the computation, the equation (4.3.2) corresponding to $r = R$ is replaced by,

(4.3.2A) $$-\frac{(R-1)(4R-2)}{16k} a_{2R-2} + \left[\frac{1}{2} + \frac{2R(2R-1)}{16k}\right] a_{2R} = b_{2R}.$$

In the first attempt at the solution of these equations, we used the direct method of Chapter 3 where the equations are written in the matrix form $\underset{\sim}{M}\,\underset{\sim}{a} = \underset{\sim}{b}$, the matrix $\underset{\sim}{M}$ is inverted and the successive column vectors $\underset{\sim}{b}$

are computed by the post-multiplication of a matrix with a column vector. It soon became apparent that a large number of terms were needed in the Chebyshev expansions of w and θ_0. Since the direct method would then first involve the inversion of a large matrix, the following iterative scheme was devised, where the number of terms required in each expansion was determined automatically as the integration proceeded.

Consider first the integration over one step δt so that $k = 1/\delta t$ is given. The values of b_{2r} are known from the previous integration. Let $a_{2r}^{(j)}$ denote the j^{th} iteration on the unknown quantity a_{2r}. Equations (4.3.2) and (4.3.2A) can be written as,

$$(4.3.3) \quad a_{2r}^{(j+1)} = \frac{2k}{(k+r^2)} b_{2r} + \frac{(2r-1)(r-1)}{4(k+r^2)} a_{2r-2}^{(j+1)} + \frac{(2r+1)(r+1)}{4(k+r^2)} a_{2r+2}^{(j)}$$

for $r = 1, 2, \ldots\ldots, R-1$, together with

$$(4.3.4) \qquad a_0^{(j+1)} = 2b_0 + \frac{1}{2k} a_2^{(j+1)}$$

$$(4.3.5) \text{ and } \quad a_{2R}^{(j+1)} = \frac{8k}{4k+R(2R-1)} b_{2R} + \frac{(R-1)(2R-1)}{4k+R(2R-1)} a_{2R-2}^{(j+1)}$$

The iteration was started by assuming that $a_{2r}^{(1)} = 2b_{2r}$ for all r. From equation (4.3.3) with $r = 1$, the value of $a_2^{(2)}$ can be computed using the values of $a_4^{(1)}$ and b_2. With $r = 2$, we next compute $a_4^{(2)}$ using the newly found value $a_2^{(2)}$ with $a_6^{(1)}$ and b_4. This evaluation of $a_{2r}^{(2)}$ is continued until we find an $a_{2r}^{(2)}$ which is smaller than some prescribed value 1×10^{-p}, say.

To p decimal places, this is taken to be the last term required, and it is corrected using equation (4.3.5). These values of $a_{2r}^{(2)}$ are compared with the previously found values $a_{2r}^{(1)}$ to see if there is any change. If there is, we start a new iteration $a_{2r}^{(3)}$ in the same way at $r = 1$. This iteration is continued until $a_{2r}^{(j+1)}$ and $a_{2r}^{(j)}$ are the same for all r. Finally a_0 is computed using equation (4.3.4). This gives us the Chebyshev series for w and we compute θ_1 from the equation,

$$C_{2r}(\theta_1) = C_{2r}(w) - C_{2r}(\theta_0).$$

Thus, we find a new right hand side, and the process is continued. This scheme was programmed for the UTECOM computer in basic machine language. For the particular problem considered, two integrations were performed with $k = 200, 400$. Following the integrations in Chapter 3, the two results were combined by k^2- extrapolation in the deferred approach to the limit. These extrapolated values of the coefficients b_{2r} are given for $t = 0{\cdot}09$, $0{\cdot}16$ and $0{\cdot}25$ to $6D$ in Table 4.1.

r	$t = 0.09$	$t = 0.16$	$t = 0.25$
0	+0.958 604	+0.930 530	+0.898 494
1	-0.424 186	-0.379 585	-0.334 207
2	-0.045 481	-0.062 806	-0.074 213
3	-0.007 465	-0.015 291	-0.023 411
4	-0.001 588	-0.004 674	-0.009 030
5	-0.000 405	-0.001 668	-0.003 981
6	-0.000 118	-0.000 666	-0.001 933
7	-0.000 038	-0.000 291	-0.001 011
8	-0.000 014	-0.000 136	-0.000 560
9	-0.000 005	-0.000 067	-0.000 325
10	-0.000 002	-0.000 035	-0.000 197
11	-0.000 001	-0.000 019	-0.000 123
12	0	-0.000 011	-0.000 079
13		-0.000 006	-0.000 052
14		-0.000 004	-0.000 035
15		-0.000 002	-0.000 024
16		-0.000 001	-0.000 017
17		-0.000 001	-0.000 012
18		-0.000 001	-0.000 009
19		0	-0.000 006
20			-0.000 005
21			-0.000 003
22			-0.000 003
23			-0.000 002
24			-0.000 002
25			-0.000 001
26			-0.000 001
27			-0.000 001
28			-0.000 001

The coefficients b_{2r}

$$\theta(x,t) = \frac{1}{2} b_0 + \sum_{r=1}^{\infty} b_{2r} T_{2r}(\operatorname{arctanh} x)$$

Table 4.1

These results indicate that the series expansions are slowly convergent, and that over the range of t considered, the number of terms is increasing with t. To check the accuracy of these results, the values of θ along $x = 0$ were computed using equation (4.1.3). The comparison is given in Table 4.2, together with the values of θ, computed from the series, for $x = \infty$ (which should be zero).

t	$\theta(0,t)$ by quadrature	$\theta(0,t)$ from series	$\theta(\infty,t)$ from series
0.09	+0.864 198	+0.864 199	−0.000 001
0.16	+0.793 860	+0.793 861	+0.000 001
0.25	+0.726 315	+0.726 321	+0.000 003

Table 4.2

The agreement along $x = 0$ is seen to be quite good, any discrepancy can easily be accounted for by round-off and truncation errors in the summation of the series. This is also true along $x = \infty$.

Because of these results, it was decided to proceed no further with the computation and to discard the method as a failure. To expect anyone to sum a Chebyshev series of 29 terms to compute a value of θ correct only to 5D was considered to be too much of an imposition!

4.4 Conclusion

To pose the problem in a slightly different form:, we have attempted to use the Chebyshev series method of Chapters 2 and 3, to solve the equation

$$(4.4.1) \quad (1-\xi^2)^2 \frac{\partial^2\theta}{\partial\xi^2} - 2\xi(1-\xi^2)\frac{\partial\theta}{\partial\xi} = \frac{\partial\theta}{\partial t}$$

for $-1 \leq \xi \leq 1$, with given initial and boundary conditions. In spite of the simple form of the resulting algebraic equations, the solution although tractable, gives series expansions for θ which are long and very slowly convergent. The reasons for this are not at all obvious to the author. It may be conjectured that the solution of any equation with singular points at the boundaries might behave in a similar fashion. Alternatively, it might be that the transformation $\xi = \tanh x$ used in solving equations (4.1.1) and (4.1.2) is a particularly bad one to use, in spite of the simplicity of the resulting equations. (It might be worth noting here that in reference (10), the authors used up to 96 terms in the series to obtain a significant result). There may be another transformation of the space variable, which although perhaps more algebraically cumbersome, will give a more rapidly convergent Chebyshev series. The author is at present of the opinion that it is the singularities introduced by the transformation from an infinite to a finite range, which will prevent any similar method from being successful. We do, however, live and learn.

CHAPTER 5.

THE EXPANSION OF FUNCTIONS IN ULTRASPHERICAL POLYNOMIALS.

5.1 Introduction.

In this Chapter we shall consider a method for finding the expansion of an arbitrary function $f(x)$, in a series of ultraspherical polynomials $P_n^{(\lambda)}(x)$. These are defined in equation (1.1.2). For a full description of the ultraspherical polynomials, see, for example, Szegö, (reference 11). Suppose we are given a function $f(x)$ which is continuous in $-1 \leqslant x \leqslant 1$, and we want to find its expansion in an infinite series of $P_n^{(\lambda)}(x)$. If,

(5.1.1) $$f(x) = \sum_{n=0}^{\infty} a_n P_n^{(\lambda)}(x) ,$$

then from the orthogonality property, we have,

(5.1.2) $$a_n = \frac{\Gamma(2\lambda)(n+\lambda)n!\,\Gamma(\lambda)}{\sqrt{\pi}\,\Gamma(n+2\lambda)\Gamma(\lambda+\frac{1}{2})}\int_{-1}^{+1}(1-x^2)^{\lambda-\frac{1}{2}}P_n^{(\lambda)}(x)f(x)\,dx$$

In general, it is not possible to evaluate the integral occurring in this equation explicitly, and to find a_n, recourse has to be made to some suitable quadrature technique. In this Chapter, we shall consider only those functions $f(x)$ which can be represented as the solution of a linear differential equation with appropriate boundary conditions, and will solve this equation by a method similar to Clenshaw's (reference 3) for the Chebyshev polynomials $T_n(x)$. The method to be described can therefore be considered as a generalisation of Clenshaw's for use with any of the ultraspherical polynomials. In practice we are most interested in expansions in Legendre polynomials and, to a lesser extent, in the Chebyshev polynomials of the second kind.

5.2 Solution of Linear Differential Equations in Ultraspherical Polynomials.

In Chapter 1 we discussed Clenshaw's method for the solution of linear differential equations, by expansion of the dependent variable directly in a series of Chebyshev Polynomials, $T_n(x)$. Again, we suppose that we have an m th. order linear differential equation in $-1 \leq x \leq 1$, given by,

$$p_m(x)\frac{d^m y}{dx^m} + p_{m-1}(x)\frac{d^{m-1} y}{dx^{m-1}} + \cdots + p_0(x)\, y = q(x) \tag{5.2.1}$$

together with m boundary conditions, which determine the function $y = f(x)$ uniquely. We now write

$$y = \sum_{n=0}^{\infty} a_n P_n^{(\lambda)}(x) \tag{5.2.2}$$

where the coefficients a_n are to be determined, and the s th. derivative of y, $y^{(s)}(x)$ is expanded formally as

$$y^{(s)}(x) = \sum_{n=0}^{\infty} a_n^{(s)} P_n^{(\lambda)}(x) \tag{5.2.3}$$

for $s = 1, 2, ---, m$.

Let us consider for a moment, the solution of equation (5.2.1) by Chebyshev series. It is fairly obvious that even if $y = f(x)$ can be expanded in a convergent Chebyshev series, it does not necessarily follow that a convergent series can be found for all its derivatives. Consider, for example, the function $y = (1-x^2)^{1/2}$. This function is continuous in $-1 \leqslant x \leqslant 1$ and can therefore be represented by a convergent Chebyshev series. The derivative, however, is not continuous in $-1 \leqslant x \leqslant 1$, being infinite at the end points, $x = \pm 1$, so that it cannot be represented by a convergent Chebyshev expansion. This function satisfies the equation

$$(5.2.4) \qquad (1-x^2)\frac{dy}{dx} + xy = 0 \quad \text{with } y(0) = 1,$$

which is of the form given by equation (5.2.1). Each term in this equation is continuous in $-1 \leqslant x \leqslant 1$, and the formal use of the divergent series for the first derivative does lead to the correct series expansion for the function y.

This statement is true in general. Provided each term in equation (5.2.1) is continuous in $-1 \leqslant x \leqslant 1$, we can use the formal expansion for the s^{th} derivative of y, even though this series might be divergent. If any term $p_r(x)\frac{d^r y}{dx^r}$ in equation (5.2.1) is not continuous in $-1 \leqslant x \leqslant 1$, then the function $f(x)$ is not continuous in the closed interval, and so cannot be represented by such an expansion.

Clenshaw's method depended upon the use of equation (1.3.4) to give the result of equation (1.3.5), and on equation (1.3.6) to give the result of equation (1.3.8).

For expansions in terms of the ultraspherical polynomials $P_n^{(\lambda)}(x)$ we start with the relations

(5.2.5) $$P_n^{(\lambda)}(x) = \frac{1}{2(n+\lambda)}\frac{dP_{n+1}^{(\lambda)}(x)}{dx} - \frac{1}{2(n+\lambda)}\frac{dP_{n-1}^{(\lambda)}(x)}{dx}$$

and

(5.2.6) $$xP_n^{(\lambda)}(x) = \frac{n+1}{2(n+\lambda)}P_{n+1}^{(\lambda)}(x) + \frac{n+2\lambda-1}{2(n+\lambda)}P_{n-1}^{(\lambda)}(x)$$

both of which are valid for $n \geq 1$.

From equation (5.2.3),

$$y^{(s+1)}(x) = \sum_{n=0}^{\infty} a_n^{(s+1)} P_n^{(\lambda)}(x) = \sum_{n=1}^{\infty}\left[\frac{a_{n-1}^{(s+1)}}{2n+2\lambda-2} - \frac{a_{n+1}^{(s+1)}}{2n+2\lambda+2}\right]\frac{dP_n^{(\lambda)}(x)}{dx},$$

on using equation (5.2.5). On differentiating equation (5.2.3), we find,

$$y^{(s+1)}(x) = \sum_{n=1}^{\infty} a_n^{(s)} \frac{dP_n^{(\lambda)}(x)}{dx}$$

from which, on equating coefficients, we have,

(5.2.7) $$a_n^{(s)} = \frac{a_{n-1}^{(s+1)}}{2n+2\lambda-2} - \frac{a_{n+1}^{(s+1)}}{2n+2\lambda+2}, \text{ for } n \geq 1.$$

This equation is the generalisation of equation (1.3.5). For computing purposes, this equation is not as easy to use as equation (1.3.5), since the coefficients on the right hand side are functions of n. To simplify the computing, we define a related set of coefficients $b_n^{(s)}$ by writing,

(5.2.8) $$a_n^{(s)} = (n+\lambda)\, b_n^{(s)} \text{ ; all } n \geq 0,\ s = 0, 1, \ldots, m.$$

The equation then takes the simpler form

(5.2.9) $$2(n+\lambda)\, b_n^{(s)} = b_{n-1}^{(s+1)} - b_{n+1}^{(s+1)}, \quad n \geq 1.$$

Again, let $C_n(y)$ denote the coefficient of $P_n^{(\lambda)}(x)$ in the expansion of y. Then,

$$xy = \sum_{n=0}^{\infty} a_n x P_n^{(\lambda)}(x)$$

$$= \sum_{n=0}^{\infty} \left[\frac{n a_{n-1}}{2(n+\lambda-1)} + \frac{(n+2\lambda)a_{n+1}}{2(n+\lambda+1)} \right] P_n^{(\lambda)}(x)$$

on using equation (5.2.6) and rearranging terms.

Thus,

(5.2.10) $$C_n(xy) = \frac{n a_{n-1}}{2(n+\lambda-1)} + \frac{(n+2\lambda)a_{n+1}}{2(n+\lambda+1)}, \quad n \geq 0$$

and in terms of the coefficients b_n, we find,

(5.2.11) $$C_n(xy) = \frac{n}{2} b_n + \frac{1}{2}(n+2\lambda) b_{n+1}, \quad n \geq 0$$

By continued application of equation (5.2.10) we can find $C_n(x^2 y)$, $C_n(x^3 y)$ etc. Equation (5.2.10) is considerably more cumbersome than equation (1.3.7), and even in terms of the coefficients b_n, the equation for $C_n(xy)$ is not arithmetically simple. No further simplification appears to be possible.

In general, equations (5.2.7) and (5.2.9) are only valid for $n \geq 1$, since a_n, b_n have not yet been defined for negative values of n. (For the Chebyshev polynomials $T_n(x)$, $a_{-n} = a_n$ for all values of n). It will be shown in Section 5.6, that for all λ except those for which 2λ is an integer, we must take $a_{-n} = b_{-n} = 0$ for $n \geq 1$.

5.3 Boundary Conditions.

These are generally given at either $x = 0$ or $x = \pm 1$.

For completeness, the values of $P_n^{(\lambda)}(x)$ at these points are given here

$$(5.3.1)\quad \begin{cases} P_n^{(\lambda)}(1) = \dfrac{\Gamma(n+2\lambda)}{\Gamma(2\lambda).\ n!} \\ P_n^{(\lambda)}(-1) = (-1)^n P_n^{(\lambda)}(1) \\ P_{2n+1}^{(\lambda)}(0) = 0 \quad , \quad n \geqslant 0 \\ P_{2n}^{(\lambda)}(0) = \dfrac{(-1)^n \Gamma(n+\lambda)}{n!\,\Gamma(\lambda)} \quad , \quad n \geqslant 0 \end{cases}$$

These results are valid for all values of λ, except $\lambda = 0$.

If we know that y is either an odd or an even function of x, then since $P_n^{(\lambda)}(x)$ is even when n is even and odd when n is odd, we have

$$(5.3.2)\quad \begin{cases} \text{for } y \text{ even, } & a_{2n+1} \text{ and } b_{2n+1} = 0 \ , \ n \geqslant 0 \\ \text{for } y \text{ odd, } & a_{2n} \text{ and } b_{2n} = 0 \ , \ n \geqslant 0 \end{cases}$$

5.4 Method of Solution.

From the differential equation with associated boundary conditions, we obtain an infinite set of linear algebraic equations in the unknowns $b_n^{(s)}$ for $s = 0, 1, \ldots$ $\ldots, m$ and all $n \geqslant 0$. The numerical solution of these equations can be performed by the two methods described by Clenshaw (reference 3). These are the method of recurrence and the iterative method.

In the recurrence method it is assumed that $b_n^{(s)} = 0$ for $n > N$, where N is not known a priori. Guessing a suitable N and giving arbitrary values to $b_N^{(s)}$, the equations can be solved to give $b_{N-1}^{(s)}, b_{N-2}^{(s)}, \ldots\ldots, b_0^{(s)}$. In general the boundary conditions are not satisfied by one such solution, and linear combinations have to be made of two or more such solutions with different values of $b_N^{(s)}$. The method is in general fairly quick, the main disadvantage being that N may be chosen either too small or too large. In the former case the required accuracy for the coefficients will not be obtained, in which case the computation must be repeated with a larger N. If N is chosen too large, more computation than necessary will have been done. In general a solution by recurrence is direct and rapid although care must be taken that figures are not lost from the most significant end when linear combinations of solutions are taken. If this does occur, the solution may be improved using the iterative method.

The iterative scheme starts with some initial guess for the b_n which satisfies the boundary conditions. From these values equation (5.2.9) can be used to compute b_n', b_n'' etc. When all $b_n^{(s)}$ have been found, these values can be used to compute a new b_n from the recurrence relation, again satisfying the boundary conditions. This procedure is continued until the desired accuracy is reached. However, the iterative scheme does not always converge, or it may only converge slowly. In such cases the recurrence method must be used.

5.5 Expansion in Legendre Polynomials.

We shall now consider in some detail the expansion of a function $f(x)$ in terms of the Legendre polynomials $P_n(x)$. Writing,

$$y^{(s)}(x) = \sum_{n=0}^{\infty} a_n^{(s)} P_n(x),$$

equations (5.2.8) - (5.2.11) become

$$(5.5.1)\quad \begin{cases} a_n^{(s)} = (n+\tfrac{1}{2})\, b_n^{(s)} \ ; \quad \text{all } n, \text{ all } s \\ (2n+1) b_n^{(s)} = b_{n-1}^{(s+1)} - b_{n+1}^{(s+1)}, \quad n \geq 1 \\ c_n(xy) = \dfrac{n}{2n-1}\, a_{n-1} + \dfrac{n+1}{2n+3}\, a_{n+1}, \quad n \geq 0 \\ c_n(xy) = \dfrac{n}{2}\, b_{n-1} + \tfrac{1}{2}(n+1)\, b_{n+1}, \quad n \geq 0 \end{cases}$$

respectively.

For an expansion in Legendre polynomials, a meaning can be given to a_{-n}, b_{-n} for $n = 1, 2, 3, \ldots$. From equation (5.2.6) with $\lambda = 1/2$, we have

$$(5.5.2)\quad x P_n(x) = \frac{n+1}{2n+1} P_{n+1}(x) + \frac{n}{2n+1} P_{n-1}(x).$$

This relation can be used to recur forwards i.e. to find $P_{n+1}(x)$ given $P_n(x)$ and $P_{n-1}(x)$, or to recur backwards to find $P_{n-1}(x)$ in terms of $P_n(x)$ and $P_{n+1}(x)$. With $n = 0$, we see from equation (5.5.2) that $P_{-1}(x)$ is indeterminate. We define

$$P_{-1}(x) = -P_0(x)$$

then putting n successively equal to -1, -2, - - - - we find that $P_{-2}(x) = -P_1(x)$, $P_{-3}(x) = -P_2(x)$ and in general,

$$P_{-n}(x) = -P_{n-1}(x)$$

For the coefficients $a_n^{(s)}$ and $b_n^{(s)}$, we must have,

$$(5.5.3)\quad \begin{cases} a_{-n}^{(s)} = -a_{n-1}^{(s)} \\ \text{whence } b_{-n}^{(s)} = b_{n-1}^{(s)} \end{cases}$$

for $n = 0, 1, 2, \ldots$ and all values of s.

We shall now consider a simple example, using the above results to find the expansion of a function in terms of Legendre polynomials.

Example 5.1. Suppose we want to find the Legendre expansion of e^{x^2} for $-1 \leq x \leq 1$. This function satisfies the equation

$$\frac{dy}{dx} - 2xy = 0 \quad \text{with } y(0) = 1.$$

Then with

$$y^{(s)}(x) = \sum_{n=0}^{\infty} a_n^{(s)} P_n(x) \quad \text{for } s = 0, 1$$

and using equations (5.5.1) we find,

$$(n + \tfrac{1}{2}) b_n' - [n b_{n-1} + (n+1) b_{n+1}] = 0$$

With this equation written in the form

$$(5.5.4) \qquad b_{n-1} = \frac{1}{2n}\left[(2n+1) b_n' - 2(n+1) b_n\right];$$

and using the second of equations (5.5.1) in the form,

$$(5.5.5) \qquad b_{n-1}' = b_{n+1}' + (2n+1) b_n$$

we can readily compute b_n, b_n' and hence a_n by the recurrence method. Since e^{x^2} is an even function,

$b_{2n+1} = 0$ and $b_{2n}' = 0$ for all n.

The complete computation is shown in Table 5.1

n	b_n	b'_n	$a_n = (n+\frac{1}{2}) b_n$	true a_n	$P_n(0)$
0	102 08866		51 04433.0	1.46265	+1.000 000
1		87 63917			
2	14 68505		36 71262.5	1.05198	-0.500 000
3		14 21392			
4	1 42339		6 40525.5	0.18354	+0.375 000
5		1 40341			
6	10030		65195.0	0.01868	-0.312 500
7		9951			
8	553		4700.5	0.00135	+0.273 438
9		550			
10	25		262.5	0.00008	-0.246 094
11		25			
12	1		12.5		+0.225 586

$$e^{x^2} = 1.46265\, P_0(x) + 1.05198\, P_2(x) + 0.18354\, P_4(x) + 0.01868\, P_6(x) + 0.00135\, P_8(x) + 0.00008\, P_{10}(x)$$

Table 5.1

As a starting point we have taken $b_{12} = 1$, $b_{14} = b_{16} = \dots = 0$ and $b'_{13} = b'_{15} = \dots = 0$. With these starting values, equations (5.5.4) and (5.5.5) can be used to compute b_n, b'_n for all $n < 12$, and hence a_n. These values of a_n have to be multiplied by a constant γ which is determined from the as yet unsatisfied boundary condition. This gives,

$$\gamma \sum_{n=0}^{12} a_n P_n(0) = 1$$

from which we find $\gamma = 0.286\,545 \times 10^{-6}$. The coefficients a_n are given to 5D. As a check we find that for $x = 1$, $e = 2.71828$

5.6 The coefficients $a_n^{(s)}$, $b_n^{(s)}$ for negative n.

The use of equations (5.2.9) and (5.2.11) gives rise to recurrence relations where we might have to assign a meaning to a_n or b_n for negative values of n. We have seen for the Legendre polynomials that $a_{-n}^{(s)} = -a_{n-1}^{(s)}$ and $b_{-n}^{(s)} = b_{n-1}^{(s)}$ for all values of n. A similar analysis can be used for all ultraspherical polynomials of order λ, when 2λ is an integer.

Suppose $2\lambda = m$, where m is an integer. From the recurrence relation, equation (5.2.6), we find

$$P_{-1}^{(\lambda)}(x) = P_{-2}^{(\lambda)}(x) = \cdots\cdots = P_{-(m-1)}^{(\lambda)}(x) = 0$$

with $P_{-m}^{(\lambda)}(x)$ being indeterminate. Defining,

$$P_{-m}^{(\lambda)}(x) = -P_0^{(\lambda)}(x),$$

then

$$P_{-(m+r)}^{(\lambda)}(x) = -P_r^{(\lambda)}(x) \text{ for all } r \geq 0.$$

For the coefficients $a_n^{(s)}$, we have,

$$\text{(5.6.1)} \quad \begin{cases} a_{-(m+r)}^{(s)} = -a_r^{(s)}, \quad r \geq 0 \\ \text{with } a_{-1}^{(s)} = a_{-2}^{(s)} = \cdots\cdots = a_{-(m-1)}^{(s)} = 0, \end{cases}$$

and for the coefficients $b_n^{(s)}$,

$$\text{(5.6.2)} \quad \begin{cases} b_{-(m+r)}^{(s)} = b_r^{(s)}, \quad r \geq 0 \\ \text{with } b_{-1}^{(s)} = b_{-2}^{(s)} = \cdots\cdots = b_{-(m-1)}^{(s)} = 0. \end{cases}$$

When 2λ is not an integer, we have simply

$$a_{-n}^{(s)} = b_{-n}^{(s)} = 0 \text{ for } n \geq 1.$$

5.7 Expansion in Chebyshev Polynomials of the Second Kind.

The Chebyshev Polynomials of the Second Kind $U_n(x)$ are obtained by putting $\lambda = 1$ in equation (1.1.2).

Writing,

$$y^{(s)}(x) = \sum_{n=0}^{\infty} a_n^{(s)} U_n(x)$$

equations (5.2.8) - (5.2.11) become

$$(5.7.1) \quad \left\{ \begin{array}{l} a_n^{(s)} = (n+1) b_n^{(s)} \text{ for all } n, s \\ 2(n+1) b_n^{(s)} = b_{n-1}^{(s+1)} - b_{n+1}^{(s+1)}, \quad n \geq 1 \\ c_n(xy) = \frac{1}{2} a_{n-1} + \frac{1}{2} a_{n+1}, \quad n \geq 0 \\ c_n(xy) = \frac{n}{2} b_{n-1} + \frac{1}{2}(n+2) b_{n+1}, \quad n \geq 0 \end{array} \right.$$

Let us now look again at the expansion of e^{x^2} for $-1 \leq x \leq 1$ in terms of the $U_n(x)$ polynomials. Substituting the direct expansions for y and y' into the differential equation and equating coefficients of $U_n(x)$ to zero for all n, we find after some algebra,

$$(5.7.2) \qquad b_{n-1} = \frac{1}{n}\left[(n+1) b_n' - (n+2) b_{n+1}\right]$$

If we write the second of equations (5.7.1) in the form

$$(5.7.3) \qquad b_{n-1}' = b_{n+1}' + 2(n+1) b_n ,$$

we can proceed in exactly the same way as in Section 5.5. The results of this computation, starting with $b_{12} = 1$, $b_{14} = b_{16} = \ldots = 0$; $b_{13}' = b_{15}' = \ldots = 0$ is given in Table 5.2

n	b_n	b'_n	$a_n = (n+1)b_n$	true a_n
0	303 74805		303 74805	1.32819
1		194 47854		
2	28 40301		85 20903	0.37259
3		24 06048		
4	2 20658		11 03290	0.04824
5		1 99468		
6	13360		93520	0.00409
7		12428		
8	656		5904	0.00026
9		620		
10	27		297	0.00001
11		26		
12	1		13	

$$e^{x^2} = 1\cdot 32819\, U_0(x) + 0\cdot 37259\, U_2(x) + 0\cdot 04824\, U_4(x)$$
$$+ 0\cdot 00409\, U_6(x) + 0\cdot 00026\, U_8(x) + 0\cdot 00001\, U_{10}(x)$$

Table 5.2

In order to satisfy the boundary condition that $y(0) = 1$ we must multiply the first computed a_n by $0\cdot 437\ 268 \times 10^{-7}$ to give the true a_n .

5.8 Summation of Series.

In this section we suppose that a series expansion for $f(x)$, to the required accuracy, has been found and is given by

$$f(x) = \sum_{n=0}^{N} a_n P_n^{(\lambda)}(x)$$

To sum this series for a given x, we can either evaluate $P_n^{(\lambda)}(x)$ for all n and sum, or we can use the method described by Clenshaw (reference 8). For the ultraspherical polynomials $P_n^{(\lambda)}(x)$, we construct a sequence d_N, d_{N-1}, ------, d_0 where,

(5.8.1) $$\begin{cases} d_n - \dfrac{2(n+\lambda)}{(n+1)} x\, d_{n+1} + \dfrac{(n+2\lambda)}{(n+2)} d_{n+2} = a_n, \quad n \leq N \\ \text{with} \quad d_{N+1} = d_{N+2} = 0 \end{cases}$$

Then for all $\lambda \neq 0$, the function $f(x)$ is given by

(5.8.2) $$f(x) = d_0$$

To investigate the effect of round-off errors in d_n and the subsequent error in $f(x)$, suppose ε_n is the error in d_n. Then ε_n satisfies the recurrence relation,

(5.8.3) $$\varepsilon_n - \frac{2(n+\lambda)}{(n+1)} x\, \varepsilon_{n+1} + \frac{(n+2\lambda)}{(n+2)} \varepsilon_{n+2} = 0$$

This is a second order recurrence relation with two linearly independent solutions given by

$$\frac{n!}{\Gamma(n+\alpha)} P_{n-1}^{(\alpha,\alpha)}(x) \quad \text{and} \quad \frac{n!}{\Gamma(n+\alpha)} Q_{n-1}^{(\alpha,\alpha)}(x).$$

Here $P_{n-1}^{(\alpha,\alpha)}(x)$ is the Jacobi polynomial of degree $n-1$ with $\beta = \alpha = \lambda - 1/2$, and $Q_{n-1}^{(\alpha,\alpha)}(x)$ is the Jacobi function of the second kind. (For a complete description of these functions, the reader is referred to Szegö, reference 11). Now, a rounding error $\varepsilon(M)$ in either d_M or a_M introduces an error $\varepsilon_r(M)$ in d_r $(r \leqslant M)$, given by

$$\varepsilon_r(M) = \frac{r!}{\Gamma(r+\alpha)} \left\{ \ell P_{r-1}^{(\alpha,\alpha)}(x) + m Q_{r-1}^{(\alpha,\alpha)}(x) \right\}$$

where ℓ, m are constants which can be determined from the conditions,

$$\varepsilon(M) = \frac{M!}{\Gamma(M+\alpha)} \left\{ \ell P_{M-1}^{(\alpha,\alpha)}(x) + m Q_{M-1}^{(\alpha,\alpha)}(x) \right\}$$

and $$0 = \frac{(M+1)!}{\Gamma(M+1+\alpha)} \left\{ \ell P_M^{(\alpha,\alpha)}(x) + m Q_M^{(\alpha,\alpha)}(x) \right\}$$

Solving these two equations for ℓ and m, we find that

$$(5.8.4)\quad \varepsilon_r(M) = \frac{\varepsilon(M)\, M!\, \Gamma(M+2\alpha+1)(x^2-1)^{\alpha}}{\Gamma(M+\alpha)\, 2^{2\alpha}\, \Gamma(M+\alpha+1)} \left\{ P_M^{(\alpha,\alpha)}(x) Q_{r-1}^{(\alpha,\alpha)}(x) - P_{r-1}^{(\alpha,\alpha)}(x) Q_M^{(\alpha,\alpha)}(x) \right\}$$

The error in $f(x)$ due to this error in d_M or a_M is then given simply by $\varepsilon_0(M)$. Before putting $r = 0$ in equation (5.8.4), we write $P_{r-1}^{(\alpha,\alpha)}(x)$ in terms of $P_r^{(\alpha,\alpha)}(x)$ and $P_{r+1}^{(\alpha,\alpha)}(x)$, and $Q_{r-1}^{(\alpha,\alpha)}(x)$ in terms of $Q_r^{(\alpha,\alpha)}(x)$ and $Q_{r+1}^{(\alpha,\alpha)}(x)$ from the recurrence relation for $P_r^{(\alpha,\alpha)}(x)$ and $Q_r^{(\alpha,\alpha)}(x)$. Then, on putting $r = 0$, we find,

$$(5.8.5)\quad \left\{ \begin{aligned} \varepsilon_0(M) &= \varepsilon(M)\, P_M^{(\alpha,\alpha)}(x) \cdot \frac{\Gamma(M+2\alpha+1) \cdot \Gamma(1+\alpha)}{\Gamma(M+\alpha+1) \cdot \Gamma(1+2\alpha)} \\ &= \varepsilon(M) \cdot P_M^{(\lambda)}(x) \end{aligned} \right.$$

from the definition of the ultraspherical polynomial $P_M^{(\lambda)}(x)$ in terms of the Jacobi polynomial $P_M^{(\alpha,\alpha)}(x)$ where $\alpha = \lambda - \frac{1}{2}$. This analysis is valid for all $\lambda \neq 0$, and Clenshaw (reference 8) has shown for this case that $\varepsilon_0(M) = \varepsilon(M)\,T_M(x)$.

This error is exactly the same as that found from summing the series for $f(x)$ using directly the values of the ultraspherical polynomials. The use of the recurrence relation, equation (5.8.1), provides a rapid method for evaluating $f(x)$ without recourse to tables of $P_m^{(\lambda)}(x)$. This will be most useful in electronic computers where storage space is at a premium. In particular, for series expansions in Legendre polynomials, since $|P_n(x)| \leq 1$ for all x in $-1 \leq x \leq 1$, then $|\varepsilon_0(M)| \leq |\varepsilon(M)|$.

5.9 Conclusions.

In this Chapter we have described a method whereby the coefficients in the expansion of an arbitrary function $f(x)$ in an infinite series of ultraspherical polynomials $P_n^{(\lambda)}(x)$, may be obtained to any required degree of accuracy without using quadrature. The function $f(x)$ is assumed to satisfy some linear differential equation with associated boundary conditions. This differential equation can then be solved directly to give the unknown coefficients.

Of all the ultraspherical polynomials, we have seen in Chapter 1 that the Chebyshev polynomials of the first kind are most useful to the numerical analyst. From equations (5.2.7) - (5.2.11) we see that these polynomials give the simplest arithmetic forms for $a_n^{(s)}$ in terms of $a_{n-1}^{(s+1)}$ and $a_{n+1}^{(s+1)}$, and for $C_n(xy)$ etc.

An expansion of Legendre polynomials gives the "best" polynomial approximation to f(x) in the least squares sense in the range $-1 \leq x \leq 1$. In Chapter 6, we shall make use of these expansions in the numerical solution of Fredholmtype integral equations.

Of the other ultraspherical polynomials, occasional use is made of the Chebyshev polynomials of the second kind. The remaining polynomials appear to be of academic interest only.

CHAPTER 6.

LINEAR INTEGRAL EQUATIONS.

6.1 Introduction.

In this Chapter we investigate the numerical solution of non-singular linear integral equations by the direct expansion of the unknown function $f(x)$ in a series of Chebyshev polynomials $T_n(x)$. The use of polynomial expansions is not new, and was first described by Crout (reference 12). He writes $f(x)$ as a Lagrangian-type polynomial over the range in x, and determines the unknown coefficients in this expansion by evaluating the functions and integral arising in the equation at chosen points x_i. A similar method (known as collocation) is used here for cases where the kernel is not separable. From the properties of expansion of functions in Chebyshev polynomials, as given in Chapter 1, we may expect greater accuracy in this case when compared with other polynomial expansions of the same degree. This is well borne out in comparison with one of Crout's examples.

The most common method of solution of integral equations is by the use of finite differences. Fox and Goodwin (reference 13) have made a thorough investigation of these methods, using the Gregory quadrature formula for the evaluation of the integral. Other methods for the algebraization of the integral equation using Gaussian quadrature have been described by Kopal (reference 14).

The crux of the problem is to find easily the Chebyshev expansion of the given functions in the equation. To find these, we restrict ourselves to functions which can be represented as the solution of some linear differential equation with associated boundary conditions. The solution of the differential equation can then be found directly in terms of Chebyshev series by Clenshaw's method (reference 3), outlined in Chapter 1.

Linear integral equations can be divided into two types depending upon the limits of the integral. An equation of the form

(6.1.1) $$f(x) = F(x) + \lambda \int_a^b K(x,y) f(y)\, dy ,$$

where F, K are given functions; λ, a, b are finite constants and $f(x)$ is the unknown function, is known as a "Fredholm equation". When the upper limit of the integral is not a constant, but is the variable x, the equation takes the form

(6.1.2) $$f(x) = F(x) + \lambda \int_a^x K(x,y) f(y)\, dy$$

and is known as a "Volterra equation".

We shall consider only equations of the Fredholm type, and in order to use Chebyshev polynomials we must change the range of the vaiable x from $a \leq x \leq b$ to either $-1 \leq x \leq 1$ or $0 \leq x \leq 1$. In the former case we use the $T_n(x)$ polynomials, defined by equation (1.1.1), and in the latter case the shifted polynomials $T_n^*(x)$, defined by equation (1.1.5).

Before proceeding with the discussion of methods of solution, we shall need results for

(i) the product of two Chebyshev expansions

and (ii) the integral of a function whose Chebyshev expansion is given.

6.2 Product of two Chebyshev expansions.

Suppose,

(6.2.1)
$$\begin{cases} f(x) = \frac{1}{2} a_0 + \sum_{n=1}^{\infty} a_n T_n(x) \\ g(x) = \frac{1}{2} b_0 + \sum_{n=1}^{\infty} b_n T_n(x) \end{cases}$$
and

and we want to find the Chebyshev expansion of the product of $f(x)$ and $g(x)$. From the relation,

(6.2.2)
$$2\, T_m(x)\, T_n(x) = T_{m+n}(x) + T_{|m-n|}(x)$$

we find that

(6.2.3)
$$\begin{cases} f(x)\, g(x) = \frac{1}{2} d_0 + \sum_{n=1}^{\infty} d_n T_n(x) \\ d_n = \frac{1}{2}\Big[a_0 b_n + \sum_{m=1}^{\infty} a_m \left(b_{|m-n|} + b_{m+n} \right) \Big], \quad n \geq 0. \end{cases}$$
where

A similar result holds for expansions in terms of the $T_n^*(x)$ polynomials. If,

(6.2.4)
$$\begin{cases} f(x) = \frac{1}{2} A_0 + \sum_{n=1}^{\infty} A_n T_n^*(x) \\ g(x) = \frac{1}{2} B_0 + \sum_{n=1}^{\infty} B_n T_n^*(x) \end{cases}$$
and

then

(6.2.5)
$$\begin{cases} f(x) g(x) = \frac{1}{2} D_0 + \sum_{n=1}^{\infty} D_n T_n^*(x) \\ D_n = \frac{1}{2}\Big[A_0 B_n + \sum_{m=1}^{\infty} A_m \left(B_{|m-n|} + B_{m+n} \right) \Big], \quad n \geq 0. \end{cases}$$
where

6.3 Integral of $f(x)$.

With $f(x)$ defined as in equation (6.2.1), we want the Chebyshev expansion of $I(x)$, where

$$I(x) = \int_{-1}^{x} f(x)\,dx \tag{6.3.1}$$

Now $I(x)$ is the solution of

$$\frac{dI}{dx} = f(x) \quad \text{with} \quad I(-1) = 0 \tag{6.3.2}$$

On writing, $\quad I(x) = \frac{1}{2} b_0 + \sum_{n=1}^{\infty} b_n T_n(x),$

equating coefficients of $T_n(x)$ in equation (6.3.2), and using equation (1.3.5) we find,

$$b_0 = a_0 - \frac{1}{2} a_1 - 2 \sum_{n=2}^{\infty} \frac{(-1)^n}{n^2-1} a_n, \tag{6.3.3}$$

(6.3.4) and $\quad b_n = \dfrac{a_{n-1} - a_{n+1}}{2n} \quad \text{for } n \geq 1.$

In many problems, we want $I(1)$ and this is given by,

$$I(1) = a_0 - 2 \sum_{n=1}^{\infty} \frac{a_{2n}}{4n^2-1}. \tag{6.3.5}$$

In solving Fredholm equations, we require the integral of the product of two functions between the limits -1 and $+1$. Defining $f(x)$ and $g(x)$ as in equation (6.2.1), and using equations (6.2.3) and (6.3.5), we find

$$\begin{aligned} \int_{-1}^{1} f(x)g(x)\,dx = {} & a_0 \left(\frac{1}{2} b_0 - \sum_{r=1}^{\infty} \frac{b_{2r}}{4r^2-1} \right) \\ & + \sum_{n=1}^{\infty} a_n \left[b_n - \sum_{r=1}^{\infty} \frac{b_{|n-2r|} + b_{n+2r}}{4r^2-1} \right] \end{aligned} \tag{6.3.6}$$

Similar results can be found for expansions in terms of the $T_n^*(x)$ polynomials. Defining $f(x)$ as in equation (6.2.4), then if

$$I(x) = \int_0^x f(x)\,dx = \tfrac{1}{2}B_0 + \sum_{n=1}^{\infty} B_n T_n^*(x),$$

we find,

(6.3.7) $$\begin{cases} B_0 = \frac{1}{2}A_0 - \frac{1}{4}A_1 - \sum_{n=2}^{\infty} \frac{(-1)^n A_{2n}}{n^2-1} \\ B_n = \frac{A_{n-1} - A_{n+1}}{4n}, \quad \text{for } n \geq 1 \end{cases}$$

For $\int_0^1 f(x)\,dx$, we find,

(6.3.8) $$I(1) = \tfrac{1}{2}A_0 - \sum_{n=1}^{\infty} \frac{1}{4n^2-1} A_{2n}.$$

Finally, for the integral of the product of two functions, if $f(x)$ and $g(x)$ are defined as in equation (6.2.4) then

(6.3.9) $$\int_0^1 f(x)g(x)\,dx = \tfrac{1}{2}A_0\left[\tfrac{1}{2}B_0 - \sum_{r=1}^{\infty}\frac{1}{4r^2-1}B_{2r}\right] + \tfrac{1}{2}\sum_{n=1}^{\infty}A_n\left[B_n - \sum_{r=1}^{\infty}\frac{B_{|n-2r|} + B_{n+2r}}{4r^2-1}\right]$$

We are now in a position to examine in detail the numerical solution of Fredholm-type integral equations. The method depends entirely upon whether the kernel $K(x, y)$ is separable or not. In Section 6.4 we will discuss the case when the kernel is separable; and compare the method with one of Crout's examples in Section 6.5. In Sections 6.6 and 6.7 we will investigate the case of non-separable kernels.

6.4 Separable Kernel.

In general, when the kernel is separable we will have

(6.4.1) $$K(x, y) = \sum_{m=1}^{M} g_m(x) h_m(y)$$

The Fredholm integral equation can then be written

(6.4.2) $$f(x) = F(x) + \lambda \sum_{m=1}^{M} g_m(x) \int_{-1}^{1} h_m(y) f(y)\,dy$$

where the range in x has been normalised to $-1 \leq x \leq 1$.

$F(x)$, $g_m(x)$, $h_m(y)$ are given functions and we assume that their Chebyshev expansions are known. Further, let us approximate to $f(x)$ by a polynomial of degree N, i.e.

$$f(x) = \tfrac{1}{2}a_0 + \sum_{n=1}^{N} a_n T_n(x).$$

If $F(x) \not\equiv 0$, we choose N to be the degree to which $F(x)$ is given to the required accuracy. If $F(x) \equiv 0$, then N can only be estimated a priori from, perhaps, some physical criterion. If N is originally chosen too small, this will be apparent from the series expansion for $f(x)$. The calculation will then have to be repeated with larger N. If N is chosen too large initially, then unnecessary extra work will have been done. Many integral equations, however, arise from physical problems where something is known of the form of $f(x)$ which will enable us to make a reasonable guess for N. Now

$$I_m = \int_{-1}^{1} h_m(y) f(y)\,dy$$

is a constant depending upon $a_0, a_1, ----, a_N$ and can be evaluated using equation (6.3.6). If $C_n(G)$ denotes the coefficient of $T_n(x)$ in the Chebyshev expansion of a function $G(x)$, then on equating coefficients of $T_n(x)$ on each side of equation (6.4.2) we find,

$$(6.4.3) \qquad a_n = C_n(F) + \lambda \sum_{m=1}^{M} C_n(g_m) I_m(a_0, \ldots, a_N) \text{ for } n = 0, 1, \ldots, N$$

This gives a system of $(N+1)$ linear equations for the unknown coefficients $a_0, a_1, ---, a_N$.

These equations can be solved numerically by standard methods to give the Chebyshev expansion of $f(x)$. From this series the value of the function can be found for any x in the range $-1 \leqslant x \leqslant 1$, by the method of reference 8.

An exactly similar analysis holds for the range $0 \leqslant x \leqslant 1$, when the $T_n^*(x)$ polynomials are used.

Example 6.1. Let us consider the integral equation

$$f(x) = -\frac{2}{\pi}\cos(\tfrac{1}{2}\pi x) + 2\int_0^1 \cos\tfrac{1}{2}\pi(x-y)\, f(y)\, dy,$$

whose solution is given by $f(x) = \sin(\frac{1}{2}\pi x)$. The kernel is separable with $M = 2$ where,

$$I_1 = \int_0^1 f(y)\cos(\tfrac{1}{2}\pi y)\,dy \text{ and } I_2 = \int_0^1 f(y)\sin(\tfrac{1}{2}\pi y)\,dy.$$

Using Clenshaw's method, we find,

$$\begin{aligned}\begin{matrix}\sin\\ \cos\end{matrix}(\tfrac{1}{2}\pi x) = {} & +0{\cdot}602\,194 \pm 0{\cdot}513\,625\,T_1^*(x) - 0{\cdot}103\,546\,T_2^*(x) \\ & \mp 0{\cdot}013\,732\,T_3^*(x) + 0{\cdot}001\,359\,T_4^*(x) \pm 0{\cdot}000\,107\,T_5^*(x) \\ & - 0{\cdot}000\,007\,T_6^*(x).\end{aligned}$$

In this example, we see that to $6D$ we can represent the expansion of $F(x)$ by a polynomial of degree 6. Consequently we take $N = 6$, and assume that

$$f(x) = \frac{1}{2}A_0 + \sum_{n=1}^{6} A_n T_n^*(x)$$

Using equation (6.3.9), we find

$$\begin{bmatrix} I_1 \\ I_2 \end{bmatrix} = \begin{aligned} & +0{\cdot}318\,309\,A_0 \mp 0{\cdot}173\,950\,A_1 - 0{\cdot}249\,298\,A_2 \pm 0{\cdot}109\,413\,A_3 \\ & -0{\cdot}020\,740\,A_4 \pm 0{\cdot}022\,008\,A_5 - 0{\cdot}013\,169\,A_6 \end{aligned}$$

With these values we find on solving equation (6.4.3) the following Chebyshev expansion for $f(x)$,

$$\begin{aligned} f(x) = {} & 0{\cdot}60220 + 0{\cdot}51362\,T_1^*(x) - 0{\cdot}10355\,T_2^*(x) - 0{\cdot}01373\,T_3^*(x) \\ & + 0{\cdot}00136\,T_4^*(x) + 0{\cdot}00011\,T_5^*(x) - 0{\cdot}00001\,T_6^*(x) \end{aligned}$$

This expansion can be compared with that for $\sin(\frac{1}{2}\pi x)$ from which we see that there is an error of approximately 1×10^{-5}. Although starting with the expansion of all the given functions to 6D, some accuracy has been lost in the sixth decimal place due to rounding errors.

With this Chebyshev expansion for $f(x)$ we might conclude from the rate of convergence of the last three coefficients, that the truncation error will be less than 1×10^{-5}. With a round-off error in each term less than $\frac{1}{2} \times 10^{-5}$ we might conclude just from the series expansion that the error in $f(x)$ will be less than 4×10^{-5}. Consequently we can assume that the expansion will give values of $f(x)$ correct to 4D for all values of x in $0 \leq x \leq 1$. This we know to be correct, being a generous upper estimate of the error.

Finally, we note that whenever the kernel is separable, the integral equation is satisfied for all values of x when determining the relations between the coefficients A_n.

6.5 Comparison with Crout's method.

We shall now compare by means of an example, the Chebyshev series expansion with the method of Crout. In this problem, the kernel is again separable, although it has a discontinuity in the first derivative.

Example 6.2.

$$f(x) = \lambda \int_0^L K(x,y)\, f(y)\, dy$$

where
$$K(x,y) = \begin{cases} \dfrac{x(L-y)}{EIL} & \text{for } y \geq x \\[2ex] \dfrac{y(L-x)}{EIL} & \text{for } y \leq x. \end{cases}$$

This integral equation arises in the problem of the buckling of a beam of length L. It is an eigen-value problem in which we want to find those values of λ for which a non-trivial solution exists. In particular we wish to find the first mode of buckling where the mid-point of the beam is an anti-node. The analytic solution for this mode of buckling is

$$f(x) = \sin \frac{\pi x}{L} \quad \text{with} \quad \lambda = \pi^2 \frac{EI}{L^2}$$

Defining $\xi = \frac{x}{L}$, $\eta = \frac{y}{L}$, $\mu = \frac{\lambda L^2}{EI}$ and writing,

$$f(L\xi) \equiv u(\xi) \text{ and } f(L\eta) \equiv u(\eta),$$

the equation can be written as,

$$u(\xi) = \mu \left\{ (1-\xi)\int_0^\xi \eta u(\eta)\,d\eta + \xi \int_\xi^1 (1-\eta) u(\eta)\,d\eta \right\}.$$

Again, the kernel is separable although each integral contains the variable as a limit. Write,

$$u(\xi) = \tfrac{1}{2}A_0 + \sum_{n=1}^{\infty} A_n T_n^*(\xi),$$

$$I(\xi) = \int_0^\xi \eta u(\eta)\,d\eta \text{ and } J(\xi) = \int_\xi^1 (1-\eta)u(\eta)\,d\eta$$

The function $I(\xi)$ satisfies the equations,

$$\frac{dI}{d\xi} = \xi u(\xi) \quad \text{with} \quad I(0) = 0$$

On writing $I(\xi) = \frac{1}{2}\alpha_0 + \sum_{n=1}^{\infty} \alpha_n T_n^*(\xi)$ we find at once,

$$\alpha_0 = 2\sum_{n=1}^{\infty} (-1)^{n+1}\alpha_n \text{ where } \alpha_n = \frac{1}{16n}\left(A_{n-2} + 2A_{n-1} - 2A_{n+1} - A_{n+2}\right)$$

for $n \geq 1$. A similar result can be found for the coefficients β_n in the Chebyshev expansion for $J(\xi)$. Returning to the integral equation, if $C_n^*(G)$ denotes the coefficient of $T_n^*(\xi)$ in the Chebyshev expansion of $G(\xi)$ then,

$$C_n^*(u) = \mu C_n^*\left[I - \xi(I - J)\right] \text{ for all } n.$$

On simplifying this expression we find the following 3 term recurrence relation for A_n, valid for all $n \geq 2$,

(6.5.1) $(n+1)A_{n-2} + \left[16n(n^2-1)\varepsilon - 2n\right]A_n + (n-1)A_{n+2} = 0,$

where $\varepsilon = 1/\mu$. Corresponding to $n = 0$, and using the values for α_0 and β_0 we find,

$$(6.5.2) \quad (96\varepsilon - 6)A_0 + 7A_2 - 36\sum_{n=2}^{\infty}\frac{1}{(n^2-1)(4n^2-1)}A_{2n} = 0$$

A corresponding equation can be found for $n = 1$, but since we are interested only in the first mode of buckling which gives a solution symmetrical about $\xi = 1/2$, we have,

$$A_{2n+1} = 0 \ , \quad n \geq 0$$

Rewriting equation (6.5.1) with $2n$ in place of n gives

$$(6.5.3) \quad (2n+1)A_{2n-2} + \left[32(4n^2-1)\varepsilon - 4n\right]A_{2n} + (2n-1)A_{2n+2} = 0, \quad n \geq 1$$

Equations (6.5.2) and (6.5.3) completely define the problem for symmetrical solutions.

Following Crout, we assume that $u(\xi)$ can be approximated by a polynomial of degree four, so that,

$$u(\xi) = \tfrac{1}{2}A_0 + A_2 T_2^*(\xi) + A_4 T_4^*(\xi)$$

The three equations for A_0, A_2, A_4 obtained from equations (6.5.2) and (6.5.3) can be written in the matrix form

$$\underset{\sim}{M}\,\underset{\sim}{A} = \varepsilon\,\underset{\sim}{A}$$

where $\underset{\sim}{A}$ is the column vector $\{A_0, A_2, A_4\}$ and $\underset{\sim}{M}$ is the matrix,

$$\begin{pmatrix} +\frac{1}{16} & -\frac{7}{96} & +\frac{1}{120} \\ -\frac{1}{32} & +\frac{1}{24} & -\frac{1}{96} \\ 0 & -\frac{1}{192} & +\frac{1}{120} \end{pmatrix}$$

The largest eigenvalue of this matrix corresponds to $\mu = 9{\cdot}86958$ so that,

$$\lambda = 9{\cdot}86958 \; \frac{EI}{L^2} .$$

Crout finds $\lambda = 9{\cdot}87605 \frac{EI}{L^2}$, and these two numerically found solutions must be compared with the analytic solution,

$$\lambda = 9{\cdot}86960 \; \frac{EI}{L^2} .$$

Using the Chebyshev expansion to the same order as Crout's Lagrangian-type expansion we have found a much better approximation to the eigenvalue. The errors are 2×10^{-5} and 645×10^{-5} respectively, although the great accuracy in the Chebyshev case seems slightly fortuitous since on repeating the calculation with a sixth degree polynomial, the eigenvalue is found to be $\lambda = 9{\cdot}86966 \frac{EI}{L^2}$ an error of 6×10^{-5} which is larger than for the fourth degree case.

For the eigenfunction $f(x)$, if we normalise the solution so that $f(L/2) = 1$, we find,

$$f(x) = 0{\cdot}47230 - 0{\cdot}49971 \, T_2^*\left(\frac{x}{L}\right) + 0{\cdot}02799 \, T_4^*\left(\frac{x}{L}\right).$$

The comparison with Crout's solution, and the analytic solution is shown in Table 6.1.

	EXACT	CROUT		CHEBYSHEV EXPANSIONS			
	$\lambda = 9.86960 \frac{EI}{L^2}$	$\lambda = 9.87605 \frac{EI}{L^2}$		$\lambda = 9.86958 \frac{EI}{L^2}$		$\lambda = 9.86966 \frac{EI}{L^2}$	
x/L	$\sin \frac{\pi x}{L}$	4th degree	$\lvert error \rvert \times 10^5$	4th degree	$\lvert error \rvert \times 10^5$	6th degree	$\lvert error \rvert \times 10^5$
0.0, 1.0	0	0	0	0.00058	58	−0.00004	4
0.1, 0.9	0.30902	0.30716	186	0.30878	24	+0.30906	4
0.2, 0.8	0.58779	0.58716	63	0.58862	83	0.58785	6
0.3, 0.7	0.80902	0.80918	16	0.81000	98	0.80907	5
0.4, 0.6	0.95106	0.95119	13	0.95142	36	0.95107	1
0.5, 0.5	1.00000	1.00000	0	1.00000	0	+1.00000	0
		$10^{10} \sum (error)^2 =$	38990	$10^{10} \sum (error)^2 =$	21729		

Table 6.1

For the given tabular points, the maximum error in the Chebyshev expansion (98×10^{-5}) is less than in Crout's case (186×10^{-5}). Also, the sum of the squares of the errors at these points is less for the Chebyshev expansion.

Taking a sixth degree expansion for $f(x)$ we find,

$$f(x) = 0{\cdot}47202 - 0{\cdot}49943\, T_2^*\left(\tfrac{x}{L}\right) + 0{\cdot}02795\, T_4^*\left(\tfrac{x}{L}\right) - 0{\cdot}00060\, T_6^*\left(\tfrac{x}{L}\right)$$

The maximum error at the given points has now been reduced to 6×10^{-5}, a considerable improvement in accuracy obtained with little extra computation.

6.6 Non-separable kernel.

In most problems where a numerical approach is required the kernel will not be separable. There are two possible methods of approach. We can try to approximate to the kernel by a function which is separable, and then use the method of Section 6.4. Alternatively, we can consider the equation as it stands and proceed by a method of collocation.

Suppose that the range of the independent variable x has been normalised to $-1 \leq x \leq 1$ and we have the following Fredholm equation,

(6.6.1) $$f(x) = F(x) + \lambda \int_{-1}^{1} K(x,y) f(y)\, dy,$$

where λ, $F(x)$, $K(x,y)$ are given and we have to find $f(x)$.

As before, write

$$f(x) = \tfrac{1}{2} a_0 + \sum_{n=1}^{N} a_n T_n(x)$$

where N in general is not known a priori but might be estimated from perhaps, some physical grounds. In order to determine the $(N+1)$ constants $a_0, a_1, ----, a_N$ we write down the integral equation at each of $(N+1)$ points x_i, say, where $i = 1, 2, ..., (N+1)$. Equation (6.6.1) is then replaced by the $(N+1)$ equations

$$(6.6.2)\quad f(x_i) = F(x_i) + \lambda \int_{-1}^{1} K(x_i, y) f(y)\, dy \; ; \; i = 1, 2, ..., N+1.$$

For each value of x_i, we now compute the Chebyshev expansion for $K(x_i, y)$ either from a differential equation or by some curve fitting process. Using equation (6.3.6), we obtain the value of

$$I(x_i, 1) = \int_{-1}^{1} K(x_i, y) f(y)\, dy$$

in terms of the coefficients $a_0, a_1, ----, a_N$. The quantity $F(x_i)$ is known immediately, and using Tables of Chebyshev Polynomials (reference 1) we can write down $f(x_i)$ in terms of $a_0, a_1, ----, a_N$ for each value of x_i. Equation (6.6.2) becomes

$$(6.6.3)\quad f(x_i) = F(x_i) + \lambda I(x_i, 1) \text{ for } i = 1, 2, ..., N+1.$$

which is a system of $(N+1)$ linear equations for the unknown coefficients. These can be solved by standard methods.

We shall illustrate the method by means of an example taken from reference 13.

<u>Example 6.3</u>

$$f(x) \pm \frac{1}{\pi} \int_{-1}^{1} \frac{1}{[1 + (x-y)^2]} f(y)\, dy = 1$$

Let us consider first the equation with positive sign.

We approximate to the function $f(x)$ by means of a polynomial of degree 6. Since $f(x)$ is an even function of x, we write

$$f(x) = \tfrac{1}{2} a_0 + a_2 T_2(x) + a_4 T_4(x) + a_6 T_6(x),$$

and only consider positive values of x_i, which have been chosen as,

$$x_i = 0,\ 0{\cdot}5,\ 0{\cdot}8 \text{ and } 1{\cdot}0$$

The kernel $K(x_i, y)$ can be considered as satisfying a differential equation of zero order with polynomial coefficients, given by

(6.6.4) $$(1 + x_i^2) K(x_i, y) - 2x_i\, y K(x_i, y) + y^2 K(x_i, y) = 1$$

If we write

$$K(x_i, y) = \tfrac{1}{2} b_0(x_i) + \sum_{n=1}^{\infty} b_n(x_i) T_n(y)$$

then on substitution into equation (6.6.4) and using the formula for $C_n[y\, K(x_i, y)]$ and $C_n[y^2 K(x_i, y)]$ we obtain the recurrence relation between the coefficients b_n for each value of x_i. The coefficients in the expansion of $K(x_i, y)$ for $x_i = 0, 0{\cdot}5, 0{\cdot}8$ and $1{\cdot}0$ are given in Table 6.2.

n	$b_n(0)$	$b_n(0.5)$	$b_n(0.8)$	$b_n(1.0)$
0	+1.414 214	+1.361 549	+1.252 701	+1.137 729
1	0	+0.31920	+0.42286	+0.43457
2	-0.24264	-0.12703	-0.00841	+0.04965
3	0	-0.08453	-0.06081	-0.03079
4	+0.04163	-0.00300	-0.02218	-0.01912
5	0	+0.01245	-0.00023	-0.00449
6	-0.00714	+0.00385	+0.00293	+0.00037
7	0	-0.00091	+0.00116	+0.00070
8	+0.00123	-0.00085	+0.00004	+0.00025
9	0	-0.00009	-0.00014	+0.00003
10	-0.00021	+0.00011	-0.00006	-0.00002
11	0	+0.00004	0	-0.00001
12	+0.00004	-0.00001	0	0
13	0	-0.00001	0	0
14	-0.00001	0	0	0

$$K(x_i, y) = \frac{1}{2} b_0(x_i) + \sum_{n=1}^{\infty} b_n(x_i) T_n(y)$$

Table 6.2

With these coefficients for $K(x_i, y)$ the evaluation of $I(x_i, 1)$ for each value of x_i can now be made by means of equation (6.3.6) to give

$$I(0, 1) = 0.78540\, a_0 \quad -0.71238\, a_2 \quad +0.03686\, a_4 \quad -0.04217\, a_6$$
$$I(0.5, 1) = 0.72322\, a_0 \quad -0.57161\, a_2 \quad -0.04902\, a_4 \quad -0.02328\, a_6$$
$$I(0.8, 1) = 0.63055\, a_0 \quad -0.41763\, a_2 \quad -0.10331\, a_4 \quad -0.02458\, a_6$$
$$I(1, 1) = 0.55358\, a_0 \quad -0.32602\, a_2 \quad -0.11278\, a_4 \quad -0.02975\, a_6$$

Substituting these values into equation (6.6.3) gives the following system of equations,

$$0.75000\, a_0 \; -1.22676\, a_2 \; +1.01173\, a_4 \; -1.01342\, a_6 = 1$$
$$0.73021\, a_0 \; -0.68195\, a_2 \; -0.51560\, a_4 \; +0.99259\, a_6 = 1$$
$$0.70071\, a_0 \; +0.14706\, a_2 \; -0.87608\, a_4 \; -1.00494\, a_6 = 1$$
$$0.67621\, a_0 \; +0.89622\, a_2 \; +0.96410\, a_4 \; +0.99053\, a_6 = 1$$

the solution of which gives

$$f(x) = 0.70758 + 0.04937\, T_2(x) - 0.00102\, T_4(x) - 0.00022\, T_6(x)$$

The comparison of this solution with that obtained by Fox and Goodwin is given in Table 6.3.

	$f(x) + \frac{1}{\pi}\int_{-1}^{1}\frac{1}{[1+(x-y)^2]}f(y)\,dy = 1$			$f(x) - \frac{1}{\pi}\int_{-1}^{1}\frac{1}{[1+(x-y)^2]}f(y)\,dy = 1$			
x	Fox and Goodwin to 4D	Chebyshev (6th degree)	Legendre (4th degree)	Fox and Goodwin to 4D	Chebyshev (6th degree)	Legendre (4th degree)	x
0	0.6574	0.65741	0.65745	1.9191	1.91903	1.91925	0
±0.25	0.6638	0.66385	0.66397	1.8997	1.89958	1.89966	±0.25
±0.50	0.6832	0.68318	0.68323	1.8424	1.84240	1.84261	±0.50
±0.75	0.7149	0.71482	0.71432	1.7520	1.75208	1.75318	±0.75
±1.00	0.7557	0.75571	0.75576	1.6397	1.63971	1.63987	±1.00

<u>Table 6.3</u>

Taking the integral equation with negative sign and proceeding as before, we find

$$f(x) = 1.77447 - 0.14003\,T_2(x) + 0.00490\,T_4(x) + 0.00037\,T_6(x)$$

The comparison of this solution with Fox and Goodwin's is also given in Table 6.3. Fox and Goodwin have presented their results only to 4D with an estimated maximum error of 1×10^{-4} due to round-off, and we see that the results found here agree exactly to within the prescribed error.

Of the computational labour in this solution of the problem, most was spent in the determination of the Chebyshev expansions of $K(x_i, y)$. With these expansions found, comparatively little labour was necessary for the evaluation of $I(x_i, 1)$ and the solution of the equations for the coefficients a_n. Had we found it necessary to use a higher degree polynomial for $f(x)$, all previous results for $K(x_i, y)$ and $I(x_i, 1)$ can be used again. When the degree of the polynomial approximation to $f(x)$ is not known a priori, we can start with a small N and increase the degree until the necessary accuracy in the solution is reached.

6.7 Use of Legendre Polynomials.

In the above example, since the limits of integration are from -1 to $+1$, this suggests expanding all functions in terms of the Legendre polynomials $P_n(x)$. The evaluation of $I(x_i, 1)$ is then almost trivial due to the orthogonality property of the Legendre polynomials in the range $-1 \leq x \leq 1$. For suppose

$$f(x) = \sum_{n=0}^{N} a_n P_n(x),$$

and for a given x_i, we find that

$$K(x_i, y) = \sum_{n=0}^{M} b_n(x_i) P_n(y)$$

where in general $M \neq N$, but let us suppose $M > N$.

Then since

$$\int_{-1}^{1} P_n(x) P_m(x)\, dx = \frac{2}{2n+1} \delta_{m,n}$$

we have that

$$(6.7.1) \quad I(x_i, 1) = \int_{-1}^{1} K(x_i, y) f(y) dy = \sum_{n=0}^{N} \frac{2 a_n b_n(x_i)}{2n+1}$$

This equation is considerably simpler than equation (6.3.6) for Chebyshev polynomials. The problem is now one of finding the expansion of $K(x_i, y)$ in terms of Legendre polynomials. This can be found by the method described in Chapter 5, provided the function satisfies some linear differential equation. However, we shall find in general that the recurrence relation between the coefficients b_n is more complicated for Legendre polynomials than for Chebyshev polynomials. The computing time saved in using equation (6.7.1) instead of equation (6.3.6) will generally be more than off-set in the computation of the expansions $K(x_i, y)$.

The integral equation of Example 6.3 has been solved by writing $f(x)$ as the fourth degree polynomial,

$$f(x) = a_0 P_0(x) + a_2 P_2(x) + a_4 P_4(x)$$

To determine the three unknown coefficients a_0, a_2 and a_4 we have used collocation at the points $x_i = 0, 0\cdot 5$ and $1\cdot 0$.

The expansions in Legendre polynomials of the kernel

$K(x_i, y)$ are given in Table 6.4, where we have written,

$$K(x_i, y) = \frac{1}{1 + (x_i - y)^2} = \sum_{n=0}^{\infty} b_n(x_i) P_n(y).$$

The coefficients $b_n(x_i)$ are again computed from equation (6.6.4) using the results for $C_n[y K(x_i, y)]$ and $C_n[y^2 K(x_i, y)]$, for expansions in Legendre Polynomials.

n	$b_n(0)$	$b_n(0.5)$	$b_n(1.0)$
0	+0.78540	+0.72322	+0.55357
1		+0.36820	+0.45365
2	−0.35398	−0.16775	+0.08067
3		−0.14610	−0.04544
4	+0.08296	−0.00911	−0.03538
5		+0.02631	−0.00989
6	−0.01722	+0.00950	+0.00052
7		−0.00207	+0.00163
8	+0.00339	−0.00231	+0.00067
9		−0.00030	+0.00008
10	−0.00067		−0.00005
11			−0.00003
12	+0.00013		−0.00001
13			
14	−0.00003		

$$K(x_i, y) = \sum_{n=0}^{\infty} b_n(x_i) P_n(y)$$

Table 6.4

Substituting these expansions into the integral equation with positive sign and using equation (6.7.1), we find the following equations for the coefficients a_0, a_2, a_4

$$1.50000\, a_0 - 0.54507\, a_2 + 0.38089\, a_4 = 1$$

$$1.46042\, a_0 - 0.14636\, a_2 - 0.28970\, a_4 = 1$$

$$1.35241\, a_0 + 1.01027\, a_2 + 0.99750\, a_4 = 1$$

the solution of which give

+ve sign ; $f(x) = 0.69107 + 0.06615\, P_2(x) - 0.00146\, P_4(x)$

Repeating the calculations for the integral equation with negative sign, we find,

−ve sign ; $f(x) = 1.82129 - 0.18971\, P_2(x) + 0.00829\, P_4(x)$.

These results are tabulated in Table 6.3 and agree excellently to 3D with the previously obtained results.

6.8 Conclusions.

In this Chapter we have considered the use of Chebyshev polynomials in the numerical solution of integral equations of the Fredholm type. The method described here is not as versatile as the finite-difference techniques, since it depends on the Chebyshev expansions of the functions arising in the equations being readily computed. However, in cases where the method can be used without a prohibitive amount of labour, we obtain the value of the function throughout the range of x, instead of at a discrete number of points.

When comparing the method of Chebyshev expansions with Crout's Lagrange-type polynomial expansions to the same degree, a greater accuracy is obtained. Furthermore, from the magnitudes of the coefficients in the Chebyshev expansion, some estimate can generally be made to its accuracy.

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S U M M A R Y.

In this thesis, two applications of Chebyshev polynomials to problems in numerical analysis have been described. Starting with Clenshaw's method for the solution of linear ordinary differential equations by expanding the dependent variable and its derivatives directly in Chebyshev series, the numerical solution of the one dimensional heat equation has been considered. The partial differential equation is first reduced to a system of ordinary differential equations by the method first proposed by Hartree and Womersley. This resulting system of equations is solved using Clenshaw's method. Two particular problems have been worked out in detail and indicate that the method is a useful one. A second application of Chebyshev series is made in the solution of linear non-singular integral equations of the Fredholm-type. Compared with the polynomial approximation method proposed by Crout, the Chebyshev method gives greater accuracy. Finally a generalisation of Clenshaw's method is made into the solution of ordinary differential equations by expansions in series of ultraspherical polynomials. This gives, in particular, a rapid means of finding expansions in Legendre polynomials of functions satisfying simple differential equations.