An Algorithm for Summing Orthogonal Polynomial Series and their Derivatives with Applications to Curve-Fitting and Interpolation

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1. Introduction and Summary. Clenshaw [1, 2] has described a simple and effective method for summing a Chebyshev series based on the recurrence relation between the Chebyshev coefficients. He has further pointed out that the same method could be used to sum a series of any set of functions which are generated by a linear recurrence relation [1]. Such a set of functions is a set of orthogonal polynomials [3, 4].

This paper describes the application of Clenshaw's technique to the summing of orthogonal polynomial series and extends his principle to the evaluation of any derivative of an orthogonal polynomial series. Applications to least square curve-fitting are discussed and a convenient method is described for interpolating first and higher order derivatives of a function tabulated at equidistant or non-equidistant points.

2. Summing the Polynomial Series. Any set of polynomials which are orthogonal over an interval of the real line or orthogonal over a discrete set of real numbers can be shown to satisfy a three-term recurrence relation [4, 5]

$$p_r(x) = (\gamma_r x - \alpha_r)p_{r-1}(x) - \beta_r p_{r-2}(x) \qquad \text{for } r \geqq 2 \tag{1}$$

with

$$p_1(x) = (\gamma_1 x - \alpha_1)p_0(x)$$

and

$$p_0(x) = \gamma_0 .$$

In these equations $p_r(x)$ is the polynomial of degree r and α_r, β_r and γ_r are constant coefficients which are usually simple and well known.

The recurrence relation (1) can be used to sum a polynomial series

$$f(x) = \sum_{r=0}^{N} c_r p_r(x) \tag{2}$$

by two methods. In the first, due to Forsythe [5], the partial sum

$$S_n(x) = \sum_{r=0}^{n} c_r p_r(x) \tag{3}$$

is calculated from $S_{n-1}(x)$ immediately after $p_n(x)$ is generated by the recurrence relation, for increasing values of n till $n = N$. Then $f(x) = S_N(x)$.

An alternative procedure is based on Clenshaw's method for summing a Cheby-

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shev series. A set of quantities B_r is defined by the formulae

$$(4)\qquad \begin{aligned} B_r &= 0 \quad \text{for } r > N, \\ B_r &= c_r + (\gamma_{r+1}x - \alpha_{r+1})B_{r+1} - \beta_{r+2}B_{r+2} \quad \text{for } 0 \leqq r \leqq N. \end{aligned}$$

By substituting the recurrence relation (1) into (2) and using (4) it can be shown that the series is given simply by

$$(5)\qquad f(x) = \gamma_0 B_0 .$$

Since B_0 can be calculated by successively evaluating the quantities B_N, B_{N-1}, etc. the series is quickly summed with less than $3N$ multiplications and additions, approximately N multiplications faster than Forsythe's method.

The Clenshaw procedure for summing a Chebyshev series is a special case of this process and is obtained by substituting in (1) and (4) the coefficients which generate the Chebyshev polynomials:

$$\alpha_r = 0, \qquad \beta_r = 1 \quad \text{for all } r; \quad \gamma_r = 2 \quad \text{for } r \geqq 2; \qquad \gamma_0 = \gamma_1 = 1.$$

3. Errors. To examine the possibility that errors might build up disastrously during the calculation, suppose that ϵ_r is the error introduced during the calculation of B_r from B_{r+1} and B_{r+2} due both to rounding and to inaccuracies in the coefficients α_{r+1}, γ_{r+1} and β_{r+2}. If the total error in B_r is given by E_r then for $r \leqq N$

$$(6)\quad B_r + E_r = c_r + \epsilon_r + (\gamma_{r+1}x - \alpha_{r+1})(B_{r+1} + E_{r+1}) - \beta_{r+2}(B_{r+2} + E_{r+2})$$

from which it follows that

$$(7)\qquad E_r = \epsilon_r + (\gamma_{r+1}x - \alpha_{r+1})E_{r+1} - \beta_{r+2}E_{r+2} .$$

Clearly since $E_r = 0$ for $r > N$ the errors E_r obey the same recurrence relation as the quantities B_r. The final error is therefore given by

$$(8)\qquad \gamma_0 E_0 = \sum_{r=0}^{N} \epsilon_r p_r(x).$$

This shows that the rounding error introduced in the rth step, ϵ_r, only contributes an error $\epsilon_r p_r(x)$ to the final answer and does not increase the errors introduced in each of the following r steps. This is a generalization of a similar result obtained by Clenshaw for a Chebyshev series and shows that errors do not build up appreciably when a polynomial series is summed by Clenshaw's procedure.

A similar error analysis of Forsythe's method shows that the error accumulation is greater than in Clenshaw's method. Since Forsythe's method is also about N multiplications slower, Clenshaw's procedure is to be preferred for both accuracy and speed.

4. Summing the Derivatives of Polynomial Series. The first derivative of the polynomial series

$$(9)\qquad f'(x) = \sum_{r=1}^{N} c_r p_r'(x)$$

can be evaluated in a manner similar to Clenshaw's technique for summing the series. By taking the derivative of (1) a new recurrence relation involving the derivatives of the polynomials $p_r'(x)$ is obtained

$$p_r'(x) = (\gamma_r x - \alpha_r)p_{r-1}'(x) - \beta_r p_{r-2}'(x) + \gamma_r p_{r-1}(x) \quad \text{for } r \geqq 2 \tag{10}$$

with

$$p_1'(x) = \gamma_1 p_0(x).$$

By substituting (10) into (9) and using the quantities B_r defined in (4), it follows that

$$f'(x) = \sum_{r=1}^{N} B_r \gamma_r p_{r-1}(x). \tag{11}$$

The right-hand side of (11) can be treated as a polynomial series. It can therefore be summed by defining a new set of quantities, B_r', such that

$$\begin{aligned} B_r' &= 0 \quad \text{for } r > N, \\ B_r' &= \gamma_r B_r + (\gamma_r x - \alpha_r)B_{r+1}' - \beta_{r+1}B_{r+2}' \quad \text{for } 1 \leqq r \leqq N. \end{aligned} \tag{12}$$

The series in (11) is then given by

$$f'(x) = \gamma_0 B_1'. \tag{13}$$

The derivative of the series at any value of x can therefore be obtained by calculating successively the set of quantities

$$B_N, B_{N-1}, \cdots, B_0, \quad B_N', B_{N-1}', \cdots, B_1'.$$

Since the series is still given by $\gamma_0 B_0$ it follows that both the series and the derivative can be evaluated with as few as $6N$ multiplications and additions.

An error analysis can be carried out similar to that in the previous section. Quantities E_r and ϵ_r are defined as in (6) and (7). Let $\gamma_r \epsilon_r'$ be the rounding error introduced in the calculation of B_r' in (12) and let E_r' be the total error in B_r'. Then following an argument similar to that used in the derivation of (7) it can be shown that

$$E_r' = \gamma_r(E_r + \epsilon_r') + (\gamma_r x - \alpha_r)E_{r+1}' - \beta_{r+1}E_{r+2}'. \tag{14}$$

It follows that the total error in the derivative is

$$\gamma_0 E_1' = \sum_{r=1}^{N} [\epsilon_r p_r'(x) + \epsilon_r' \gamma_r p_{r-1}(x)] \tag{15}$$

which is approximately twice the error in the series if $\epsilon_r \approx \epsilon_r' \gamma_r$. However, since the derivative may be smaller in magnitude, the percentage error in the derivative may be higher than in the series.

The same principle can be extended to evaluate higher order derivatives of the series. We define sets of quantities for $0 \leqq k \leqq N - 1$,

$$\begin{aligned} B_r^{k+1} &= 0 \quad \text{for } r > N, \\ B_r^{k+1} &= \gamma_t B_r^k + (\gamma_t x - \alpha_t)B_{r+1}^{k+1} - \beta_{t+1}B_{r+2}^{k+1} \quad \text{for } N \geqq r \geqq k + 1, \\ B_r^0 &= c_r \quad \text{for } 0 \leqq r \leqq N \end{aligned} \tag{16}$$

in which $t = r - k$. To calculate the mth derivatives, $0 \leqq m \leqq N$, the sets

$$\{B_r^0\}, \{B_r^1\}, \cdots, \{B_r^m\}$$

are generated successively and the mth derivative is given by

$$f^m(x) = m!\gamma_0 B_m{}^m. \tag{17}$$

This takes less than $3N(m + 1)$ multiplications and additions and there is no disastrous error accumulation.

5. Application to Curve Fitting and Interpolation. Besides its obvious application to series of the orthogonal polynomials found in applied mathematics the algorithm described above can be used to improve Forsythe's method of least square curve-fitting [5]. In this Forsythe has described a method for calculating the coefficients α_r, β_r, γ_r and c_r for a series of orthogonal polynomials which fits in the least square sense a set of experimental points which are not necessarily equidistant. Given these coefficients the above algorithm may be used to evaluate the fitted function or any of its derivatives for any value of x.

If the degree of Forsythe's orthogonal polynomial series is one less than the number of points being curve-fitted, Forsythe's series fits the points exactly and can therefore be used for interpolation. A comparison of the number of arithmetic operations involved shows, however, that this method would be slower than Aitken's interpolation method [6]. Since Aitken's procedure also permits an easy estimate of the error, the use of Forsythe's polynomial series for simple interpolation has little or no advantage over Aitken's method.

However, when it is coupled with the algorithm for evaluating derivatives of the polynomial series a simple method is discovered for interpolating a first or higher order derivative of the tabulated function. It has been used successfully for this purpose on a number of physical problems [7]. It was found that large errors may appear in the calculation of the derivatives, especially the higher derivatives. These arise because of cancellations during the calculation of α_r, β_r, and c_r especially when two or more of the points in the table are close together. In such cases other methods of interpolating the derivatives would be equally inaccurate.

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