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

\[
\int_a^b w(x)f(x)\,dx = \sum_{i=1}^{n} A_i^{(n)}f(x_i^{(n)}) + \sum_{j=1}^{n+1} B_j^{(n)}f(x_j^{(n)}) + R_n(f),
\]

where \(x_i^{(n)}, i = 1, \ldots, n\), 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 \(A_i^{(n)}\) 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 \(w(x) = (1 - x^2)\lambda^{-\frac{1}{2}}\) 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 \(x_i^{(n)}\), \(j = 1, 2, \ldots, n + 1\), 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 \(\{x_i^{(n)}\}_{i=1}^n\) and \(\{x_j^{(n)}\}_{j=1}^{n+1}\) both ordered decreasingly.

**Theorem 1.** We have

\[
B_j^{(n)} = \frac{h_n}{k_nQ_{2n+1}'(x_j^{(n)})}, \quad j = 1, 2, \ldots, n + 1,
\]

and all \(B_j^{(n)} > 0\) if and only if the nodes \(x_i^{(n)}\) and \(x_j^{(n)}\) 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 \(x_i^{(n)}\) are simple and distinct from the \(x_i^{(n)}\).

Assume now that the nodes \(x_i^{(n)}\) and \(x_j^{(n)}\) interlace, i.e., \(x_{n+1}^{(n)} < x_n^{(n)} < \cdots < x_1^{(n)} < x_1^{(n)}\). Since the polynomial \(Q_{2n+1}\) vanishes precisely at the nodes \(x_{n+1}^{(n)}\) and \(x_1^{(n)}\), 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 \(x_1^{(n)}\), \(x_1^{(n)}\), \(x_2^{(n)}\), \(x_2^{(n)}\), \(x_3^{(n)}\), \(x_3^{(n)}\), 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

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

we obtain

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

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

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

The existence of nodes $x_j^{(n)} > \xi_1^{(n)}$ and $x_j^{(n)} < \xi_n^{(n)}$ 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

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

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 $x_j^{(n)}$ and $\xi_i^{(n)}$ interlace.

**Proof.** Letting

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

in (1.1), we have

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

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

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

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

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

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

for $j = 1, \ldots, n$.  

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

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

(4.2)

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

$p_{n+1}(x)$ 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 $A_i^{(n)}$, $B_i^{(n)}$ 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 $p_2(x) = x^2 - \frac{1}{4}$ 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 $w(x) = (1 - x^2)^{\frac{1}{2}}$. Recalling again (4.1), we choose $p_{n+1}(x) = 2^{-n}T_{n+1}(x)$, and obtain

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

(4.3)

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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