MATHEMATICS OF COMPUTATION, VOLUME 30, NUMBER 136
OCTOBER 1976, PAGES 812–817

A Note on Extended Gaussian Quadrature Rules

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Abstract. Extended Gaussian quadrature rules of the type first considered by Kronrod are examined. For a general nonnegative weight function, simple formulas for the computation of the weights are given, together with a condition for the positivity of the weights associated with the new nodes. Examples of nonexistence of these rules are exhibited for the weight functions $(1 - x^2)^{\lambda - 1/2}$, e^{-x^2} and e^{-x}. Finally, two examples are given of quadrature rules which can be extended repeatedly.

1. Introduction. A quadrature rule of the type

$$\int_a^b w(x)f(x)\,dx = \sum_{i=1}^{n} A_i^{(n)} f(\xi_i^{(n)}) + \sum_{j=1}^{n+1} B_j^{(n)} f(x_j^{(n)}) + R_n(f), \tag{1.1}$$

where $\xi_i^{(n)}$, $i = 1, \ldots, n$, are the zeros of the nth-degree orthogonal polynomial $\pi_n(x)$ belonging to the nonnegative weight function $w(x)$, can always be made of polynomial degree $3n + 1$ by selecting as nodes $x_j^{(n)}$, $j = 1, 2, \ldots, n + 1$, the zeros of the polynomial $p_{n+1}(x)$, of degree $n + 1$, satisfying the orthogonality relation

$$\int_a^b w(x)\pi_n(x)p_{n+1}(x)x^k\,dx = 0, \qquad k = 0, 1, \ldots, n. \tag{1.2}$$

The polynomial $p_{n+1}(x)$ is unique up to a normalization factor and can be constructed, for example, as described by Patterson [4]. Unfortunately, the zeros of $p_{n+1}(x)$ are not necessarily real, let alone contained in $[a, b]$. We call (1.1) an *extended Gaussian quadrature rule*, if the polynomial degree is $3n + 1$, and all nodes $x_j^{(n)}$ are real and contained in $[a, b]$.

The only known existence result relates to the weight function $w(x) = (1 - x^2)^{\lambda - 1/2}$, $-a = b = 1$, $0 \leqslant \lambda \leqslant 2$, for which Szegö [9] proves that the zeros of $p_{n+1}(x)$ are all real, distinct, inside $[-1, 1]$, and interlaced with the zeros $\xi_i^{(n)}$ of the ultraspherical polynomial $\pi_n(x)$.

Kronrod [3] considers the case $\lambda = 1/2$ and computes nodes and weights for the corresponding rule (1.1) up to $n = 40$. For the same weight function, Piessens [6] constructs an automatic integration routine using a rule of type (1.1) with $n = 10$. Further accounts of Kronrod rules, including computer programs, can be found in [8], [2].

Patterson [4] derives a sequence of quadrature formulas by successively iterating the process defined by (1.1) and (1.2). Starting with the 3-point Gauss-Legendre rule, he adds four new abscissas to obtain a 7-point rule, then eight new nodes to obtain a 15-point rule and continues the process until he reaches a 127-point rule. The procedure,

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Received December 2, 1975.
AMS (MOS) subject classifications (1970). Primary 65D30; Secondary 33A65.
*Work performed while the author held a fellowship from the Consiglio Nazionale delle Ricerche, Italy.

even carried one step further to include a 255-point rule, is made the basis of an automatic numerical integration routine in [5].

Ramsky [7] constructs the polynomial $p_{n+1}(x)$ satisfying condition (1.2) for the Hermite weight function up to $n = 10$ and notes that the zeros are all real only when $n = 1, 2, 4$.

In all papers [3], [4] and [5], all weights are positive; however in [7], for $n = 4$, two (symmetric) weights $A_i^{(n)}$ are negative.

We first study a rule of type (1.1) with polynomial degree at least $2n$ and give simple formulas for the weights $A_i^{(n)}$ and $B_j^{(n)}$, together with a condition for the positivity of the weights $B_j^{(n)}$. We then construct the polynomial $p_{n+1}(x)$ in (1.2) for the weight functions $w(x) = (1 - x^2)^{\lambda - 1/2}$ on $[-1, 1]$, $\lambda = 0(.5)5, 8$, $w(x) = e^{-x^2}$ on $[-\infty, \infty]$, and $w(x) = e^{-x}$ on $[0, \infty]$, in each case up to $n = 20$, and give examples in which $p_{n+1}(x)$ has complex roots. We compute the extended Gaussian quadrature rules, whenever they exist, and give further examples of rules with negative weights $A_i^{(n)}$. Finally, we give two examples of quadrature rules which can be extended repeatedly.

2. The Weights $A_i^{(n)}$ and $B_j^{(n)}$. Let $k_n > 0$ be the coefficient of x^n in $\pi_n(x)$, and $h_n = \int_a^b w(x)\pi_n^2(x)\,dx$. Consider a rule of type (1.1) with real nodes $x_j^{(n)}$, $j = 1, 2, \ldots, n + 1$, and polynomial degree at least $2n$. Let $q_{n+1}(x) = \prod_{j=1}^{n+1}(x - x_j^{(n)})$ and define $Q_{2n+1}(x) = \pi_n(x)q_{n+1}(x)$. We assume the two sets of nodes $\{\xi_i^{(n)}\}_{i=1}^{n}$ and $\{x_j^{(n)}\}_{j=1}^{n+1}$ both ordered decreasingly.

THEOREM 1. *We have*

$$B_j^{(n)} = \frac{h_n}{k_n Q'_{2n+1}(x_j^{(n)})}, \qquad j = 1, 2, \ldots, n + 1, \tag{2.1}$$

and all $B_j^{(n)} > 0$ if and only if the nodes $x_j^{(n)}$ and $\xi_i^{(n)}$ interlace.

Proof. Applying (1.1) to $f_k(x) = \pi_n(x)q_{n+1}(x)/(x - x_k^{(n)})$, $k = 1, 2, \ldots, n + 1$, we obtain

$$\int_a^b w(x)f_k(x)\,dx = B_k^{(n)}\pi_n(x_k^{(n)})q'_{n+1}(x_k^{(n)}) = B_k^{(n)}Q'_{2n+1}(x_k^{(n)}). \tag{2.2}$$

Since $q_{n+1}(x)/(x - x_k^{(n)}) = x^n + t_{n-1}(x)$, where $t_{n-1}(x)$ is a polynomial of degree at most $n - 1$, we have, by the orthogonality of $\pi_n(x)$,

$$\int_a^b w(x)f_k(x)\,dx = \int_a^b w(x)\pi_n(x)x^n\,dx = h_n/k_n. \tag{2.3}$$

Since $h_n/k_n > 0$, we see that $Q'_{2n+1}(x_k^{(n)}) \neq 0$, and (2.1) follows from (2.2) and (2.3). Note in particular that the nodes $x_j^{(n)}$ are simple and distinct from the $\xi_i^{(n)}$.

Assume now that the nodes $x_j^{(n)}$ and $\xi_i^{(n)}$ interlace, i.e., $x_{n+1}^{(n)} < \xi_n^{(n)} < x_n^{(n)} < \cdots < \xi_1^{(n)} < x_1^{(n)}$. Since the polynomial Q_{2n+1} vanishes precisely at the nodes $x_j^{(n)}$ and $\xi_i^{(n)}$, and by normalization, $Q_{2n+1}(x) > 0$ for $x > x_1^{(n)}$, it is clear that the derivative Q'_{2n+1} will be alternately positive and negative at the nodes $x_1^{(n)}, \xi_1^{(n)}, x_2^{(n)}, \xi_2^{(n)}, \ldots$, hence, in particular; $Q'_{2n+1}(x_j^{(n)}) > 0$, $j = 1, 2, \ldots, n + 1$. By (2.1), therefore, $B_j^{(n)} > 0$.

Vice versa, suppose the weights $B_j^{(n)}$, $j = 1, 2, \ldots, n+1$, are positive. Applying (1.1) to the function

$$f_i(x) = \pi_n^2(x)/((x - \xi_{i+1}^{(n)})(x - \xi_i^{(n)})), \qquad i = 1, \ldots, n-1,$$

we obtain

$$0 = \int_a^b w(x) f_i(x)\, dx = \sum_{j=1}^{n+1} B_j^{(n)} f_i(x_j^{(n)}). \tag{2.4}$$

Since all the nodes $x_j^{(n)}$ are distinct from any $\xi_i^{(n)}$, the sum in (2.4) can be zero only if at least one of the numbers $f_i(x_j^{(n)})$ is negative. It follows that at least one node $x_j^{(n)}$, say $x_{j_i}^{(n)}$, satisfies the inequality

$$\xi_{i+1}^{(n)} < x_{j_i}^{(n)} < \xi_i^{(n)}, \qquad i = 1, \ldots, n-1.$$

The existence of nodes $x_1^{(n)} > \xi_1^{(n)}$ and $x_{n+1}^{(n)} < \xi_n^{(n)}$ follows similarly by considering $f_0(x) = \pi_n^2(x)/(\xi_1^{(n)} - x)$ and $f_n(x) = \pi_n^2(x)/(x - \xi_n^{(n)})$, respectively. Having thus accounted for at least $n+1$, hence exactly $n+1$, nodes $x_j^{(n)}$, the interlacing property is established.

THEOREM 2. *We have*

$$A_i^{(n)} = H_i^{(n)} + \frac{h_n}{k_n Q'_{2n+1}(\xi_i^{(n)})}, \qquad i = 1, \ldots, n, \tag{2.5}$$

where $H_i^{(n)}$ are the Christoffel numbers for the weight function $w(x)$. The inequalities

$$A_i^{(n)} < H_i^{(n)}, \qquad i = 1, \ldots, n, \tag{2.6}$$

hold if and only if the nodes $x_j^{(n)}$ and $\xi_i^{(n)}$ interlace.

Proof. Letting

$$f_i(x) = q_{n+1}(x)\pi_n(x)/(x - \xi_i^{(n)}), \qquad i = 1, \ldots, n,$$

in (1.1), we have

$$\int_a^b w(x) f_i(x)\, dx = A_i^{(n)} Q'_{2n+1}(\xi_i^{(n)}). \tag{2.7}$$

Applying the n-point Gaussian rule to f_i, and noting that the remainder is

$$\frac{f_i^{(2n)}(\xi)}{(2n)!k_n^2} \int_a^b w(x)\pi_n^2(x)\, dx = \frac{h_n}{k_n},$$

we find that

$$\int_a^b w(x) f_i(x)\, dx = H_i^{(n)} Q'_{2n+1}(\xi_i^{(n)}) + h_n/k_n. \tag{2.8}$$

From the last two relations, (2.5) follows, since again, $Q'_{2n+1}(\xi_i^{(n)}) \neq 0$.

If the nodes $x_j^{(n)}$ and $\xi_i^{(n)}$ interlace, then $Q'_{2n+1}(\xi_i^{(n)}) < 0$ for all i, proving (2.6). Vice versa, if (2.6) holds, consider

$$f_j(x) = q_{n+1}^2(x)/((x - x_{j+1}^{(n)})(x - x_j^{(n)})), \qquad j = 1, \ldots, n.$$

By applying (1.1) we have

$$\int_a^b w(x)f_j(x)\,dx = \sum_{i=1}^{n} A_i^{(n)} f_j(\xi_i^{(n)}), \tag{2.9}$$

and from the n-point Gaussian rule, with remainder, similarly as above,

$$\int_a^b w(x)f_j(x)\,dx = \sum_{i=1}^{n} H_i^{(n)} f_j(\xi_i^{(n)}) + h_n/k_n^2. \tag{2.10}$$

By subtracting (2.9) from (2.10) we obtain

$$\sum_{i=1}^{n} (H_i^{(n)} - A_i^{(n)}) f_j(\xi_i^{(n)}) = -h_n/k_n^2 < 0. \tag{2.11}$$

Since $H_i^{(n)} - A_i^{(n)} > 0$, $i = 1, \ldots, n$, inequality (2.11) is possible only if at least one of the numbers $f_j(\xi_i^{(n)})$ is negative. This means that at least one $\xi_i^{(n)}$, say $\xi_{i_j}^{(n)}$, satisfies the inequality

$$x_{j+1}^{(n)} < \xi_{i_j}^{(n)} < x_j^{(n)}, \qquad j = 1, \ldots, n,$$

which, as before, implies the interlacing property.

Clearly, Theorems 1 and 2 both apply to the extended Gaussian quadrature rules, if one chooses $q_{n+1}(x) = p_{n+1}(x)$.

3. Numerical Results. We have constructed the polynomial $p_{n+1}(x)$ satisfying condition (1.2) for $w(x) = (1 - x^2)^{\lambda - 1/2}$, $\lambda = 0(.5)5, 8$, up to $n = 20$, by using an algorithm similar to the one described in [4]. When the zeros of these polynomials are all real, the corresponding weights $A_i^{(n)}$ and $B_j^{(n)}$ were computed by means of (2.1) and (2.5). For all rules thus obtained, the nodes always satisfy the interlacing property; nevertheless, in some cases we find negative weights $A_i^{(n)}$. Cases of complex zeros also occur. A brief list of the values of λ and n, for which negative weights and complex zeros were observed, is reported in the following table (where $k(i)l$ denotes the sequence of integers $k, k + i, k + 2i, \ldots, l$).

λ	n $(A_i^{(n)} < 0)$	n (complex zeros)
4	13, 15	———
4.5	7(2)13, 16	15, 17, 19
5	7, 9, 14, 16	11(2)19, 20
8	3, 5, 6, 8	7, 9(1)20

Similarly, we examined $w(x) = e^{-x^2}$ and $w(x) = e^{-x}$, again up to $n = 20$. In the first case, studied already in [7] up to $n = 10$, we have confirmed that extended Gaussian rules exist only for $n = 1, 2, 4$. For the second weight function, when $n = 1$, the zeros of $p_2(x)$ are real, but one is negative, while for $2 \leqslant n \leqslant 20$ some of the zeros are complex.

4. Extended Gauss-Chebyshev Rules. The extension of Gauss-Chebyshev rules can be carried out explicitly by virtue of the identity

$$2T_n(x)U_{n-1}(x) = U_{2n-1}(x), \tag{4.1}$$

where $T_n(x)$ and $U_n(x)$ are the nth-degree Chebyshev polynomials of first and second kind, respectively.

When $w(x) = (1 - x^2)^{-1/2}$ we may choose $p_{n+1}(x) = 2^{-n+1}(x^2 - 1)U_{n-1}(x)$, $n \geq 2$, and (1.1) becomes the Gauss-Chebyshev rule of closed type (see for example [1])

$$\int_{-1}^{1} (1 - x^2)^{-1/2} f(x)\,dx = \frac{\pi}{2n}\left[\sum_{i=1}^{2n-1} f(x_i^{(n)}) + \frac{1}{2}f(-1) + \frac{1}{2}f(1)\right] + R_n(f), \quad n \geq 2, \tag{4.2}$$

where

$$x_i^{(n)} = \cos\frac{i\pi}{2n}, \qquad i = 1, 2, \ldots, 2n - 1.$$

$p_{n+1}(x)$ satisfies the required orthogonality condition (1.2) by virtue of (4.1). As a matter of fact, (1.2) holds for all $k \leq 2n - 2$, $n \geq 2$. Since the coefficients $A_i^{(n)}$, $B_j^{(n)}$ are uniquely determined, they must be as in (4.2), which is known to have not only degree $3n + 1$, but in fact degree $4n - 1$. For $n = 1$ we have $p_2(x) = x^2 - 3/4$ and (1.1) coincides with the 3-point Gauss-Chebyshev rule.

A natural way of iterating the process is to add $2n$ new nodes, namely the zeros of $T_{2n}(x)$, so that, by virtue of (4.1), the new rule will have as nodes the zeros of $(x^2 - 1)U_{4n-1}(x)$ and polynomial degree $8n - 1$. In general, after p extensions, having reached a rule with $2^p n + 1$ nodes, we add $2^p n$ new nodes, namely the zeros of $T_{2^p n}(x)$, to get a rule of the type (4.2) with $2^{p+1}n + 1$ nodes and polynomial degree $2^{p+2}n - 1$.

In a similar way we may extend the Gaussian quadrature rule for the weight function $w(x) = (1 - x^2)^{1/2}$. Recalling again (4.1), we choose $p_{n+1}(x) = 2^{-n}T_{n+1}(x)$, and obtain

$$\int_{-1}^{1} (1 - x^2)^{1/2} f(x)\,dx = \frac{\pi}{2(n+1)} \sum_{i=1}^{2n+1} (1 - [x_i^{(n)}]^2) f(x_i^{(n)}) + R_n(f), \tag{4.3}$$

the Gaussian rule constructed over the $2n + 1$ zeros

$$x_i^{(n)} = \cos\frac{i\pi}{2(n+1)}, \qquad i = 1, 2, \ldots, 2n + 1,$$

of the polynomial $U_{2n+1}(x)$. It has polynomial degree $4n + 1$. As before, the process may be iterated.

Acknowledgement. I am grateful to Professor Walter Gautschi for many constructive suggestions and constant guidance during this work.

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