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A Note on the Optimal Addition of Abscissas to Quadrature Formulas of Gauss and Lobatto Type

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Abstract. An improved method for the optimal addition of abscissas to quadrature formulas of Gauss and Lobatto type is given.

1. Introduction. We consider the quadrature formula

$$\int_{-1}^{+1} f(x)\,dx \simeq \sum_{k=1}^{N} \alpha_k f(x_k) + \sum_{k=1}^{N+1} \beta_k f(\xi_k), \tag{1}$$

where the x_k's are the abscissas of the N-point Gaussian quadrature formula. We want to determine the additional abscissas ξ_k and the weights α_k and β_k so that the degree of exactness of (1) is maximal. This problem has already been discussed by Kronrod [1] and Patterson [2] and it is well known that the abscissas ξ_k must be the zeros of the polynomial $\phi_{N+1}(x)$ which satisfies

$$\int_{-1}^{+1} P_N(x)\phi_{N+1}(x)x^k\,dx = 0, \qquad k = 0, 1, \cdots, N, \tag{2}$$

where $P_N(x)$ is the Legendre polynomial of degree N. Thus, $\phi_{N+1}(x)$ must be an orthogonal polynomial with respect to the weight function $P_N(x)$. Then, the weights α_k and β_k can be determined so that the degree of exactness of (1) is $3N + 1$ if N is even and $3N + 2$ if N is odd.

Szegö [3] proved that the zeros of $\phi_{N+1}(x)$ and $P_N(x)$ are distinct and alternate on the interval $[-1, +1]$. Kronrod [1] gave a simple method for the computation of the coefficients of $\phi_{N+1}(x)$. This method requires the solution of a triangular system of linear equations, which is, unfortunately, very ill-conditioned. Patterson [2] expanded $\phi_{N+1}(x)$ in terms of Legendre polynomials. The coefficients of this expansion satisfy a linear system of equations which is well-conditioned, although its construction requires a certain amount of computing time.

The present note proposes the expansion of $\phi_{N+1}(x)$ in a series of Chebyshev polynomials. We also give explicit formulas for the weights α_k and β_k. Finally, we consider the optimal addition of abscissas to Lobatto rules. As compared with Patterson's method, our method has three advantages:

(i) It leads to a considerable saving in computing time since the formulas are much simpler.

(ii) The loss of significant figures through cancellation and round-off is slightly reduced, as we verified experimentally. This is in agreement with some theoretical results given by Gautschi [4].

(iii) It is applicable for every value of N, while Patterson's method fails in the

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Lobatto case for $N = 7, 9, 17, 22, 27, 35, 36, 37, 40, \cdots$, since some of the denominators in his recurrence formulae become zero.

2. Optimal Addition of Abscissas to Gaussian Quadrature Formulas. It is evident that $\phi_{N+1}(x)$ is an odd or even function depending on whether N is even or odd. Thus, $\phi_{N+1}(x)$ can be expressed as

$$\phi_{N+1}(x) = \sum_{k=0}^{m}{}' b_k T_{2k}(x), \quad \text{if } N \text{ is odd,} \tag{3}$$

and

$$\phi_{N+1}(x) = \sum_{k=0}^{m} b_k T_{2k+1}(x), \quad \text{if } N \text{ is even,} \tag{4}$$

where $m = [(N + 1)/2]$.

It is clear that the polynomial $\phi_{N+1}(x)$ is only defined to within an arbitrary multiplicative constant. For the sake of convenience, we assume $b_m = 1$.

From (2), we derive the condition

$$\int_{-1}^{+1} P_N(x)\phi_{N+1}(x)T_k(x)\,dx = 0, \qquad k = 0, 1, \cdots, N. \tag{5}$$

In order to calculate the coefficients b_k, $k = 0, 1, \cdots, m - 1$, (3) or (4) is substituted in (5). This leads to the system of equations

$$\begin{aligned} b_{m-1} &= \tau_1 - 1, \\ b_{m-k} &= \sum_{j=1}^{k-1} b_{m-k+j}\tau_j + \tau_k, \qquad k = 2, 3, \cdots, m, \end{aligned} \tag{6}$$

where

$$\tau_k = -\int_{-1}^{+1} P_N(x)T_{N+2k}(x)\,dx \Big/ \int_{-1}^{+1} P_N(x)T_N(x)\,dx. \tag{7}$$

In order to derive a recurrence formula for τ_k, we consider the integral

$$J = \int_{-1}^{+1} [xP_N(x) - P_{N+1}(x)]T_l(x)\,dx. \tag{8}$$

Using a well-known property of the Chebyshev polynomials, we obtain

$$J = \frac{1}{2}\int_{-1}^{+1} [xP_N - P_{N+1}]\, d\left(\frac{T_{l+1}}{l+1} - \frac{T_{l-1}}{l-1}\right), \tag{9}$$

and, by integrating by parts, this integral can be expressed as

$$J = \frac{N}{2(l+1)} I_{N,l+1} - \frac{N}{2(l-1)} I_{N,l-1}, \tag{10}$$

where

$$I_{N,l} = \int_{-1}^{+1} P_N(x)T_l(x)\,dx. \tag{11}$$

On the other hand, using a property of the Legendre polynomials, (8) can be transformed into

$$J = \frac{1}{N+1} \int_{-1}^{+1} (1 - x^2) T_l(x) \, d(P_N(x)),$$

which can be expressed as

$$J = \frac{2+l}{2(N+1)} I_{N,l+1} + \frac{2-l}{2(N+1)} I_{N,l-1}. \tag{12}$$

Since $\tau_k = I_{N,N+2k}/I_{N,N}$, the recurrence formula

$$\tau_{k+1} = \frac{[(N+2k-1)(N+2k) - (N+1)N](N+2k+2)}{[(N+2k+3)(N+2k+2) - (N+1)N](N+2k)} \tau_k, \tag{13}$$

where $\tau_1 = (N+2)/(2N+3)$ can be easily derived from (10) and (12).

System (6) is easier to construct than the corresponding system of Patterson [2], inasmuch as his method requires a set of recursions of variable lengths, while in our method only one recursion is needed. Moreover, further economy is achieved in solving the equation $\phi_{N+1}(x) = 0$, since, using a modification of Clenshaw's algorithm of summation, an odd or even Chebyshev series can be evaluated more efficiently than an odd or even Legendre series [5, p. 10]. Indeed, the computing time can be halved.

Explicit formulas for the weights are

$$\alpha_k = \frac{C_N}{P_N'(x_k)\phi_{N+1}(x_k)} + \frac{2}{NP_{N-1}(x_k)P_N'(x_k)}, \qquad k = 1, 2, \cdots, N, \tag{14}$$

$$\beta_k = \frac{C_N}{\phi_{N+1}'(\xi_k)P_N(\xi_k)}, \qquad k = 1, 2, \cdots, N+1, \tag{15}$$

where $C_N = 2^{2N+1}(N!)^2/(2N+1)!$.

3. Optimal Addition of Abscissas to Lobatto Quadrature Formulas. We now consider the quadrature formula

$$\int_{-1}^{+1} f(x) \, dx \simeq \sum_{k=0}^{N+1} \alpha_k f(x_k) + \sum_{k=1}^{N+1} \beta_k f(\xi_k), \tag{16}$$

where the x_k's are abscissas of the Lobatto quadrature formula. Consequently, $x_0 = -1$, $x_{N+1} = +1$ and $x_1, x_2, \cdots, x_N$ are the zeros of the Jacobi polynomial $P_N^{(1,1)}(x)$. It is our purpose to determine the free abscissas ξ_k and the weights α_k and β_k so that the degree of exactness of (16) is maximal. Then, ξ_k must be a zero of the polynomial $\phi_{N+1}(x)$ which satisfies

$$\int_{-1}^{+1} (1 - x^2) P_N^{(1,1)}(x) \phi_{N+1}(x) T_k(x) \, dx = 0, \qquad k = 0, 1, 2, \cdots, N. \tag{17}$$

Again, we express $\phi_{N+1}(x)$ in terms of Chebyshev polynomials as in (3) or (4), according to the parity of N. The coefficients b_k can be found by solving the system (6) where

$$\tau_k = -\int_{-1}^{+1} (1 - x^2) P_N^{(1,1)} T_{N+2k} \, dx \Big/ \int_{-1}^{+1} (1 - x^2) P_N^{(1,1)} T_N \, dx. \tag{18}$$

Using the relation

$$\int_{-1}^{+1} (1 - x^2)P_N^{(1,1)} T_l \, dx = \frac{1}{N+2} [(l+2)I_{N+1,l+1} - (l-2)I_{N+1,l-1}],$$

where $I_{N,l}$ is defined by (11), the recurrence formula

$$(19) \quad \tau_{k+1} = \frac{[(N+2k-1)(N+2k-2) - (N+1)(N+2)](N+2k+2)}{[(N+2k+3)(N+2k+4) - (N+1)(N+2)](N+2k)} \tau_k$$

can be derived from (13).

The starting value for (19) is

$$\tau_1 = 3(N+2)/(2N+5).$$

The expressions for the weights are

$$(20) \quad \alpha_k = \frac{C_N}{2P_N'(x_k)\phi_{N+1}(x_k)} + \frac{2}{(N+1)(N+2)[P_{N+1}(x_k)]^2}, \quad \text{for } k = 1, 2, \cdots, N,$$

$$(21) \quad \alpha_0 = \alpha_{N+1} = \frac{2}{(N+2)(N+1)} - \frac{C_N}{2(N+1)\phi_{N+1}(1)},$$

$$(22) \quad \beta_k = \frac{N+2}{2(N+1)} \frac{C_N}{[P_N(\xi_k) - \xi_k P_{N+1}(\xi_k)]\phi_{N+1}'(\xi_k)}, \qquad k = 1, 2, \cdots, N+1,$$

where $C_N = 2^{2N+3}[(N+1)!]^2/(2N+3)!$.

Appendix. Computer program. In this appendix, we describe a FORTRAN program for the construction of the quadrature formula (1). A listing of this program is reproduced in the supplement at the end of this issue. A program for the construction of the quadrature formula (11) may be obtained from the authors.

The program consists of three subroutines: the main subroutine KRONRO and two auxiliary subroutines ABWE1 and ABWE2, which are called by KRONRO.

In KRONRO the coefficients of the polynomial $\phi_{N+1}(x)$ are calculated.

In ABWE1 the abscissas x_k and weights α_k are calculated.

In ABWE2 the abscissas ξ_k and weights β_k are calculated.

The abscissas are calculated using Newton-Raphson's method. Starting values for this iterative process are provided by [6]

$$x_k \simeq \left(1 - \frac{1}{8N^2} + \frac{1}{8N^3}\right) \cos\left(\frac{2k - 1/2}{2N+1} \pi\right)$$

and

$$\xi_k \simeq \left(1 - \frac{1}{8N^2} + \frac{1}{8N^3}\right) \cos\left(\frac{2k - 3/2}{2N+1} \pi\right).$$

The program has been tested on the computer IBM 370/155 of the Computing Centre of the University of Leuven, for $N = 2(1)50(10)200$. The computations were carried out in double precision (approximately 16 significant figures). For $N = 200$, the maximal absolute error of the abscissas is 8.6×10^{-16} and of the weights 3.3×10^{-15}.

For $N = 50$, the computing time is 1.7 sec., for $N = 100$, 6.4 sec. and for $N = 200$, 24.7 sec.

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