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# "USES OF CHEBYSHEV POLYNOMIALS"

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# POWER EXPANSIONS OF STRONG CONVERGENCE.

## § 1. PARTIAL SUMS OF POWER SERIES.

The conventional Taylor Series expansion of a function f(z):-

$$f(z) = f(o) + \frac{f'(o)}{1!} z + \frac{f''(o)}{2!} z^2 + \ldots. \qquad (1.1)$$

is an abbreviation for the more precise formula:-

$$f(z) = \lim_{n\to\infty} S_n,$$

where the polynomials $S_k$ are the partial sums:

$$S_k = \sum_{r=o}^{k} \frac{f^{(r)}(o).z^r}{r!} \qquad (1.2)$$

The coefficients of the powers of z are uniquely specified, being the same in all the partial sums.

But alternatively we could consider a more flexible sequence of polynomials:-

$$R_o(z) = a_o$$
$$R_1(z) = b_o + b_1 z \qquad (1.3)$$
$$R_2(z) = c_o + c_1 z + c_2 z^2$$

where the coefficients are chosen such that, for z over a specified range, $\lim_{n\to\infty} R_n(z) = f(z)$.

Here the coefficients of equal powers of z in different polynomials need not be the same, and the coefficients may be so chosen as to be suitable for a specified range of z.

Functions may be expandable into infinite series other than power series, e.g. as a series of Legendre polynomials.

$$c_o + c_1 P_1(z) + \ldots + C_k P_k(z) + \ldots. \qquad (1.4)$$

The k'th partial sum for this series is

$$c_o + c_1 P_1(z) + \ldots + c_k P_k(z) \qquad (1.5)$$

which could be rearranged as a conventional polynomial :-

$$a_o + a_1 z + \ldots + a_k z^k \qquad (1.6)$$

Here, if the coefficients $c_i$ of the successive partial sums (1.5) are rigidly fixed, then the coefficients $a_i$ of the polynomial re-arrangement (1.6) are flexible, i.e. they differ from polynomial to polynomial.

Of course, we cannot say that the infinite series actually exists, but only its limit if the series converges. For instance, the conventional manner of writing the Taylor series for $e^x$:-

$$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \qquad (1.7)$$

is only an abbreviation of the statement:-

$$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \dots + \frac{x^n}{n!} + \epsilon_n \qquad (1.8)$$

where $\epsilon_n \to 0$ as $n \to \infty$. More precisely, we can avoid any mention of infinity and say that

$$|\epsilon_n| < \frac{e^{|x|}}{(n+1)!} \qquad (1.9)$$

which gives us much more information about the convergence of the sequence of partial sums of the Taylor series expansion (1.7).

## 2. FUNCTION SPACE

Functions which are quadratically integrable may be represented as vectors in the Function Space of Hilbert. (N.B. A so-called Hilbert Space is much more general than a Function Space).

Let the range of the functions under consideration be normalized as [0,1]. We shall examine the vectors corresponding to the successive powers of x.

First consider

$$f_0(x) = x^0 = 1 \qquad (2.1)$$

Next

$$f_1(x) = x^1, \dots\dots, f_n(x) = x^n \qquad (2.2)$$

Define the "length" of the vector representing a function f(x) as:-

$$V(x) = \left\{ \int_0^1 (f(x))^2 \cdot dx \right\}^{\frac{1}{2}} \qquad (2.3)$$

Then we get:-

$$V_0^2 = \int_0^1 (f_0(x))^2 . dx = 1, \dots\dots,$$
$$V_n^2 = \int_0^1 (f_n(x))^2 dx = \frac{1}{2n+1} \qquad (2.4)$$

The cosine of the angle between two functions f(x) and g(x) is defined as:-

$$(fg) = \frac{\int_0^1 f(x) . g(x) . dx}{\left\{ \int_0^1 (f(x))^2 . dx \right\}^{\frac{1}{2}} \left\{ \int_0^1 (g(x))^2 . dx \right\}^{\frac{1}{2}}} \qquad (2.5)$$

Thus

$$(V_0 V_1) = \frac{\int_0^1 1 \times x dx}{1 \times \frac{1}{\sqrt{3}}} = \frac{\sqrt{3}}{2} = \text{Cos } 30^\circ \qquad (2.6)$$

Hence the vectors $V_0$ and $V_1$ are not orthogonal - rather they are at a skew angle of $30^\circ$ to one another. Similarly, all the vectors corresponding to powers form a skew set.

Normalize the vectors to unit length, i.e. replace $x^n$ by $\frac{x^n}{\sqrt{2n+1}}$

As a measure of orthogonality of the vectors we shall take the hypervolume of the skew hypercube formed by the normalized vectors. This has a maximum value of 1 when the vectors are orthogonal, and equals 0 when the vectors are linearly dependent. By elementary geometry, we find that the hypervolume $v_n$ of the skew hypercube based on the first n powers (with the vectors normalized to unit length) is given by:-

$$v_n^2 = \begin{bmatrix} V_1^2 & (V_1V_2) & \dots & (V_1V_n) \\ (V_2V_1) & V_2^2 & & \vdots \\ \vdots & & \ddots & \vdots \\ (V_nV_1) & \dots & \dots & V_n^2 \end{bmatrix} = 1.3.5\dots(2n+1) \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} & \dots & \frac{1}{n} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \dots & \frac{1}{n+1} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & & \vdots \\ \vdots & & & \ddots & \vdots \\ \frac{1}{n} & \frac{1}{n+1} & \dots & & \frac{1}{2n+1} \end{bmatrix}$$

(2.7)

The determinant of the notorious Hilbert matrix appears on the right of (2.7). Evaluating this, it can be shown that:-

$$v_n = \frac{1}{\binom{2}{1}\binom{4}{2}\binom{6}{3}\cdots\binom{2n}{n}} = \frac{1}{2\times 6\times 20\times 70\times 252\times 924\times\dots\times\binom{2n}{n}}$$

(2.8)

Thus $v_n$ decreases very rapidly with n i.e. the set of vectors representing the powers becomes rapidly more skew as higher powers are introduced. This suggests that the powers are not very suitable bases for representing functions.

Weierstrass's Theorem(that any continuous function over a finite range can be approximated to any desired accuracy by a polynomial) shows that the powers $x^0, x^1, x^2, \dots$ form a complete basis in function space. But the entire set of integer powers is superfluous, and indeed the following theorem shows how redundant is the complete set:-

<u>MÜNTZ'S THEOREM</u>:- Let an infinite sequence $\lambda_k$ be such that:

$$1 \leq \lambda_1 < \lambda_2 < \dots < \lambda_k < \dots$$

Then, a necessary and sufficient condition for the sequence of functions

$$1,\ x^{\lambda_1},\ x^{\lambda_2},\ \dots,\ x^{\lambda_k},$$

to be a complete family is that the series

$$\frac{1}{\lambda_1} + \frac{1}{\lambda_2} + \dots + \frac{1}{\lambda_k} + \dots$$

be divergent.

By a "complete family" of functions we mean a family such that any continuous function can be represented within any specified accuracy as a linear combination of the functions of that family.

We observe that the harmonic series

$$1 + \tfrac{1}{2} + \tfrac{1}{3} + \tfrac{1}{4} + \ldots + \frac{1}{n} + \ldots$$

remains divergent when any finite number of terms is removed. Applying Müntz's Theorem we conclude that the sequence $1, x^1, x^2, \ldots$ remains a complete set when any finite number of powers are removed, and even infinite sequences of powers can be removed and yet leave a complete set. This is in marked contrast to orthonormal complete sets, from which none can be removed.

Actually, the family of integer powers contains in the highest degree the properties of non-specification and non-orthogonality. We shall examine the extent to which any power can be represented on a basis of lower powers:

## §3 CHEBYSHEV POLYNOMIALS

Definition:-

$$\left.\begin{aligned} T_n(x) &= \text{Cos } n \text{ Arccos } x \\ T_n^*(x) &= \text{Cos } n\text{Arccos } (2x-1) \end{aligned}\right\} \qquad (3.1)$$

These families of polynomials were invented by Chebyshev in connection with the following result, (cf (3.4) and (3.5)) which was indeed the only occasion on which he used the polynomials.

It follows from the definition (3.1) that:

$$T_n^*(x) = \tfrac{1}{2}\, 4^n x^n + \ldots \qquad (3.2)$$

Normalize the polynomials as follows:-

$$\frac{2}{4^n}\, T_n^*(x) = x^n + c_1 x^{n-1} + \ldots + c_n \qquad (3.3)$$

The upper bound of $|T_n^*(x)|$ in the range $[0,1]$ is clearly 1 (cf (3.1). Therefore,

$$x^n = -c_1 x^{n-1} - \ldots - c_n + \epsilon_n \qquad (3.4)$$

where

$$\epsilon_n = \frac{2}{4^n}\, T_n^*(x), \qquad |\epsilon_n| \leq \frac{2}{4^n} \qquad (3.5)$$

Thus (over the range $[0,1]$), $x^n$ can be approximated by an $(n-1)$ th-order polynomial with error not greater than $\frac{2}{4^n}$ e.g. $x^{10}$ can be approximated by a 9th-order polynomial with error $<2\times10^{-6}$. It can be shown (from an analysis of the maxima and minima of $T_n^*(x)$) that (3.4) gives the best possible approximation to $x^n$ by a lower order polynomial.

Equation (3.4) shows that any high integer power of x is almost a linear combination of the lower powers. If we are given any nth-order polynomial $p_n(x)$ we could use (3.4) to remove the highest power of x (ignoring $\epsilon_n$,) giving the best possible approximation to $p_n(x)$ by an $(n-1)$' th-order polynomial. A second application of (3.4) would give the best possible approximation by an $(n-2)$ th-order polynomial to the $(x-1)$ th-order polynomial, and accordingly this second application will give almost the best possible approximation to $p_n(x)$ by an $(n-2)$' th-order polynomial. The process may be continued, giving polynomials of decreasing degree approximating to $p_n(x)$.

Thus if $p_n(x) = a_0x^n + a_1x^{n-1} + \ldots + a_n$ (3.6)

then:-

$$p_n(x) = q_{n-1}(x) + \eta_1(x) \tag{3.7}$$

where

$$q_{n-1}(x) = (a_1 - a_0c_1)x^{n-1} + \ldots + (a_n - a_0c_n) \tag{3.8}$$

and

$$\eta_1(x) = \beta_nT_n^*(x) = \frac{2}{4^n}.\ T_n^*(x) \tag{3.9}$$

After the second step, similarly we get:-

$$p_n(x) = q_{n-2}(x) + \eta_2(x) \tag{3.10}$$

where

$$\eta_2(x) = \beta_{n-1}\ T^*_{n-1}(x) + \beta_nT_n^*(x) \tag{3.11}$$

and in general after m steps we have

$$p_n(x) = q_{n-m}(x) + \eta_m(x) \tag{3.12}$$

where

$$\eta_m(x) = \beta_{n-m+1}\ T^*_{n-m+1}(x) + \ldots + \beta_nT_n^*(x) \tag{3.13}$$

Finally, after n steps:-

$$p_n(x) = \beta_0T_0^*(x) + \beta_1T_1^*(x) + \ldots + \beta_nT_n^*(x) \tag{3.14}$$

In this manner the polynomial $p_n(x)$ has been rewritten as a finite Chebyshev series. For any smooth function, the coefficients of the Chebyshev series expansion decrease very rapidly. In other words a Chebyshev series in which the terms do not decay rapidly can be shown to give a highly irregular function. Thus series of Chebyshev polynomials tend to be rapidly convergent.

In a space with a skew basis, such as the power vectors of § 2, the projection of a vector can be very much greater than the length of the original vector itself e.g. In Fig. 1, the projections OB and OC of the vector OA onto the directions of OD and OE are each much longer than OA.

Fig. 1.


Fig. 1

But with an orthonormal basis, each projection has length not greater than that ofthe original vector.

It is readily verified that the Chebyshev Polynomials $T_n^*(x)$, although not themselves orthogonal, become orthogonal when integrated with respect to the weight function $\frac{2}{\pi\sqrt{x(1-x)}}$; i.e.

$$\frac{2}{\pi}\int_0^1 \frac{T_m^*\ T_n^*(x)}{\sqrt{x(1-x)}}.\ dx = \begin{cases} 0 \text{ if } m \neq n \\ 1 \text{ if } m = n \neq 0 \\ 2 \text{ if } m = n = 0 \end{cases} \tag{3.15}$$

In view of this, the Chebyshev polynomials form a complete basis which is orthonormal (with the appropriate weight function). From this we would expect the coefficients of the Chebyshev expansion of a function to decrease more rapidly than those for a power series. (Note that over the range [0,1], both $|x^n| \leq 1$ and $|T_n^*(x)| \leq 1$).

A function could be expanded as a Chebyshev series by evaluating its Taylor series, truncating to give a polynomial and then replacing each power of x by a Chebyshev expansion. But this method is inefficient since many terms of the Taylor series may be needed, there will generally be heavy cancellation between the large coefficients of the Chebyshev expansions of the individual powers of x, and this is largely a numerical process rather than an analytic process. Accordingly, the following alternative procedure is of greater interest.

## § 4 SOLUTION OF DIFFERENTIAL EQUATIONS USING CHEBYSHEV POLYNOMIALS

Most of the common transcendental functions (except the Gamma-function) satisfy linear differential equations with coefficients which are rational functions of x

e.g.

$$y'+y = 0, \; y(o) = 1 \qquad (4.1)$$

defines the function $y=e^{-x}$. Again, the Exponential Integral

$$E(\xi) = \int_{\xi}^{\infty} \frac{dt}{te^t} \qquad (4.2)$$

when differentiated gives

$$E'(\xi) = \frac{-1}{\xi e^{\xi}} \qquad (4.3)$$

Putting

$$y(\xi) = \xi e^{\xi} E(\xi) \text{ and } x = \frac{1}{\xi} \qquad (4.4)$$

we get the differential equation:-

$$x^2y' + (1+x)y = 1 \qquad (4.5)$$

Representing the solution (4.1) and (4.5) as power series, we may solve the ensuing recurrence relations got by equating coefficients so as to get the formal power series solutions of these differential equations.

$$(4.1) \longrightarrow y = 1-\frac{x}{1!} + \frac{x^2}{2!} - \frac{x^3}{3!} + \qquad (4.6)$$

$$(4.5) \longrightarrow y = 1-1!x+2!x^2-3!x^3+ \qquad (4.7)$$

The first power series converges for all x, but the second power series diverges for all non-zero x. However, we never use an infinite number of terms. Suppose we take a finite series i.e. a n'th-order polynomial, and attempt to adjust its coefficients so as to get a solution of the differential equation. We find that we do not have enough parameters at our disposal - we get an over-determined system of linear equations in the coefficients. Hence the equation cannot be satisfied by an n'th order polynomial - but what will happen if we add an adjustable perturbation term to the right-hand side of the differential equation itself?

Let the differential equation be represented as:

$$Dy = \rho(x) \tag{4.8}$$

Let $p_n(x)$ be an n'th-order polynomial such that:-

$$Dp_n(x) = \rho(x) + \tau x^n \tag{4.9}$$

where $\tau$ is undetermined. Then forD such as in (4.1) and (4.5), we now have (n+2)coefficients at our disposal and (n+2) relations between them (including the initial condition). Solving these for $\tau$ and the coefficients of $p_n(x)$, we get a polynomial which is an exact solution of the perturbed differential equation (4.9). But with a perturbation term of the form $\tau x^n$, the perturbation is largely concentrated near the upper end of the range [01]. This suggests that it would be advantageous to use instead a perturbation term of the form $\tau T_n^*(x)$, in which the perturbation is distributed much more uniformly throughout the range [01[. Then the perturbed equation to be solved will be of the form:

$$Dp_n(x) = \rho(x) + \tau T_n^*(x) \tag{4.10}$$

Sometimes the following form may prove to be more suitable:

$$Dp(x) = \rho(x) + \tau T_{n+1}^*(x) \tag{4.11}$$

If these are two degrees of over-determination of the polynomial coefficient (as generally happens when D is a second-order differential operator), then a suitable perturbation term would be $\sigma T_n^*(x) + \tau T_{n+1}^*(x)$. A polynomial solution of a perturbed differential equation (4.9), (4.10) or (4.11) is in some sense an approximation to the solution of the original differential equation.

Let us examine the effect of adding any n'th order polynomial as a perturbed term of a linear ordinary differential equation.

$$Dy = \gamma_0 + \gamma_1 x + \ldots + \gamma_n x^n \tag{4.12}$$

The general solution of this linear equation may be written in the form

$$y = \sum_{k=0}^{n} \gamma_k Q_k(x) \tag{4.13}$$

where $Q_k(x)$ is the polynomial which is the general solution of

$$DQ_k(x) = x^k \tag{4.14}$$

The order of the polynomial $Q_k(x)$ need not necessarily be k.

For the operator of (4.1) $(Dy = y' + y)$ we find that:

$$Q_k(x) = \left(1 - x + \frac{x^2}{2!} + \ldots + \frac{(-1)^k x^k}{k!}\right) \underline{(-1)^k}\ k! \tag{4.15}$$

The term in brackets on the right is the truncated Taylor series for $e^{-x}$. Replacing y by $Q_k$ on the left of (4.1), we get $DQ_k(x) = x^k$.

For the operator of (4.5) $(Dy = x^2y' + (1+x)y)$, we get (cf. 4.7)

$$Q_{k+1}(x) = (1-x+2!\,x^2-3!x^3+\dots+(-1)^k\,k!x^k)\,\frac{(-1)^k}{(k+1)!} \qquad (4.16)$$

for which

$$\left(x^2\frac{d}{dx} + (1+x)\right) Q_{k+1} = x^{k+1} + \frac{(-1)^k}{(k+1)!} \qquad (4.17)$$

These may be written as

$$\left.\begin{aligned} Q_k(x) &= S_k(x)\,(-1)^k k! \\ Q_{k+1}(x) &= S_k^*(x)\,\frac{(-1)^k}{(k+1)!} \end{aligned}\right\} \qquad (4.18)$$

respectively where the $S_k(x)$ and the $S_k^*(x)$ are the appropriate partial sums

We shall apply (4.18) and (4.13) to the case where

$$Dy = \tau\, T_n^*(x) = C_0^n + C_1^n x + C_2^n x^2 + \dots + C_n^n x^n \qquad (4.19)$$

where the coefficients $C_i^n$ can be evaluated. We get for the first case

$$(4.1) \qquad y = \tau \sum_{k=0}^{n} C_k^n\, S_k(x)\,(-1)^k\, k! \qquad (4.20)$$

But in the second case, bearing in mind the constant term on the right-hand side of (4.17)

we take the function

$$y = \tau \sum_{k=0}^{n} C_{k+1}^{n+1}\; S_k^*(x)\,\frac{(-1)^k}{(k+1)!} \qquad (4.21)$$

which is a solution of the perturbed equation

$$Dy = \tau\left\{T_{n+1}^*(x) - C_0^{n+1} - \sum_{k=0}^{n} \frac{(-1)^k}{(k+1)!}\, C_{k+1}^{n+1}\right\} \qquad (4.22)$$

Both in (4.20) and (4.21), the $\tau$ is to be found by requiring y to satisfy the initial condition.

In classical analysis, a sequence of partial sums of a series may be replaced by a sequence of averages (possibly weighted) of the partial sums to give a more strongly convergent sequence - this is the so-called Cesaro summation. The process may be repeated to give Cesaro sums of 2nd order, 3rd order, ... etc. Examining (4.20) in this light, we see that (with $\tau$ suitably adjusted so as to fit any initial condition) y(x) is a Cesaro sum of the infinite series (4.6), but with a weight factor $(-1)^k\, C_k^{n+1}\, k!$ The series (4.6) is already convergent for all x, but this weight factor strongly emphasises the partial sum for largest k, which is a good approximation to the true solutions.

In the case of (4.21) the individual partial sums $S_k^*(x)$ diverge, but (4.21) gives a Cesaro sum with a weight factor $\frac{(-1)^k C_{k+1}^{n+1}}{(k+1)!}$, This (k+1)! in the denominator assigns low weight to the diverging terms of large k, and it can be shown that these weights are the best possible, in the sense that (4.21) has the lowest possible maximum error in representing the true solution of the unperturbed differential equation (4.5). Thus the convergent partial runs $S_k(x)$ have been made more rapidly convergent, and the divergent $S_k^*(x)$ have been made convergent.

More generally, if the range is $[0,\alpha]$ adjust the T's to the new range, replacing $T_n^*(x)$ by $T_n^*\left[\frac{x}{\alpha}\right]$, in which event $C_k^n$

7 (cf (4.18) must be replaced by $\frac{Ck^n}{\alpha^k}$, while (4.13) and (4.18) give

$$y^*(x) = \tau \sum_{k=0}^{n} C_k^n \alpha^{-k} Q_k(x) \qquad (4.23)$$

as the solution of a differential equation with a perturbation term $\tau T_n^*\left[\frac{x}{\alpha}\right]$, where $\tau$ is to be adjusted so as to fit the initial conditions.

If a is small then $\alpha^{-k}$ will be very large for large k, sc that the weight emphasises the higher partialsums. This corresponds to the fact that both a Taylor series solution and an asymptotic expansion are good near the origin. Conversely, if $\alpha$ is large the divergence-producing character of the $Q_k(x)$ is counteracted, so that the so-called "$\tau$-method" (i.e. adding a perturbation term $\tau T_n^*\left(\frac{x}{a}\right)$) is likely to give better convergence over a large range than the Taylor series expansion.

Lanczos' $\tau$-method can be shown to give results identical with Clenshaw's procedure for finding solutions of ordinary differential equations directly in the form of series of Chebyshev polynomials.

## 5 ESTIMATION OF ERROR OF $\tau$-METHOD

The errors of the Taylor series method and of the $\tau$-method may be estimated a priori as follows:-

The remainder after n terms of a Taylor series expansion of f(x) whose (n+1)'st derivative exists, (where x is in the range 0 to 1) may be expressed as

$$\eta_T(x) = \frac{f^{(n+1)}(\theta x) x^{n+1}}{(n+1)!} \qquad (5.1)$$

where $\theta$ is somewhere in the range

$$0 \leqslant \theta \leqslant 1 \qquad (5.2)$$

Alternatively, the remainder may be expressed in Lagrange's form:-

$$\eta_T(x) = \frac{x^{n+1} \int_0^x f^{(n+1)}(\xi).G(x-\xi).d\xi}{(n+1)! \int_0^x G(x-\xi).d\xi} \qquad (5.3)$$

where G is an auxiliary Green's Function with G>0 everywhere

If we expand f(x) in a series of Chebyshev polynomials, it turns out that

$$\eta(x) = \frac{2\int_0^1 f^{(n+1)}(\xi).\ G(x,\xi).d\xi}{4^{n+1}(n+1)!\int_0^1 G(x,\xi).d\xi} \qquad (5.4)$$

where $G(x,\xi)$ is some other Green's function and

$G(x,\xi)>0$ for all x and $\xi$. Applying the Mean Value Theorem to (5.4), we get:-

$$\eta(x) = \frac{2}{4^{n+1}(n+1)!}\ f^{(n+1)}(\phi x) \qquad (5.5)$$

where $\phi$ is somewhere in the range

$$0\leqslant\phi\leqslant1 \qquad (5.6)$$

Comparing (5.5) with (5.1), we see that the error bounds for the Taylor series are better then those for the Chebyshev series when $0<x<<1$; but that over the entire range 0 to 1 the bounds (5.5) for the truncation error of the Chebyshev series are very much smaller than those for the Taylor series expansion, in view of the additional factor $\frac{2}{4^{n+1}}$ in (5.5).

The Green's Function $G(x,\xi)$ in the Chebyshev remainder term (5.4) has the following general form for all x:-

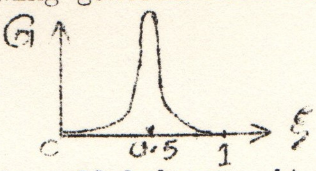


Fig. 2.

Hence if $f^{(n+1)}(\xi)$ is well-behaved, it follows from (5.4) that $\phi\simeq\frac{1}{2}$. Therefore,

$$\eta(x) \simeq \frac{2}{4^{\,n+1}(n+1)!}\ f^{(n+1)}(\tfrac{1}{2}) \qquad (5.7)$$

Comparing (5.7) and (5.1) with $x\simeq\frac{1}{2}$, we see that if $f^{(n+1)}(x)$ is well-behaved the error bound for a truncated Chebyshev series is roughly $2^{-n}$ that for the truncated Taylor series, The error for the Taylor series is concentrated near the upper end of the range 0 to 1 (in view of the term $x^{n+1}$ in (5.1), but the error for the Chebyschev series is distributed much more evenly over the entire range, within greatly reduced bounds.

Converting (5.7) to a range $[0\ \alpha]$, we get approximately,

$$\eta(x) \simeq \frac{2\alpha^{n+1}}{4^{n+1}}\ \frac{\left| f^{(n+1)}\left(\frac{\alpha}{2}\right)\right|}{(n+1)!} \qquad (5.8)$$

How may the higher derivatives of f(x) be estimated? Let f(x) be defined by the linear differential equation:-

$$Df(x) = \rho(x) \qquad (5.9)$$

with appropriate boundary conditions, whereas we solve a perturbed equation:-

$$Dy^*(x) = \rho(x) - \tau T_{n+1}{}^*(x) \qquad (5.10)$$

with the same boundary condition. Defining

$$\eta(x) = f(x) - y^*(x) \qquad (5.11)$$

we see that $\eta(x)$ satisfies the inhomogeneous differential equation:-

$$D\eta(x) = -\tau T^*_{n+1}(x) \qquad (5.12)$$

with homogeneous boundary conditions. Hence we can use a Green's Function, to give:-

$$|\eta(x)| = \tau \int_0^1 T_{n+1}{}^*(\xi) . G(r,\xi).d\xi \qquad (5.13)$$

$$|\eta(x)| \leqslant \tau \int_0^1 G(x,\xi).d\xi \qquad (5.14)$$

Therefore if an upper bound $\rho$ is known for G, we have

$$|\eta(x)| \leqslant \tau\rho \qquad (5.15)$$

N.B. $\rho$ is independent of the order n.

The inequality (5.15) gives a very pessimistic estimate of $\eta$, since G is of fixed sign whilst $T^*_{n+1}(\xi)$ oscillates rapidly. Moreover it is a posteriori estimate, since $\tau$ is not known initially and is found by fitting the general polynomial solution of the perturbed equation (5.10) to the boundary conditions.

Another approach to the problem of estimating the errors of the $\tau$-method is as follows

Equations (5.12) and (3.1) give:-

$$D\eta(x) = -\tau T_{n+1}{}^*(x) = -\tau \mathrm{Cos}\,(n+1)\theta = -\tau \mathrm{Re}^{i(n+1)\theta} \qquad (5.16)$$

Although the right hand side is a rapidly fluctuating function of x (especially near x =0 and x=1), it varies smoothly with respect to $\theta$. This suggests that

$$\eta(x) = \tau B(x)\, e^{i(n+1)\theta} \qquad (5.17)$$

where B(x) varies fairly smoothly with x, i.e. most of the fluctuation of $\eta$ is catered for by the term $e^{i(n+1)\theta}$. Hence in the operator D we may neglect $\frac{d}{dx} B(x)$ in comparison with B(x), and as a result (5.16) reduces a purely algebraic equation for B(x). Solving this, we may estimate the maximum possible error $\eta$.

This is known as the "method of forced oscillations"

SINGULAR CONDITIONS

## §6 PITFALLS IN THE τ-METHOD

Consider again the exponential integral:-

$$E(x) = \int_x^\infty \frac{dt}{te^t} \tag{6.1}$$

On the negative branch, instead of (4.5) we get:-

$$-x^2y' + y(1-x) = 1 \tag{6.2}$$

Applying the τ-method, we seek a polynomial solution of the perturbed equation:-

$$x^2y^{*\prime} + y^*(1-x) = 1 + \tau T_n^*(x) \tag{6.3}$$

We have the asymptotic expansion

$$F(x) = E(-x) = \frac{e^x}{x}\left(1+\frac{1!}{x} + \frac{2!}{x^2} + \frac{3!}{x^3} + \ldots\ldots\right) \tag{6.4}$$

The τ-method error estimate appears to fail. Indeed, if $Y(x)$ is the solution of the homogeneous equation, we get the general solution

$$y(x) = y_o(x) + CY(x) \tag{6.4}$$

where $y_o(x)$ is a Particular Integral, and

$$Y(x) = \frac{1}{x} e^{\frac{1}{x}} \tag{6.5}$$

in the positive branch, but

$$Y(x) = \frac{1}{x} e^{\frac{-1}{x}} \tag{6.6}$$

in the negative branch. In the positive branch, $Y(x) \to \infty$ as $x \to 0$, so that automatically C= 0, since y(o) is finite. In the negative branch as $x \to 0$, we have $Y \to 0$, $Y' \to 0$m $Y'' \to 0$, $Y''' \to 0$,....etc. Therefore the Complementary Function $Y(x)$ cannot be excluded by any boundary condition at x=0, and a boundary condition for some positive x (e.g. x=+∞) is required for fixing the solution of (6.2) uniquely. Thus the τ -method cannot be applied with boundary conditions at x=0,

Similar troubles can arise when the τ-method is applied to Bessel's differential equation, and to any case where the homogeneous equation has a nonzero solution. However, if it is known beforehand that the solution of the differential equation has such features, then the τ-method can be adapted to such problems.

Another pitfall in the τ-method is illustrated by the following example:-

Let $$y = x^p \tag{6.7}$$

where p is fractional. Then

$$\frac{y'}{y} = \frac{p}{x} \tag{6.8}$$

$$\therefore\; xy' - py = 0,\; y(o) = 0 \tag{6.9}$$

The $\tau$-method gives disappointing results in the range 0 to 1. But x=0 is a singularity of the solution $y=x^p$, so that we can hardly expect good results over a range which includes the origin. Hence, instead of taking the range [01] and fixing y at x=0, we shall fix it at x=1. Shifting the origin, y is rewritten as $(1-x)^p$ over a range $[0\alpha]$ where $\alpha<1$, in order to avoid t e singularity. As in (4.21) we now get the following approximation to $(1-x)^p$:-

$$y = \tau \sum \frac{C_k^n}{\alpha^k} Q_k(x) \tag{6.10}$$

Now put $x = \alpha$, i.e. the very end of the range $[0\ \alpha]$. Then (6.10) becomes:-

$$(1-\alpha)^p = \tau \sum \frac{C_k^n}{\alpha^k} Q_k(a) \tag{6.11}$$

Thus we get a rational approximation to $(1-x)^p$. This forms the best Chebyshev-type approximation possible to $(1-\alpha)^p$. The error worsens as $\alpha\to 1$. In general, if a function has any singularity th n a Chebyshev expansion over a range including that singularity will give poor results.

## §7 LEGENDRE POLYNOMIAL EXPANSION

Over the entire range of the argument, Chebsyhev polynomial perturbations minimize the maximum error in the solution of the perturbed equation. But Lanczos has made the interesting discovery that if we are interested in the solution at only one point $x=\alpha$, then a solution over the range $[0\alpha]$ with the equation perturbed by a Legendre polynomial gives the best possible result at the one point $x=\alpha$. Indeed it can give accuracy at $x=\alpha$ much higher than the Chebyshev techniques, which minimizes the maximum error over the entire range $[0\alpha]$. This superiority holds only if there is no singularity within the range, so that it does not hold for, say, the exponential integral including the origin.

In order to see only this is so, consider the perturbed equation:

$$Dy(x) = \tau_1 \ P_{n+1}^*(x) \tag{7.1}$$

rather than $\tau T_{n+1}^*(x)$. To solve this, the $C_n^k$ of (4.21) could be taken as the coefficients of the Legendre polynomial $P_{n+1}^*$, rather than of $T_{n+1}^*(x)$. We know that $|\tau_1| > |\tau|$, since Chebyshev polynomials minimise the maximum error in the range.

Using the Green's Function, we get:

$$\eta(x) = \tau_1 \int_0^1 P_{n+1}^*(\xi)\ G(x,\xi).d\xi \tag{7.2}$$

Now G has a discontinuity at $x=\xi$, so that G camot be approximated by p powers of x and $\xi$. But at the end point x =1, $G(1,\xi)$ is continuous throughout the entire range $\xi = [01]$.

Therefore $G(1,\xi)$ can be well approximated by powers, according to Weierstrass' Theorem. Expand $G(1,\xi)$ in a series of Legendre polynomials.

$$G(1,\xi) = \sum_{k=0}^{n} C_k P_k^*(\xi) + \tau'\eta'(\xi) \qquad (7.3)$$

where the remainder term $\tau'\eta'$ is generally very small. Putting x=1 in (7.2) and using (7.3), we get:

$$\eta(1) = \tau_1 \int_0^1 P_{n+1}^*(\xi).\ G(1,\xi).\ d\xi$$

$$= \tau_1 \int_0^1 P_{n+1}^*(\xi) \left( \sum_{k=0}^{n} C_k P_k^*(\xi) + \tau'\eta'(\xi) \right). d\xi$$

$$= \tau_1 \sum_{k=0}^{n} \int_0^1 C_k P_{n+1}^*(\xi).P_k^*(\xi).d\xi + \tau_1\tau' \int_0^1 P_{n+1}^*(\xi).\eta'(\xi).d\xi$$

$$= \tau_1\tau' \int_0^1 P_{n+1}(\xi).\eta'(\xi).\ d\xi \qquad (7.4)$$

since the Legendre polynomials are orthogonal over the range [01]. Thus the error $\eta(1)$ at the end of the range is of the order $\tau_1\tau'$, which is generally of a higher order of smallness than $\tau_1$ itself. The requisite orthogonality properties (of polynomials with unit weight over the range [01]) are possessed only by the Legendre polynomials, so that the perturbation (7.1) is indeed the best possible for minimising the error at the end of the range.

## ANALYSIS OF EQUIDISTANT DATA

### §8 FOURIER ANALYSIS

Here we shall consider values of x over the range [-1 1] . If we take

$$\theta = \text{Arcos } x \qquad (8.1)$$

then any function f(x) is a periodic even function $f(\text{Cos } \theta)$ of the argument $\theta$, and if f(x) is an analytic function of x then $f(\text{Cos}\theta)$ is an analytic function of $\theta$. An expansion of f(x) into a series of Chebyshev polynomials $T_n(x)$ is exactly equivalent to a Fourier series expansion of $f(\text{Cos}\theta)$.
Therefore if f(x) is analytic the coefficients of both expansions will decrease very rapidly.

Thus we can apply the highly developed theory of Fourier series to Chebyshev series, and vice versa. In particular, any function f(x) which is continuous over the range [-1 1] is a continuous periodic even function of $\theta$, and thus

$$f(\text{Cos}\theta) = \tfrac{1}{2} a_0 + a_1 \text{Cos}\theta + a_2 \text{Cos } 2\theta + \cdots \qquad (8.1a)$$

$$f(x) = \tfrac{1}{2} a_0 + a_1 T_1(x) + a_2 T_2(x) + \cdots \qquad (8.1b)$$

are convergent expansions (with, moreover, rapidly decreasing coefficients), whether or not a Taylor series expansion converges.

The coefficients could be found by the standard integration process based on the orthogonality integral properties, but such integrations will generally be exceedingly difficult to perform. But if the data are given at equidistant values of $\theta$, then we could exploit the discrete orthogonality summation properties of cosines to find the coefficients of a finite Fourier series fitting at the equidistant points. It can be shown that the error of the finite Fourier series is never more than twice that resulting from using twice the number of terms with exact coefficients (i.e. found by integration, rather than by summation).

But equidistant $\theta$ do not correspond to equidistant x. Indeed if $\theta_k = \frac{k\pi}{n}$ $(k=0,1,2, \ldots,n)$ then $x_k = \mathrm{Cos}\,\frac{k\pi}{n}$, which are inconveniently spaced values of x. If we are interested in fitting a polynomial to a function which can be evaluated for any argument (e.g by a subroutine) then it is convenient to use $x_k = \mathrm{Cos}\,\frac{k\pi}{n}$ and to fit a finite Fourier sum, which gives directly a finite Chebyshev series. There is no need to rearrange a Chebyshev series into a standard polynomial - the finite Chebyshev series may most conveniently be evaluated by a form of "nested" multiplication for any value of its argument (cf. Clenshaw).

But usually we are given the values of a function at (n+1) equidistant values of x, as in an ordinary table. It would be possible to evaluate the function at the Chebyshev points by applying some interpolation procedure, but it is generally preferable to fit curves by techniques such as those in the following section.

## §9 FITTING CURVES TO PERIODIC FUNCTIONS

Consider any function $G_k(x)$ whose k'th derivative exists. Write the derivatives of $G_k(x)$ in the following unorthodix manner:-

$$\left.\begin{aligned} G_k'(x) &= G_{k-1}(x) \\ G_{k-1}'(x) &= G_{k-2}(x) \\ &\cdots\cdots \\ G_1'(x) &= G_o(x) = G(x) \end{aligned}\right\} \qquad (9.1)$$

Let f(x) be another function whose (k+1)'th derivative exists - we shall write its derivatives in the orthodox manner as

$$f'(x),\ f''(x),\ \ldots,\ f^{(k+1)}(x).$$

Integrating by parts, we get:

$$\int_a^b f^{(k+1)}(\xi)\, G_k(x-\xi).d\xi = \int G_k(x-\xi).df^{(k)}(\xi)$$

$$= \Big[ f^{(k)}(\xi).G(x-\xi)\Big]_a^b - \int f^{(k)}(\xi).dG_k(x-\xi)$$

$$= \Big[f^{(k)}(\xi).G(x-\xi)\Big]_a^b + \int_a^b f^{(k)}(\xi).\ G_{k-1}(x-\xi).d\xi \qquad (9.2)$$

Repeating this process k times, we get the following important formula for Repeated Integration by Parts:-

$$\int_a^b f'(\xi).\, G(x-\xi).d\xi = - \Big[f'(\xi).G_1(x-\xi) + f''(\xi).\,G_2(x-\xi) + \ldots + f^{(b)}(\xi).G_k(x-\xi)\Big]_a^b + \int_a^b f^{(k+1)}(\xi).G_k(x-\xi).D\xi \qquad (9.3)$$

As a special case, take b=X, and $G_k(t) = \frac{t^k}{k!}$. Then G(t)=1, $G_1(t) = t$, $G_k(t) = \frac{t^2}{2!}$ ,... etc. Applying (9.3) we get

$$f(X)-f(a) = f'(a)\,(X-a) + \ldots + f^{(k)}(a)\,\frac{(X-a)^k}{k!} + + \int_a^X f^{(k+1)}(\xi)\,\frac{(X-\xi)^k}{k!}\,.d\xi \qquad (9.4)$$

giving the Taylor series expansion with remainder term.

Next, define $G_k(t)$ by the following series expansion:-

$$G_k(t) = \text{Re} \sum_{m=1}^{\infty} \frac{e^{im\pi t}}{(im\pi)^{k+1}} \qquad (9.5)$$

Differentiating (9.5) k times, we see that for 0≤r≤k,

$$G_r(t) = \text{Re} \sum_{m=1}^{\infty} \frac{e^{im\pi t}}{(im\pi)^{r+1}} \qquad (9.6)$$

i.e. the set of functions $G_r(t)$ do satisfy equation (9.1).

In particular,

$$G(t) = \text{Re} \sum_{m=1}^{\infty} \frac{e^{im\pi t}}{im\pi} = \sum_{m=1}^{\infty} \frac{\text{Sin}m\pi t}{m\pi} \qquad (9.7)$$

We observe that each $G_r(t)$ is periodic, with period 2, i.e. $G_r(t+2) = G_r(r)$ for all t and for all r. In particular $G_r(-1) = G_r(1)$. The $G_r$ are alternatively odd and even functions of t.

Define

$$B_{r+1}(t) = - 2G_r(t-1) \qquad (9.8)$$

Then each $B_r(t)$ is likewise periodic, (0≤r≤k), with period 2.

Examining formula (9.7) for G(t), we recognise the Fourier expansion for the following saw-tooth wave, shown here over a fundamental period from -1 to +1:-

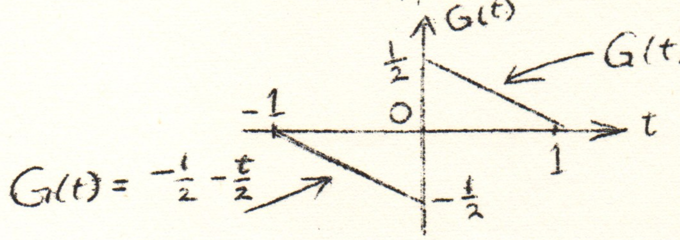


Fig. 3.

Accordingly, $B_1(t)$ is also a sawtooth wave, with the following strudture:-

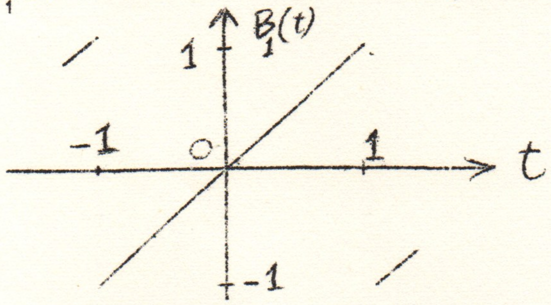


Fig. 4.

i.e.

$$\left.\begin{array}{l} B_1(t) = t \quad \text{for } -1<t<1, \\ B_1(1) = 0 \\ B_1(t+2) = B_1(t) \end{array}\right\} \qquad (9.9)$$

Comparing (9.8) and (9.5) we see that, for each r:-

$$B_r(t) = B'_{r+1}(t) \qquad (9.10)$$

Now, $B_1(t)$ is a periodic peicewise-polynomial curve of degree 1, and hence it follows from (9.10) that each $B_r(t)$ is a periodic piecewise-polynomial of degree r.

Since each $B_{r+1}(t)$ is periodic, it follows from (9.10) that, for each r:

$$\int_{-1}^{-1} B_r(t)\,dt = 0 \qquad (9.11)$$

Consider $B_2(t)$, which is a periodic function equalling a 2nd-order polynomial within the range -1 to 1. Integrating (9.9) we get, for $-1<t<1$;

$$B_2(t) = \frac{t^2}{2!} + k \qquad (9.12)$$

The constant of integration k may be evaluated by integrating (9.12) and applying (9.11):-

$$0 = \int_{-1}^{1} \left(\frac{t^2}{2!}+k\right).dt = \left[\frac{t^3}{3!} + kt\right]_{-1}^{1} = \frac{2}{6} + 2k \;.. \qquad (9.13)$$

Hence $k = \frac{-1}{6}$ and

$$B_2(t) = \frac{t^2}{2!} - \frac{1}{6} \qquad (9.14)$$

Continuing in this manner, we find that, within the range $-1<t<1$;

$$\left.\begin{aligned} B_1(t) &= t \\ B_2(t) &= \frac{t^2}{2!} - \frac{1}{6} \\ B_3(t) &= \frac{t^3}{3!} - \frac{t}{6} \\ B_4(t) &= \frac{t^4}{4!} - \frac{t^2}{12} + \frac{7}{360} \end{aligned}\right\} \qquad (9.15)$$

These happen to be the Bernouilli polynomials. (Somewhat different polynomials are also defined as Bernouilli polynomials).

Putting a=-1, b=1 in (9.3) and taking $G_k(t)$ as in (9.5), the left-hand side of (9.3) becomes

$$\int_{-1}^{1} f'(\xi).\ G(x-\xi).d\xi = \left\{ \int_{-1}^{x-0} + \int_{x+0}^{1} \right\} f'(\xi).G(x-\xi).d\xi$$

$$= \int_{-1}^{x-0} f'(\xi)\ [\tfrac{1}{2}-\tfrac{1}{2}(x-\xi)].d\xi + \int_{x+0}^{1} f'(\xi)\ [-\tfrac{1}{2}-\tfrac{1}{2}(x-\xi)].d\xi$$

$$= -\tfrac{1}{2} \int_{-1}^{1} f'(\xi)(x-\xi).d\xi + \tfrac{1}{2} \int_{-1}^{x} f'(\xi).d\xi - \tfrac{1}{2} \int_{x}^{1} f'(\xi).d\xi$$

$$= -\tfrac{1}{2} \int (x-\xi).df(\xi) + \tfrac{1}{2}\,[f(\xi)]_{-1}^{x} - \tfrac{1}{2}\,[f(\xi)]_{x}^{1}$$

$$= -\tfrac{1}{2}[(x-\xi)f(\xi)]_{-1}^{1} + \tfrac{1}{2} \int f(\xi).d(x-\xi) + f(x) - \tfrac{1}{2}f(-1) - \tfrac{1}{2}f(1)$$

$$= -\tfrac{1}{2}(x-1)f(1) + \tfrac{1}{2}(x+1)f(-1) - \tfrac{1}{2} \int_{-1}^{1} f(\xi).d\xi + f(x) - \tfrac{1}{2}f(-1) - \tfrac{1}{2}f(1)$$

$$= f(x) - \tfrac{1}{2} \int_{-1}^{1} f(\xi).d\xi - \tfrac{x}{2}[f(1)-f(-1)] \qquad (9.16)$$

Bearing in mind that $G_r(x-1)=G_r(x+1)$, the right-hand side of (9.3) becomes:

$$-[f'(\xi)G_1(x-\xi) + f''(\xi)G_2(x-\xi)+\ldots+ f^{(k)}(\xi).G_k(x-\xi)]_{-1}^{1} + \int_{-1}^{1} f^{(k+1)}(\xi)G_k(x-\xi).d\xi$$

$$= - G_1(x-1)[f'(1)-f'(-1)] - G_2(x-1)[f''(1)- f''(-1)] - \ldots - G_k(x-1)[f^{(k)}(1)-f^{(k)}(-1)]$$

$$+ \int_{-1}^{1} f^{(k+1)}(\xi).G_k(x-\xi).d\xi$$

$$= \tfrac{1}{2}B_2(x)[f'(1)-f'(-1)] + \tfrac{1}{2}B_3(x)[f''(1)-f''(-1)]+\ldots+\tfrac{1}{2}B_{k+1}(x)[f^{(k)}(1)-f^{(k)}(-1)]$$

$$+ \int_{-1}^{1} f^{(k+1)}(\xi).G_k(x-\xi).d\xi \qquad (9.17)$$

Equating (9.16) to (9.17), we get the following remarkable formula:-

$$f(x) - \tfrac{1}{2} \int_{-1}^{1} f(\xi).d\xi = \tfrac{1}{2}[f(1)-f(-1)]B_1(x) + \tfrac{1}{2}[f'(1)-f'(-1)]\ B_2(x)+\ldots+ \tfrac{1}{2}[f^{(k)}(1)-f^{(k)}(-1)]B_{k+1}(x)$$

$$+ \int_{-1}^{1} f^{(k+1)}(\xi).G_k(x-\xi).d\xi \qquad (9.18)$$

---

Note that the $B_r(x)$ are universal polynomials, independent of f(x). We recall that:-

$$G_k(x-\xi) = \mathrm{Re} \sum_{m=1}^{\infty} \frac{e^{im\pi(x-\xi)}}{(im\pi)^{k+1}} \qquad (9.19)$$

Replace f(x) by $f(x)+\frac{1}{2}\int_{-1}^{1} f(\xi).d\xi$, so that the left-hand side of (9.18) becomes simply f(x). Expand both sides of (9.18) as Fourier series, truncating the Fourier series in each case after the terms in Sin $n\pi x$ and Cos $n\pi x$, where n is any integer. Denote the truncated Fourier series for $f(x), B_r(x)$ and $G_k(x-\xi)$ by $f^*(x)$, $B_r^*(x)$ and $G_k^*(x-\xi)$ respectively. Subtracting the truncated Fourier series from both sides of (9.18), we get

$$f(x)-f^*(x) = \beta_o[B_1(x)-B_1^*(x)]+\beta_1[B_2(x)-B_2^*(x)]+\dots+\beta_k[B_{k+1}(x)-B_{k+1}^*(x)]$$
$$+\int_{-1}^{1} f^{(k+1)}(\xi)\,[G_k(x-\xi)-G_k^*(x-\xi)]d\xi \qquad (9.20)$$

where

$$\beta_r = \tfrac{1}{2}[f^{(r)}(1) - f^{(r)}(-1)] \qquad (9.21)$$

But equation (9.19) shows that:

$$G_k(x-\xi)-G_k^*(x-\xi) = \text{Re}\sum_{m=n+1}^{\infty} \frac{e^{im\pi(x-\xi)}}{(im\pi)^{k+1}} \qquad (9.22)$$

and hence we get the following important formula for the truncation error:-

$$f(x)-f^*(x)= \beta_o[B_1(x)-B_1^*(x)]+\dots+ \beta_k[B_{k+1}(x)-B_{k+1}^*(x)]$$
$$+ \text{Re}\sum_{m=n+1}^{\infty} \frac{e^{im\pi x}}{(im\pi)^{k+1}} \int_{-1}^{1} f^{(k+1)}(\xi)e^{-im\pi\xi}d\xi \qquad (9.23)$$

Thus we have expressed the error of the truncated Fourier series for f(x) in terms of known functions (viz: the truncation errors of the Fourier series for the Bernouilli polynomials), together with a remainder term. Equation (9.23) shows that this remainder term decreases very rapidly as k and/or n are increased.

Now, <u>if</u> the function f(x) (whose (k+1)st derivative has been assumed to exist) is actually periodic, then each $\beta_r=0$ (cf.(9.21)). Thus for a truly periodic function the truncation error of the Fourier series (taken as far as Sin $n\pi n$ and Cos $n\pi x$) equals:

$$f(x)-f^*(x)= \text{Re}\sum_{m=n+1}^{\infty} \frac{e^{im\pi x}}{(im\pi)^{k+1}} \int_{-1}^{1} f^{(k+1)}(\xi).\, e^{-im\pi\xi}d\xi \qquad (9.24)$$

Equation (9.24) shows that, for a periodic function f(x) which is sufficiently smooth for $f^{(k+1)}(x)$ to exist everywhere, the truncation error becomes very small if k is large, and it decreases rapidly as n is increased for fixed k.

Note that the factor $e^{-im\pi\xi}$ in the integrand of (9.24) fluctuates rapidly about its zero mean value, so that $\int_{-1}^{1} f^{(k+1)}(\xi)e^{-im\pi\xi}.d\xi$ tends to zero as $m\to\infty$ (Fubini's Theorem).

## §10 FITTING CURVES TO APERIODIC FUNCTIONS.

If f(x) is sufficiently smooth for $f^{(k+1)}(x)$ to exist for $-1\leq x\leq 1$ but f(x) is not periodic, then a highly accurate Fourier expansion of f(x) within the range x=-1 to 1 can be obtained by using (9.23).

$$f(x) = f^*(x) + \beta_0[B_1(x)-B_1^*(x)]+\ldots+\beta_k[B_{k+1}(x)-B^*_{k+1}(x)]+R_{k,n} \tag{10.1}$$

where $R_{k,n}$ is the right-hand side of (9.24). In this manner, by adding the correction terms consisting of the truncation errors of Fourier expansions of Bernouilli polynomials (with coefficients equation to $\frac{1}{2}[f^{(r)}(1)-f^{(k)}(-1)]$), f(x) can be expressed with an accuracy as high as though it were strictly periodic. This technique requires that the derivatives of f be known at the ends of the range.

Similar techniques can be applied when Fourier interpolation is used, rather than truncation of a Fourier series.

When fitting a Fourier curve to an aperiodic function, we always know the value of $\beta_0$ $\left(=\frac{1}{2}[f(1)-f(-1)]\right)$, whether or not we know any derivatives at the ends of the range. Therefore if we subtract the linear term $\beta_0 x$ from f(x) we shall get a function for which $\beta_0$ becomes zero, i.e. a function which can be regarded as being periodic without any discontinuities at x=±1. Provided that f'(x) exists for $-1<x<1$, this produces results equivalent to (10.1) with k=0 rather than the truncation term for a discontinuous function

$$f(x)-f^*(x) = \mathrm{Re}\sum_{m=n+1}^{\infty} e^{im\pi x}\int_{-1}^{1} f(\xi).e^{-im\pi\xi}.d\xi \tag{10.2}$$

(cf. (9.24) with k+1=0). Thus the removal of the linear term produces a truncation term $R_{o,n}$, which decreases much more rapidly (as n increases) than does the truncation term (10.2)

Again, when performing a Fourier analysis of an aperiodic curve the convergence of the Fourier series may be improved considerably by taking the range of x as [0,1], then extending the function over the range [-1,0] so that we have an odd function over the range [-1,1], and regarding this as being one period of an odd periolic function g(x):-

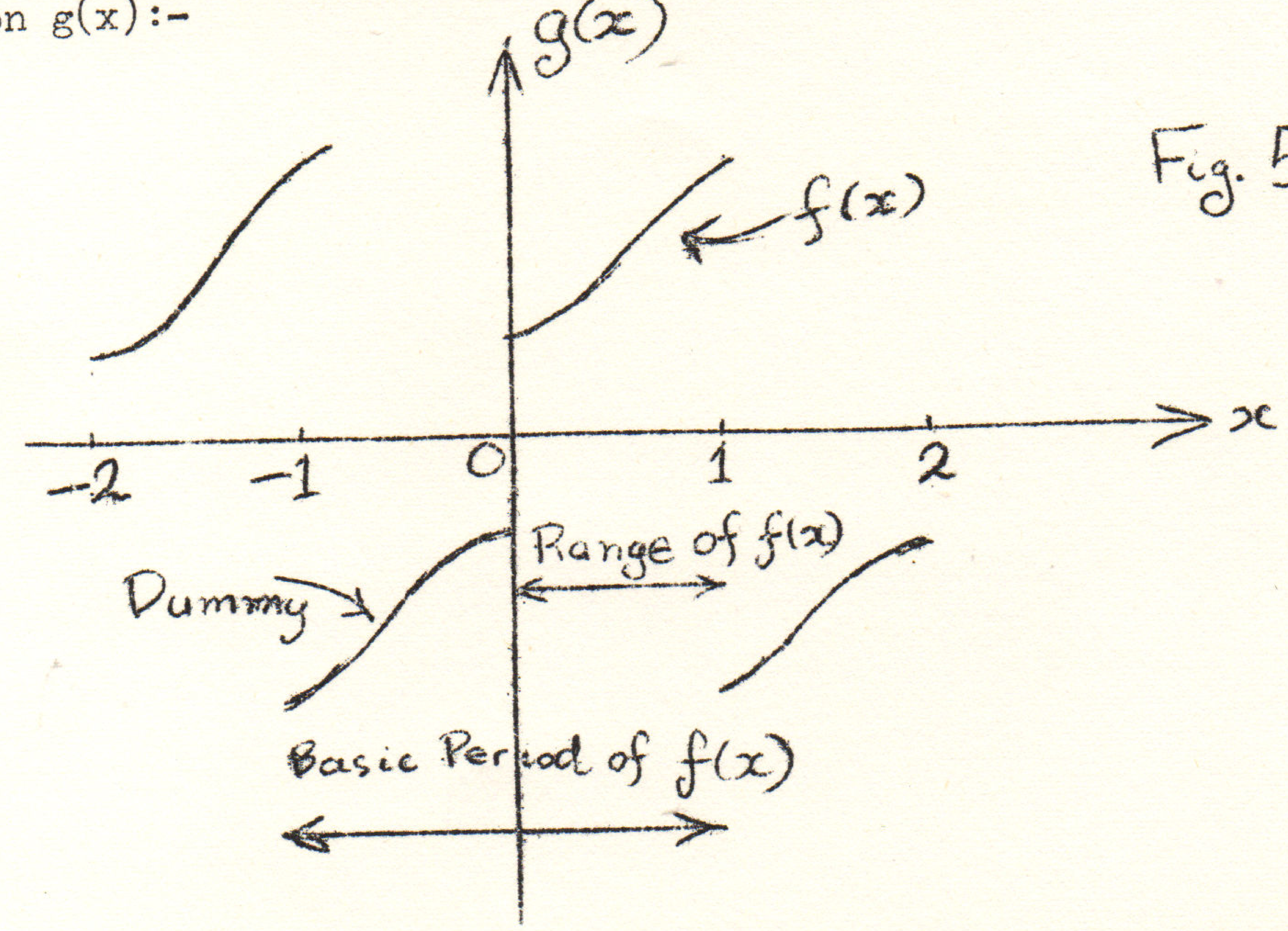


Fig. 5.

The Fourier series for $g(x)$ (which coincides with $f(x)$ for $0<x<1$) contains sine terms only, and all the $\beta_{2r+1}$ are zero.
At $x=0$, $f(x)$ and all of its even derivatives are discontinuous, but all odd derivatives are continuous.

Bearing in mind the extra jump at $x=0$, it can be shown that:-

$$g(x) = f^*(x)+f(1)\Phi_1(x)-f(0)\ \Phi_1(1-x)+ f''(1)\Phi_3(x)-f''(0)\Phi_3(1-x)$$
$$+ f^{(iv)}(1)\ \Phi_5(x)-f^{(iv)}(0)\Phi_5(1-x)+ \mathrm{Re} \sum_{m=n+1}^{\infty} \frac{e^{im\pi x}}{(im\pi)^6} \int_{-1}^{1} f^{(vi)}(\xi).e^{-im\pi\xi}d\xi \qquad (10.3)$$

where $\Phi_k(x)$ is the truncation error of the Fourier series for the Bernouilli polynomial:-

$$\Phi_k(x) = B_k(x)-B_k^*(x) \qquad (10.4)$$

It can be shown that, for $0<x<1$,

$$\left.\begin{aligned} \left|\Phi_3(x)\right| &< \frac{1}{\pi n^2} \\ \left|\Phi_5(x)\right| &< \frac{1}{2\pi^5 n^4} \end{aligned}\right\} \qquad (10.5)$$

In (10.3) the terms $f(1)\ \Phi_1(x)$ and $f(o)\Phi_1(1-x)$ are always known, and (10.5) shows that the truncation error of $f^*(x)+f(1)\Phi_1(x)-f(0)\Phi_1(1-x)$ is $0\left(\frac{1}{n^2}\right)$. If $f''(0)$ and $f''(1)$ are known or can be estimated, then the inclusion of the corresponding terms reduces the truncation error to $0\left(\frac{1}{n^4}\right)$.

Even more rapidly convergent Fourier series can be produced if we first subtract a linear term from $f(x)$, such that the modified $f(x)$ equals zero at $x=0$ and $x=1$. Then reflecting in the origin, we get a basic period of a <u>continuous</u> odd periodic function, which has a rapidly convergent Fourier expansion.

## §11. <u>INDEFINITE INTEGRATION</u>

Let a curve be fitted to $f(x)$, e.g. a Chebyshev series, or a Fourier series which may include polynomial terms as in (10.1). Then we may integrate or differentiate this curve for approximating to the integrals or derivatives of $f(x)$. Of course, the derivatives will be more uncertain than the integrals.

Many numerical techniques are available for finding definite integrals (and derivatives) of $f(x)$ or of the fitted curve, but difficulties can arise if an indefinite integral is required. For example, if Simpson's rule is used for producing a table of the indefinite integral, it will produce numerical integrals only for every second step.
But if a curve has been fitted to $f(x)$ (e.g. Chebyshev or Fourier series) then this curve may be differentiated and integrated analytically, enabling the integrals or derivatives to be found at any point of the range by evaluating analytic expressions. Such techniques may be called "global" integration (or differentiation), since they

utilise all the values at our disposal, in contrast to "local" integration by, say, the trapezoidal rule or Simpson's rule. In consequence of this, much higher accuracy can be attained by global integration than by comparable local integration techniques.

## §12 LARGE-SCALE LINEAR SYSTEMS

Insufficient time remained by this stage for the application of Chebyshev polynomials to the solution of linear equations to be discussed (cf. Golub and Varga). However, Professor Lanczos advocated that the solution of any system of linear algebraic equations

$$Av = \beta \tag{12.1}$$

where A may be a square or a rectangular matrix, should proceed (unless A is an Hermitian matrix) by replacing (12.1) by the augmented set of equations:

$$\begin{bmatrix} 0 & A \\ A^* & 0 \end{bmatrix} \begin{bmatrix} 0 \\ v \end{bmatrix} = \begin{bmatrix} \beta \\ 0 \end{bmatrix} \tag{12.2}$$

This produces a set of equations with an Hermitian matrix, and is equivalent to analysing a linear vector space in terms of both covariant and contravariant coordinates.

Most iterative procedures for solving linear equations can be adapted to the augmented equations (12.2) without actually generating the augmented matrix, but working throughout with A itself.

For a fuller account of augmented matrices (including the extension of the concept of eigenvalues and eigenvectors to matrices which are not square), consult Professor Lanczos' paper in the Proceedings of the Fifth International Mathematical Congress at Edinburgh, and his book on "Linear Differential Operators".

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