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 \((1 - x^2)^{\lambda-\frac{1}{2}}, e^{-x^2}\) and \(e^{-x}\). Finally, two examples are given of quadrature rules which can be extended repeatedly.

1. Introduction. A quadrature rule of the type

\[
\int_{a}^{b} w(x)f(x) \, dx = \sum_{i=1}^{n} A_{i}^{(n)} f(\xi_{i}^{(n)}) + \sum_{j=1}^{n+1} B_{j}^{(n)} f(x_{j}^{(n)}) + R_{n}(f),
\]

where \(\xi_{i}^{(n)}, i = 1, \ldots, n\), are the zeros of the \(n\)-th 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

\[
\int_{a}^{b} w(x)\pi_{n}(x)p_{n+1}(x)x^{k} \, dx = 0, \quad k = 0, 1, \ldots, n.
\]

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 \(w(x) = (1 - x^2)^{\lambda-\frac{1}{2}}, -a = b = 1, 0 \leq \lambda \leq 2\), 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 \(\lambda = \frac{1}{2}\) 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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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 $w(x) = (1 - x^2)x^{-\lambda/2}$ on $[-1, 1]$, $\lambda > 0$, $\lambda = 0(5), 8$, $w(x) = e^{-x^2}$ 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 $q_{n+1}(x) = \Pi_{j=1}^{n+1}(x - x_j^{(n)})$ 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

$$B_j^{(n)} = \frac{h_n}{k_n Q_{2n+1}'(x_j^{(n)})}, \quad j = 1, 2, \ldots, n + 1,$$

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

$$\int_a^b w(x)f_k(x)\,dx = B_k^{(n)}\pi_n(x_k^{(n)})q_{n+1}'(x_k^{(n)}) = B_k^{(n)}Q_{2n+1}'(x_k^{(n)}).$$

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 $\pi_n(x)$,

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

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., $x_j^{(n)} < \xi_i^{(n)} < x_j^{(n)} < \ldots < x_1^{(n)} < x_1^{(n)}$. 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 $x_j^{(n)}$, $\xi_1^{(n)}$, $x_2^{(n)}$, $\xi_2^{(n)}$, $\ldots$, hence, in particular, $Q_{2n+1}'(x_j^{(n)}) > 0$, $j = 1, 2, \ldots, n + 1$. By (2.1), therefore, $B_j^{(n)} > 0$. 

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

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

we obtain

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

Since all the nodes $x_i^{(n)}$ 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 $x_i^{(n)}$, say $x_{i_1}^{(n)}$, satisfies the inequality

$$\xi_{i+1}^{(n)} < x_{i_1}^{(n)} < \xi_i^{(n)}, \quad i = 1, \ldots, n - 1.$$

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 $x_i^{(n)}$, the interlacing property is established.

**Theorem 2.** We have

$$A_i^{(n)} = H_i^{(n)} + \frac{h_n}{k_n Q_{2n+1}^{(n)}(\xi_i^{(n)})}, \quad i = 1, \ldots, n,$$

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

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

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

**Proof.** Letting

$$f_i(x) = \pi_{n+1}(x)/(x - \xi_i^{(n)}), \quad i = 1, \ldots, n,$$

in (1.1), we have

$$\int_a^b w(x)f_i(x) \, dx = A_i^{(n)} Q_{2n+1}^{(n)}(\xi_i^{(n)}).$$

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

$$\int_a^b w(x)f_i(x) \, dx = H_i^{(n)} Q_{2n+1}^{(n)}(\xi_i^{(n)}) + h_n/k_n.$$
By applying (1.1) we have

\[ \int_a^b w(x)f(x)\,dx = \sum_{i=1}^n A_i^{(n)}f(\xi_i^{(n)}), \]

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

\[ \int_a^b w(x)f(x)\,dx = \sum_{i=1}^n H_i^{(n)}f(\xi_i^{(n)}) + h_n/k_n. \]

By subtracting (2.9) from (2.10) we obtain

\[ \sum_{i=1}^n (H_i^{(n)} - A_i^{(n)})f(\xi_i^{(n)}) = -h_n/k_n < 0. \]

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 \( f(\xi_i^{(n)}) \) is negative. This means that at least one \( \xi_i^{(n)} \), say \( \xi_{i_1}^{(n)} \), satisfies the inequality

\[ x_{i_1+1}^{(n)} < \xi_{i_1}^{(n)} < x_{i_1}^{(n)}, \quad j = 1, \ldots, n, \]

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 \( w(x) = (1 - x^2)^{\lambda-\frac{1}{2}}, \lambda = 0(.5)5, 8 \), 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 \( B_i^{(n)} \) 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 \( \lambda \) 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 \( k, k + i, k + 2i, \ldots, l \)).

<table>
<thead>
<tr>
<th>( \lambda )</th>
<th>( n ) ((A_i^{(n)} &lt; 0))</th>
<th>( n ) ((\text{complex zeros}))</th>
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<td></td>
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<td>11(2)19, 20</td>
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<td>8</td>
<td>3, 5, 6, 8</td>
<td>7, 9(1)20</td>
</tr>
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</table>

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 \( 2 \leq n \leq 20 \) 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
(4.1) 
\[ 2T_n(x)U_{n-1}(x) = U_{2n-1}(x), \]
where \( T_n(x) \) and \( U_n(x) \) are the \( n \)th-degree Chebyshev polynomials of first and second kind, respectively.

When \( w(x) = (1 - x^2)^{-\frac{1}{2}} \) 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])

\[
\int_{-1}^{1} (1 - x^2)^{-\frac{1}{2}} f(x) \, dx = \frac{\pi}{2n} \left[ \sum_{i=1}^{2n-1} f(x_i^{(n)}) + \frac{1}{2} f(-1) + \frac{1}{2} f(1) \right] + R_n(f),
\]
where

\[ x_i^{(n)} = \cos \frac{i\pi}{2n}, \quad i = 1, 2, \ldots, 2n - 1. \]

(4.2)

\( p_{n+1}(x) \) 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 \( A_j^{(n)} \), \( B_j^{(n)} \) 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 \( p_2(x) = x^2 - \frac{1}{3} \) 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 \( w(x) = (1 - x^2)^{-\frac{1}{2}} \). Recalling again (4.1), we choose \( p_{n+1}(x) = 2^{-n}T_{n+1}(x) \), and obtain

\[
\int_{-1}^{1} (1 - x^2)^{-\frac{1}{2}} f(x) \, dx = \frac{\pi}{2(n + 1)} \sum_{i=1}^{2n+1} (1 - [x_i^{(n)}]^2) f(x_i^{(n)}) + R_n(f),
\]
the Gaussian rule constructed over the \( 2n + 1 \) zeros

\[ x_i^{(n)} = \cos \frac{i\pi}{2(n + 1)}, \quad i = 1, 2, \ldots, 2n + 1, \]
of the polynomial \( U_{2n+1}(x) \). It has polynomial degree \( 4n + 1 \). As before, the process may be iterated.

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