A Note on Extended Gaussian Quadrature Rules

By Giovanni Monegato*

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

\[
\int_{a}^{b} w(x)f(x) \, dx = \sum_{i=1}^{n} A_i^{(n)}f(\xi_i^{(n)}) + \sum_{j=1}^{n+1} B_j^{(n)}f(\xi_j^{(n)}) + R_n(f),
\]

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,
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 \( A^{(4)}_i \) are negative.

We first study a rule of type (1.1) with polynomial degree at least \( 2n \) and give simple formulas for the weights \( A^{(r)}_i \) and \( B^{(r)}_i \), together with a condition for the positivity of the weights \( B^{(r)}_i \). 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 \( A^{(r)}_i \). Finally, we give two examples of quadrature rules which can be extended repeatedly.

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

**Theorem 1.** We have

\[
B^{(r)}_j = \frac{h_n}{k_nQ_{2n+1}'(x^{(n)}_j)}, \quad j = 1, 2, \ldots, n + 1,
\]

and all \( B^{(r)}_j > 0 \) if and only if the nodes \( x^{(n)}_j \) and \( x^{(n)}_j \) interlace.

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

\[
\int_a^b w(x)f_k(x)dx = B^{(n)}_k \pi_n(x^{(n)}_k)q_{n+1}(x^{(n)}_k) = B^{(n)}_k Q_{2n+1}'(x^{(n)}_k).
\]

Since \( q_{n+1}(x)/(x - x^{(n)}_k) = x^n + t_{n-1}(x) \), 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 \( Q_{2n+1}'(x^{(n)}_k) \neq 0 \), and (2.1) follows from (2.2) and (2.3).

Note in particular that the nodes \( x^{(n)}_j \) are simple and distinct from the \( x^{(n)}_j \).

Assume now that the nodes \( x^{(n)}_j \) and \( x^{(n)}_j \) interlace, i.e., \( x^{(n)}_n < x^{(n)}_n < x^{(n)}_n < \cdots < x^{(n)}_n < x^{(n)}_n \). Since the polynomial \( Q_{2n+1} \) vanishes precisely at the nodes \( x^{(n)}_j \) and \( x^{(n)}_j \), and by normalization, \( Q_{2n+1}(x) > 0 \) for \( x > x^{(n)}_1 \), it is clear that the derivative \( Q_{2n+1}' \) will be alternately positive and negative at the nodes \( x^{(n)}_j, \xi^{(n)}_1, x^{(n)}_2, \xi^{(n)}_2, \ldots \), hence, in particular; \( Q_{2n+1}'(x^{(n)}_j) > 0, j = 1, 2, \ldots, n + 1 \). By (2.1), therefore, \( B^{(r)}_j > 0 \).
Vice versa, suppose the weights $B_j^{(n)}$, $j = 1, 2, \ldots, n + 1$, are positive. Applying (1.1) to the function
\[ f_i(x) = \pi_n^2(x)/((x - \xi_{i+1}^{(n)})(x - \xi_i^{(n)})), \quad i = 1, \ldots, n - 1, \]
we obtain
\[ 0 = \int_a^b w(x)f_i(x) \, dx = \sum_{j=1}^{n+1} B_j^{(n)} f_j(x_i^{(n)}). \tag{2.4} \]
Since all the nodes $x_i^{(n)}$ are distinct from any $\xi_j^{(n)}$, the sum in (2.4) can be zero only if at least one of the numbers $f_j(x_i^{(n)})$ is negative. It follows that at least one node $x_i^{(n)}$, say $x_i^{(n)}$, satisfies the inequality
\[ \xi_{i+1}^{(n)} < x_i^{(n)} < \xi_i^{(n)}, \quad i = 1, \ldots, n - 1. \]
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
\[ A_i^{(n)} = H_i^{(n)} + \frac{h_n}{k_n Q_{2n+1}'(\xi_i^{(n)})}, \quad i = 1, \ldots, n, \tag{2.5} \]
where $H_i^{(n)}$ are the Christoffel numbers for the weight function $w(x)$. The inequalities
\[ A_i^{(n)} < H_i^{(n)}, \quad i = 1, \ldots, n, \tag{2.6} \]
hold if and only if the nodes $x_i^{(n)}$ and $\xi_i^{(n)}$ interlace.

**Proof.** Letting
\[ f_i(x) = q_{n+1}(x)\pi_n(x)/(x - \xi_i^{(n)}), \quad i = 1, \ldots, n, \]
in (1.1), we have
\[ \int_a^b w(x)f_i(x) \, dx = A_i^{(n)} Q_{2n+1}'(\xi_i^{(n)}). \tag{2.7} \]
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 $x_i^{(n)}$ 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
\[ f_j(x) = q_{n+1}^2(x)/((x - x_{j+1}^{(n)})(x - x_j^{(n)})), \quad j = 1, \ldots, n. \]
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,

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

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 $\xi_j^{(n)}$, satisfies

$$x_{j+1}^{(n)} < \xi_j^{(n)} < x_j^{(n)}, \quad j = 1, \ldots, n,$$

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 $w(x) = (1 - x^2)^{\lambda - \frac{1}{2}}$, $\lambda = 0, 0.5, 5$, 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>$n$ (complex zeros)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>13, 15</td>
<td></td>
</tr>
<tr>
<td>4.5</td>
<td>7(2)13, 16</td>
<td>15, 17, 19</td>
</tr>
<tr>
<td>5</td>
<td>7, 9, 14, 16</td>
<td>11(2)19, 20</td>
</tr>
<tr>
<td>8</td>
<td>3, 5, 6, 8</td>
<td>7, 9(1)20</td>
</tr>
</tbody>
</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
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 \( p_{n+1}(x) = 2^{-n+1}(x^2 - 1)U_n(x) \), \( n \geq 2 \), and (1.1) becomes the Gauss-Chebyshev rule of closed type (see for example [1])

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

(4.2)

where

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

\( p_{n+1}(x) \) 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 \( A_i^{(n)} \) and \( B_i^{(n)} \) 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 \( p_2(x) = x^2 - \frac{3}{4} \) 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 \( T_{2^p} p_n(x) \), to get a rule of the type (4.2) with \( 2^p + 1 n + 1 \) nodes and polynomial degree \( 2^p + 2n - 1 \).

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

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

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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Department of Computer Sciences
Purdue University
West Lafayette, Indiana 47907


