Numerical Algorithms **26:** 173–196, 2001.

Survey paper

An overview of the computational aspects of Kronrod quadrature rules *

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We present a survey of the computational aspects of Kronrod's rules, and in particular we describe recent results about their construction, error estimates and applications, including new developments that have been suggested by the Kronrod's strategy.

Keywords: quadrature rules, error evaluation, algorithms, automatic routines

AMS subject classification: 65D32

1. Introduction

Consider the problem of approximating a linear functional $L(f)$ by means of a linear combination of function values $f_{n,i}$, i.e.,

$$L(f) \approx \sum_{i=1}^{n} \alpha_{ni} f_{ni} =: Q_n(f). \tag{1.1}$$

Assuming that the right hand side converges to $L(f)$ as $n \to \infty$, a practical question is to estimate

$$\left|L(f) - Q_n(f)\right| \tag{1.2}$$

for any chosen value of $n \geqslant 1$.

A simple example of this problem is the evaluation of an integral by means of a quadrature rule, that is, for example,

$$\int_a^b f(x)\,\mathrm{d}x \approx \sum_{i=1}^{n} w_{ni} f(x_{ni}). \tag{1.3}$$

A common approach to estimate (1.2) is to consider a second rule

$$Q_m(f) = \sum_{j=1}^{m} v_{mj} f(t_{mj})$$

* Work supported by the Ministero dell'Università e della Ricerca Scientifica e Tecnologica of Italy.

with $m > n$, and then to take

$$\left|L(f) - Q_n(f)\right| \approx \left|Q_m(f) - Q_n(f)\right|, \tag{1.4}$$

provided m is such that this estimate is acceptable, i.e., sufficiently accurate.

But let us postpone the question concerning the choice of Q_m. Instead we immediately remark that the cost, in terms of function evaluations, of this error estimate is $m + n > 2n$, unless the two sets of abscissas $\{x_{ni}\}$ and $\{t_{mj}\}$ have common points. In particular, if the second set contains the first one then the total cost is only m. This is precisely the observation that in 1964 led Kronrod [35,36] to formulate the following proposal.

Consider the n-point Gauss–Legendre quadrature formula

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = \sum_{i=1}^{n} w_{ni} f(x_{ni}) + R_n^G(f) =: G_n(f) + R_n^G(f), \tag{1.5}$$

which, as we know, has degree of exactness $2n - 1$, i.e., $R_n(f) = 0$ whenever $f(x)$ is a polynomial of degree $2n - 1$. To estimate $R_n^G(f)$ we associate with (1.5) a second formula

$$\begin{aligned}\int_{-1}^{1} f(x)\,\mathrm{d}x &= \sum_{i=1}^{n} A_{ni} f(x_{ni}) + \sum_{j=1}^{n+1} B_{nj} f(y_{nj}) + R_{2n+1}^K(f)\\ &=: K_{2n+1}(f) + R_{2n+1}^K(f),\end{aligned} \tag{1.6}$$

where the first set of nodes $\{x_{ni}\}$ is precisely the one used in (1.5), while all the other $3n + 2$ parameters $\{A_{ni}\}$, $\{B_{nj}\}$ and $\{y_{nj}\}$ are chosen in such a way that formula (1.6) reaches its maximum degree of exactness, i.e., if possible, at least $3n + 1$. This formula, if it exists with real and distinct nodes, can also be interpreted as a Gaussian rule with n prescribed internal (and simple) nodes.

If such a formula exists (with real and distinct nodes), then we are able to estimate the integral and the error term using a total of $2n + 1$ function values. Notice that if we would associate with (1.5) a second Gauss–Legendre rule with $m = n + 1$ nodes, this would have only degree of exactness $2n + 1$, while the total cost would still be $2n + 1$. Furthermore, while when the function $f(x)$ is smooth a $(n + 1)$-point Gaussian rule is generally sufficiently accurate to be taken as reference in (1.4), in general, when the function $f(x)$ is not smooth the reference Gaussian rule must have about double number of points. Formula (1.6) is adequate in both cases and, at the same time, minimizes the total cost. Furthermore, as noted in [48], $n + 1$ is the minimum number of nodes one has to add to the n-point Gaussian formula in order to obtain an extended rule with degree of exactness greater than $2n - 1$.

Incidentally we notice that Merson in 1957, Sarafyan in 1966 and Fehlberg in 1968 (to mention a few of the people who worked on the problem we describe next; see [31])

applied a similar idea in the context of embedded Runge–Kutta methods for initial value ODEs

$$\begin{cases} y' = f(x, y), \quad x > 0, \\ y(0) = y_0. \end{cases}$$

More precisely, in order to estimate the local truncation error associated with a Runge–Kutta method, at a minimum cost, they constructed couples of Runge–Kutta methods, of given orders p and $p+1$ of the following type:

$$\begin{cases} y_{n+1} = y_n + h \sum_{i=1}^{r} a_i K_i \\ K_1 = f(x_n, y_n) \\ K_i = f\left(x_n + b_i h, y_n + h \sum_{j=1}^{i-1} c_{ij} K_j \right), \quad i = 2, \ldots, r \end{cases} \tag{1.7}$$

$$\begin{cases} y^*_{n+1} = y_n + h \sum_{i=1}^{r^*} a^*_i K_i, & r^* > r \\ K_1 = f(x_n, y_n) \\ K_i = f\left(x_n + b_i h, y_n + h \sum_{j=1}^{i-1} c_{ij} K_j \right), \quad i = 2, \ldots, r^* \end{cases} \tag{1.8}$$

where the coefficients $\{a_i\}$, $\{a^*_i\}$, $\{b_i\}$ and $\{c_{ij}\}$ are chosen so that r^* is minimum. Notice that all K_i of (1.7) are included in (1.8), so that no function values are wasted.

Turning back to our quadrature formulas (1.5) and (1.6), it is of interest to observe, as firstly done independently by Mysovskih in 1964 [49] and by Barrucand in 1970 [4], that the new nodes $\{y_{nj}\}$ required by (1.6) must coincide with the zeros of the polynomial $E_{n+1}(x)$, of exact degree $n+1$, which is uniquely defined, up to a constant factor, by the orthogonality relationship

$$\int_{-1}^{1} P_n(x) E_{n+1}(x) x^k \, \mathrm{d}x = 0, \quad k = 0, 1, \ldots, n, \tag{1.9}$$

where $P_n(x)$ is the Legendre polynomial of degree n and $E_{n+1}(x) = c_n \prod_{j=1}^{n+1} (x - y_{nj})$. In other words, the polynomial $E_{n+1}(x)$ is orthogonal, with respect to the variable-sign weight function $P_n(x)$, to all polynomials of lower degree.

Thus, the existence of (1.6) with real and distinct nodes $\{y_{nj}\}$, possibly in $[-1, 1]$, is related to the properties of the zeros of $E_{n+1}(x)$ defined by (1.9).

The numerical results produced by Kronrod show that, at least for the values of n considered, all nodes of (1.6) are real, distinct and in $(-1, 1)$. Moreover, all the corresponding coefficients $\{A_{ni}\}$ and $\{B_{nj}\}$ are positive.

Barrucand in his paper also pointed out that the polynomials $E_{n+1}(x)$ defined by (1.9) were already studied several decades earlier by Szëgo in [69]. Actually, these new

polynomials were first introduced, in a different context, by Stieltjes in 1894 (see [2]). In particular Szëgo proved that all zeros of $E_{n+1}(x)$ are real, distinct and in $(-1, 1)$; moreover, they interlace with those of $P_n(x)$. Monegato in 1978 [45], using some inequalities obtained by Szëgo in his paper, showed that all weights $\{A_{ni}\}$ and $\{B_{nj}\}$ are positive. Therefore, all the numerical evidences produced by Kronrod were indeed confirmed by these theoretical results.

Finally, Rabinowitz in [65] proved that the exact degree of exactness of (1.6) is precisely $3n + 1$ when n is even, and $3n + 2$ when n is odd.

These results have also been extended to formulas of type (1.6) with a Jacobi weight function, i.e., of the form

$$\int_{-1}^{1} (1-x)^{\alpha}(1+x)^{\beta} f(x)\,\mathrm{d}x \approx \sum_{i=1}^{n} A_{ni}^{(\alpha,\beta)} f\left(x_{ni}^{(\alpha,\beta)}\right) + \sum_{j=1}^{n+1} B_{nj}^{(\alpha,\beta)} f\left(y_{nj}^{(\alpha,\beta)}\right). \tag{1.10}$$

In particular, when $\alpha = \beta = \mu - \frac{1}{2}$, with $0 < \mu \leqslant 2$, it has been proved (see [64]) that all nodes $\{y_{nj}^{(\alpha,\beta)}\}$ are in $(-1, 1)$ and interlace with those of $\{x_{ni}^{(\alpha,\beta)}\}$. We recall that the latters are the zeros of the Jacobi polynomial of degree n, denoted by $P_n^{(\alpha,\beta)}(x)$ (see [65]). Moreover, for $0 < \mu \leqslant 1$ all coefficients of (1.10) are certainly positive (see [40]). The cases $\mu = 0$ and $\mu = 1$ are exceptional, in the sense that the corresponding Kronrod extensions coincide with the classical Lobatto–Gauss–Chebyshev and Gauss–Chebyshev rules, respectively (see [48]).

Further results on existence and on nonexistence of Kronrod type extensions of Gaussian rules associated with integrals of the form

$$\int_{a}^{b} w(x) f(x)\,\mathrm{d}x \tag{1.11}$$

for some particular (nonnegative) weight functions $w(x)$, including the Laguerre and the Hermite cases, have been obtained by several authors (see [28,47,50,60]).

Also the Radau and Lobatto cases have been considered, that is, the Kronrod type extensions of Gauss–Radau and Gauss–Lobatto quadrature formulas; corresponding results can be found in [3,13,17,28,48,52,63].

The connection between Kronrod formulas and the properties of the polynomials $E_{n+1}(x)$ stimulated much research work on these latters. Fundamental contributions in this direction were accomplished by Ehrich [16,21] and Peherstorfer [57,59]. Other questions of interest, such as interpolation on the zeros of $E_{n+1}(x)$ and of $P_n(x)E_{n+1}(x)$, have been investigated by Ehrich and Mastroianni [23,24].

These theoretical results are certainly quite rich and deep, particularly if compared with the few ones available till about twenty years ago.

Since several survey papers have treated these questions (see, for instance, [21, 28,48,50]), in this work we will concentrate our attention mainly on the computational questions and aspects of Kronrod rules. Therefore, in the next section we will describe the numerical procedures that since Kronrod's work have been proposed to construct

rule (1.6). Then, in section 3 we will discuss the behaviour of the remainder term of Kronrod's rules, particularly from the point of view of its role in the construction of an automatic integrator. Finally, in the last section we will present some generalizations and applications of these rules.

2. Construction

Kronrod computed the coefficients of $E_{n+1}(x) = x^{n+1} + a_1 x^n + \cdots$ by solving the corresponding linear triangular system which springs from (1.9), hence determined the zeros of $E_{n+1}(x)$. Unfortunately this procedure suffers a severe loss of accuracy, because of the great difference in magnitude between the coefficients a_i. To produce nodes correct to 16 (decimal) digits, for $n \leqslant 40$ he had to carry out the computation using about 65 digits.

A fairly stable algorithm was proposed by Patterson [52], who suggested to expand $E_{n+1}(x)$ in terms of Legendre polynomials. The coefficients of this expansion, which are obtained by solving a linear triangular system, are much more equilibrated.

However, as pointed out in [46], a better approach could have been derived directly from a relationship contained in Szëgo's paper. Not aware of this, Piessens and Branders independently obtained by their own essentially the same algorithm (see [63]). By expanding $E_{n+1}(x)$ in terms of Chebyshev polynomials (of the first kind) $T_k(x)$, that is,

$$E_{n+1}(x) = T_{n+1}(x) + a_1 T_{n-1}(x) + \cdots + \begin{cases} a_{n/2} T_1(x) & n \text{ even}, \\ \dfrac{1}{2} a_{(n+1)/2} T_0(x) & n \text{ odd}, \end{cases} \tag{2.1}$$

the coefficients $\{a_k\}$ are then given by the following recurrence relations:

$$\begin{cases} f_1 = \dfrac{n+1}{2n+3} \\ f_{k+1} = \dfrac{(2k+1)(n+k+1)}{(k+1)(2n+2k+3)} f_k, \quad k = 1, \ldots, m-1, \\ a_1 = -f_1 \\ a_k = -f_k - \sum_{i=1}^{k-1} f_i a_{k-i}, \quad k = 2, \ldots, m, \end{cases} \tag{2.2}$$

where $m = \lfloor (n+1)/2 \rfloor$.

The above approaches separate the computation of the nodes of (1.6) from that of the corresponding weights, in the sense that after having obtained the representation of $E_{n+1}(x)$ one computes its zeros hence, using known representations, the corresponding coefficients. Incidentally, here we remark that having determined the expansion (2.1), the computation of its zeros and the weights of (1.6) can be performed very efficiently by proceding as follows.

Recalling the known relationships (see [70, (4.7.14)])

$$\begin{cases} T_k'(x) = kU_{k-1}(x), \\ U_k'(x) = P_{k-1}^{(2)}(x), \end{cases}$$

where $P_k^{(\lambda)}(x) \equiv P_k^{(\lambda-1/2,\lambda-1/2)}(x)$ denotes the ultraspherical polynomial defined in [67], first we notice that besides (2.1) we also have, for example,

$$E_{n+1}'(x) = (n+1)U_n(x) + (n-1)a_1U_{n-2}(x) + \cdots + a_{\lfloor n/2 \rfloor},$$
$$E_{n+1}''(x) = (n+1)P_{n-1}^{(2)}(x) + (n-1)a_1P_{n-3}^{(2)}(x) + \cdots + a_{\lfloor (n-2)/2 \rfloor}.$$

Therefore, using the well-known three-term recurrence relations which are satisfied by the above orthogonal polynomials, and the Clenshaw summation algorithm, one can compute efficiently the values of $E_{n+1}(x)$, $E_{n+1}'(x)$ and $E_{n+1}''(x)$, hence, use a third order iterative method such as the Laguerre one to compute the zeros of $E_{n+1}(x)$. Good starting points for such computation are the "odd" zeros of $T_{2n+1}(x)$, i.e.,

$$y_{nj}^{(0)} = \cos\left(\frac{2j-1}{2n+1}\frac{\pi}{2}\right), \quad j = 1, 3, \ldots.$$

This choice is suggested by the property (see [16,21])

$$P_n(x)E_{n+1}(x) = \gamma_n T_{2n+1}(x) + o(1), \quad n \to \infty, \tag{2.3}$$

which holds uniformly in any interval of the type $[-1+\varepsilon, 1-\varepsilon]$, with $\varepsilon > 0$. We remark that the accuracy of this initial guess is quite good: for example, it is of about 2 (decimal) digits for $n = 20$ and of 3–4 digits for $n = 30$; it increases with n.

Also the computation of the coefficients $\{A_{ni}\}$ and $\{B_{nj}\}$ can be performed using the quite simple representations:

$$\begin{aligned} A_{ni} &= \frac{c_n}{P_{n-1}^{(3/2)}(x_{ni})E_{n+1}(x_{ni})}, \quad i = 1, \ldots, n, \\ B_{nj} &= \frac{c_n}{P_n(y_{nj})E_{n+1}'(y_{nj})}, \qquad j = 1, \ldots, n+1, \end{aligned} \tag{2.4}$$

where

$$c_n = \frac{2^{2n+1}}{2n+1}\left(\frac{n!}{(2n)!}\right)^2.$$

They follow from the known expressions

$$A_{ni} = \frac{1}{P_n'(x_{ni})E_{n+1}(x_{ni})}\int_{-1}^{1}\frac{P_n(x)E_{n+1}(x)}{x - x_{ni}}\,\mathrm{d}x,$$
$$B_{nj} = \frac{1}{P_n(y_{nj})E_{n+1}'(y_{nj})}\int_{-1}^{1}\frac{P_n(x)E_{n+1}(x)}{x - y_{nj}}\,\mathrm{d}x,$$

once we replace the above integrals by the $(n+1)$-point Gauss–Legendre rule (including its remainder term, whose value turns out to be c_n).

Since the iterative method proposed to compute the zeros of $E_{n+1}(x)$ require very few iterations, no matter how large n is, the complexity of this approach is essentially $O(n^2)$. This approach is also generalized to the case of an ultraspherical weight function (see [46]).

Gautschi et al. (see [12,30]) proposed to compute simultaneously all the unknown nodes and all the weights of (1.6), by solving the nonlinear system which follows from (1.6) when we replace in it $f(x)$ by $P_k(x)$, $k = 0, 1, \ldots, 3n+1$. This will have exactly $3n+2$ unknowns: the A_{ni}'s, the B_{nj}'s and the y_{nj}'s. Newton's method is then applied. Very good starting values for the the ierative process can be taken from the asymptotic results obtained by Ehrich in [16,21]. Recalling also (2.3), these are:

$$
\begin{aligned}
x_{ni} &= \cos\phi_{ni}, \quad \phi_{ni} = \frac{i - 1/4 + o(1)}{n + 1/2}\pi, \\
y_{nj} &= \cos\theta_{nj}, \quad \theta_{nj} = \frac{j - 3/4 + o(1)}{n + 1/2}\pi, \\
A_{ni} &= \frac{\pi}{2n + 3/2}\sin\phi_{ni}\big[1 + o(1)\big], \\
B_{nj} &= \frac{\pi}{2n + 3/2}\sin\theta_{nj}\big[1 + o(1)\big],
\end{aligned}
$$

and they are valid whenever $x_{ni}, y_{nj} \in [-1+\varepsilon, 1-\varepsilon]$, $\varepsilon > 0$ fixed. In practice they can be used for all nodes and weights.

A fixed point method to compute the additional nodes $\{y_{nj}\}$ is examined by Ehrich in [14]. It follows from the relationship

$$
\int_{-1}^{1} P_n(x)E_{n+1}(x)\left[\frac{E_{n+1}(x)}{x - y_{nj}}\right]\mathrm{d}x = 0, \quad j = 1, \ldots, n+1,
$$

a consequence of (1.9), after having rewritten it in the new form

$$
\begin{aligned}
y_{nj}\int_{-1}^{1} P_n(x)\prod_{k=1,k\neq j}^{n+1}(x - y_{nk})^2\,\mathrm{d}x &= \int_{-1}^{1} P_n(x)\prod_{k=1,k\neq j}^{n+1}(x - y_{nk})^2 x\,\mathrm{d}x, \\
j &= 1, \ldots, n+1.
\end{aligned}
$$

This method is locally convergent with order 2. It can be implemented in a way that every iteration step involves a number of arithmetic operation that depends quadratically on the number of nodes; furthermore, it provides aposteriori error estimates. Finally, it can be used to construct extensions of more general rules, like those of Patterson that we will describe in section 4.

Since it is well known that the construction of Gaussian rules can be reduced to an eigenvalue problem for a symmetric tridiagonal matrix, usually called Jacobi matrix, in [33] Kautsky and Elhay presented a first attempt to generalize this approach by including, among other situations, the Kronrod case. In particular, they generalized the

concept of Jacobi matrix for nonnegative weight functions to the situation where the weight function changes sign within the interval of orthogonality. Notice that while in the first case a complete sequence of orthogonal polynomials exist, in the second only a few orthogonal polynomials may exist.

But the key result in this direction have been obtained very recently by Laurie (see [41]). In this paper, an $O(n^2)$ procedure for computing specifically the Kronrod rule is described. It represents an efficient way of reducing the construction of (1.6) to the well-studied problem of computing a Gaussian rule from the recurrence coefficients. Here we shall simply report a short description of the main ideas this procedure is based on.

Let $\{p_j\}_{j=0}^{\infty}$ be a sequence of monic orthogonal polynomials with respect to the inner product

$$(f, g) = \int_{-1}^{1} f(x)g(x)w(x)\,\mathrm{d}x. \tag{2.5}$$

Then the p_j's satisfy a recurrence relation of the form

$$\begin{cases} p_0(x) = 1 \\ p_1(x) = x - a_0 \\ p_{k+1}(x) = (x - a_k)p_k(x) - b_k^2 p_{k-1}(x), \quad k = 1, 2, \ldots, \end{cases} \tag{2.6}$$

with coefficients

$$\begin{aligned} a_k &= \frac{(p_k, xp_k)}{(p_k, p_k)}, && k = 0, 1, \ldots, \\ b_k &= \left[\frac{(p_k, p_k)}{(p_{k-1}, p_{k-1})}\right]^{1/2}, && k = 1, 2, \ldots. \end{aligned} \tag{2.7}$$

The $2n - 1$ coefficients $\{a_k\}_{k=0}^{n-1}$ and $\{b_k\}_{k=1}^{n-1}$ determine the symmetric tridiagonal matrix

$$T_n = \begin{pmatrix} a_0 & b_1 & & & & & \\ b_1 & a_1 & b_2 & & & & \\ & \cdot & \cdot & \cdot & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & b_{n-2} & a_{n-2} & b_{n-1} \\ & & & & & b_{n-1} & a_{n-1} \end{pmatrix} \in \mathbb{R}^{n\times n} \tag{2.8}$$

with spectral factorization

$$\begin{aligned} &T_n = W_n \Lambda_n W_n^{\mathrm{T}}, && W_n W_n^{\mathrm{T}} = I, \\ &\Lambda_n = \mathrm{diag}[\lambda_1, \lambda_2, \ldots, \lambda_n]. \end{aligned} \tag{2.9}$$

Due to the positivity of the b_k's, the eigenvalues λ_j are distinct and all entries of the first row of W_n are nonvanishing. Moreover, it is well known that the nodes and weights of the Gaussian rule

$$\int_{-1}^{1} w(x) f(x)\,\mathrm{d}x \approx \sum_{i=1}^{n} w_{ni} f(x_{ni}) \tag{2.10}$$

are given by

$$\begin{cases} x_{ni} = \lambda_i, \\ w_{ni} = \left(e_1^{\mathrm{T}} W_n e_i\right)^2, \end{cases} \qquad 1 \leqslant i \leqslant n, \tag{2.11}$$

where e_i denotes the ith axis vector.

Assuming that we already know the coefficients a_k and b_k needed, the nodes and weights of (2.8) can be computed in $\mathrm{O}(n^2)$ arithmetic operations by the well-known Golub–Welsch algorithm.

Laurie [41] showed that if the Kronrod extension (1.6) exists with real and distinct nodes $\{\tilde{x}_{ni}\}_{i=1}^{2n+1}$ and positive weights $\{\widetilde{w}_{ni}\}_{i=1}^{2n+1}$, then we can associate with it a symmetric tridiagonal matrix of the form

$$\widetilde{T}_{2n+1} = \begin{pmatrix} \tilde{a}_0 & \tilde{b}_1 & & & & & \\ \tilde{b}_1 & \tilde{a}_1 & \tilde{b}_2 & & & & \\ & \cdot & \cdot & \cdot & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & \tilde{b}_{2n-1} & \tilde{a}_{2n-1} & \tilde{b}_{2n} \\ & & & & & \tilde{b}_{2n} & \tilde{a}_{2n} \end{pmatrix} \in \mathbb{R}^{(2n+1)\times(2n+1)} \tag{2.12}$$

with spectral factorization

$$\begin{aligned} &\widetilde{T}_{2n+1} = \widetilde{W}_{2n+1} \widetilde{\Lambda}_{2n+1} \widetilde{W}_{2n+1}^{\mathrm{T}}, \qquad \widetilde{W}_{2n+1} \widetilde{W}_{2n+1}^{\mathrm{T}} = I, \\ &\widetilde{\Lambda}_{2n+1} = \operatorname{diag}\left[\tilde{\lambda}_1, \tilde{\lambda}_2, \ldots, \tilde{\lambda}_{2n+1}\right] \end{aligned} \tag{2.13}$$

such that

$$\begin{cases} \tilde{x}_{ni} = \tilde{\lambda}_i, \\ \widetilde{w}_{ni} = \left(e_1^{\mathrm{T}} \widetilde{W}_{2n+1} e_i\right)^2, \end{cases} \qquad 1 \leqslant i \leqslant 2n+1. \tag{2.14}$$

Moreover, under the above assumptions on the Kronrod rule, Laurie proved the following fundamental result (see [41]).

Theorem 1. Let $\widehat{T}_n$ and $\check{T}_n$ denote the leading and trailing $n \times n$ principal submatrices of $\widetilde{T}_{2n+1}$, respectively. Then, $\widehat{T}_n$ and $\check{T}_n$ have the same eigenvalues. Moreover, for n odd

$$\begin{cases} \tilde{a}_{j-1} = a_{j-1}, \\ \tilde{b}_j = b_j, \end{cases} \qquad 1 \leqslant j \leqslant \frac{3n+1}{2}, \tag{2.15}$$

and, for n even,

$$\begin{cases} \tilde{a}_j = a_j, & 0 \leqslant j \leqslant \dfrac{3n}{2}, \\ \tilde{b}_j = b_j, & 1 \leqslant j \leqslant \dfrac{3n}{2}. \end{cases} \tag{2.16}$$

Notice that $\widehat{T}_n \equiv T_n$.

A major consequence of this result is (see [13,41]) that the existence of a Kronrod rule with real and distinct nodes and positive weights, is equivalent to the existence of a real solution of the following inverse eigenvalue problem.

Corollary 1. Let the first $n-1$ entries $\tilde{a}_{n+1}, \tilde{b}_{n+2}, \tilde{a}_{n+2}, \ldots$ of the $n \times n$ symmetric tridiagonal matrix

$$\breve{T}_n = \begin{pmatrix} \tilde{a}_{n+1} & \tilde{b}_{n+2} & & & & & \\ \tilde{b}_{n+2} & \tilde{a}_{n+2} & \tilde{b}_{n+3} & & & & \\ & \cdot & \cdot & \cdot & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & \tilde{b}_{2n-1} & \tilde{a}_{2n-1} & \tilde{b}_{2n} \\ & & & & & \tilde{b}_{2n} & \tilde{a}_{2n} \end{pmatrix} \tag{2.17}$$

be determined by (2.15) when n is odd, and by (2.16) when n is even, the remaining ones being unknown. Then the eigenvalues of $\breve{T}_n$ coincide with those of the matrix $\widehat{T}_n$, i.e., of (2.8), if and only if there is a $(2n+1)$-point Kronrod quadrature rule (1.6) with real nodes and positive weights.

Therefore, for example, in the case we know that a Kronrod rule exists with real nodes and positive weights, and the recurrence coefficients associated with its weight function are also known, its construction is equivalent to the determination of the unknown terms of $\breve{T}_n$, that is, of $\widetilde{T}_{2n+1}$ defined by (2.12), hence, to the solution of the eigenvalue problem defined by (2.13) and (2.14).

A first algorithm implementing these ideas has been presented by Laurie in [41]. The unknown coefficients, that is the last n entries of $\breve{T}_n$, are computed explicitly through a five-term recurrence relation of certain mixed moments. The existence of the Kronrod rule with real nodes and positive weights is equivalent to the positivity of all $\tilde{b}_i$'s. A pseudocode for this method is presented at the end of the paper [41].

Calvetti et al. in [13] propose a variant of the above algorithm which does not explicitly determine the tridiagonal matrix $\widetilde{T}_{2n+1}$, whose entries could be very sensitive to round-off errors.

In both cases, the construction of the Kronrod rule is performed, starting from the recursion coefficients a_j and b_j defined by (2.7), in only $O(n^2)$ arithmetic operations. These algorithms can also be applied to the computation of the Kronrod extensions of Gauss–Radau and Gauss–Lobatto formulas.

A further generalization of the second algorithm above, which allows the construction of Kronrod rules even when some of the nodes and weights are complex (conjugate) or all nodes are real but some of the corresponding weights are negative, have been proposed in [1].

The description of these algorithms is quite involving and fairly long; therefore we omit it and address the reader to the original articles.

Of course these algorithms can also be used to investigate the existence of Kronrod extensions associated with a given weight function; see [13,41]. They also establish a connection with analogous results for the Gaussian quadrature formulas. Besides giving rise to efficient numerical procedures, this is certainly fashinating. However, at least for the standard case (1.6), this approach has the same computational cost ($O(n^2)$) of the more traditional algorithm based on relations (2.1), (2.2) and (2.4). In this case, without a rigorous numerical testing, it does not seem to be possible to decide a priori which one of the two is faster.

3. Error behaviour and estimates

The drawback of the error estimate (1.4) is that it provides only information about the error in the less accurate value $Q_n(f) = G_n(f)$. The value $Q_m(f) = K_{2n+1}(f)$ is used only to obtain the error estimate. However, this value is often much more accurate than $G_n(f)$, especially when f is smooth. Actually, its degree of accuracy is related to the smoothness of f.

In the following table we report the performances, in terms of relative errors (their absolute values), of $G_7(f)$ and $K_{15}(f)$ when these rules are applied to the functions

$$f_1(x) = |x|, \qquad f_2(x) = x^4|x|, \qquad f_3(x) = x^{10}|x|. \tag{3.1}$$

Then we report the analogous results we have obtained when the integrand function $f(x)$ is

$$f_{4,k}(x) = (1-x)^{k/2}, \quad k = 1, 3, 5, 9. \tag{3.2}$$

A few attempts have been made to estimate the higher accuracy of $K_{2n+1}(f)$ with respect to $G_n(f)$; see [6,15,19,40,64]. This because the integral approximation one has at his disposal, after having estimated the accuracy of $G_n(f)$, is indeed $K_{2n+1}(f)$.

Table 1
Relative errors for the functions $f_i(x)$, $i = 1, 2, 3$, in (3.1).

i	G_7	K_{15}
1	2.95E−2	7.34E−3
2	1.65E−4	2.16E−6
3	6.56E−5	3.10E−9

Table 2
Relative errors for the functions (3.2).

k	G_7	K_{15}
1	3.70E−4	2.02E−05
3	9.01E−6	4.28E−08
5	4.63E−7	3.39E−10
9	5.95E−9	1.44E−12

From a theoretical point of view an explanation can be given by looking at the best error bounds for $R_n^G(f)$ and $R_{2n+1}^K(f)$, when $f \in C^s[-1, 1]$. These are of the type

$$\begin{aligned} \left|R_n^G(f)\right| &\leqslant c_s\left(R_n^G\right)\left\|f^{(s)}\right\|_\infty, \\ \left|R_{2n+1}^K(f)\right| &\leqslant c_s\left(R_{2n+1}^K\right)\left\|f^{(s)}\right\|_\infty, \end{aligned}$$

with

$$c_s(R_n) = \sup_{\|f^{(s)}\|_\infty \leqslant 1} \left|R_n(f)\right|.$$

In particular, Brass and Förster [8] have shown that

$$\frac{c_{2n}(R_{2n+1}^K)}{c_{2n}(R_n^G)} < cn^{1/4}\left(\frac{16}{25\sqrt{5}}\right)^n.$$

Moreover (see [18]), for every $s = 1, 2, \ldots$

$$\lim_{n\to\infty} \frac{c_s(R_{2n+1}^K)}{c_s(R_n^G)} = 2^{-s};$$

actually (see [15]),

$$\lim_{n\to\infty} \frac{c_s(R_{2n+1}^G)}{c_s(R_{2n+1}^K)} = 1.$$

When f is only of bounded variation, $K_{2n+1}(f)$ is still twice as good as $G_n(f)$ (see [21]).

In the case of high order constants we have

$$c_{3n+2+k}\left(R_{2n+1}^K\right) \sim \frac{2^{-3n}n^{-5/2}}{(3n+2+k)!}$$

with $k = 0$ when n is even, and $k = 1$ when n is odd, and (see [7])

$$c_{2m}\left(R_m^G\right) = \frac{2^{2m+1}}{2m+1}\frac{(m!)^4}{[(2m)!]^3}.$$

Therefore, if we consider the m-point Gaussian rule, with $2m-1 = 3n+2+k$, that is the Gaussian rule having the same degree of exactness of the $(2n+1)$-point Kronrod formulas, we have

$$\frac{c_{3n+2+k}(R_n^K)}{c_{2m}(R_m^G)} \sim n^{-5/2}.$$

Indeed, when these two rules are applied to a smooth function, the Kronrod one gives a higher accuracy. Notice that although they have the same degree of exactness, the Kronrod rule uses a larger number of points. If instead we compare the $(2n+1)$-point Kronrod rule with the $(2n+1)$-point Gaussian one, the latter is superior. Indeed, in this case we have (see [21])

$$\frac{c_{3n+2+k}(R_{2n+1}^G)}{c_{3n+2+k}(R_{2n+1}^K)} < 3^{-n+1}$$

for $n \geqslant 15$, and

$$\lim_{n\to\infty}\left(\frac{c_{3n+2+k}(R_{2n+1}^G)}{c_{3n+2+k}(R_{2n+1}^K)}\right)^{1/n} = \sqrt{\frac{6^6}{7^7}} = \frac{1}{4.2013\ldots}.$$

From a practical point of view reasonable estimates are derived starting from a mixture of theoretical results and empirical evidences. The basic idea is to estimate the smoothness of $f(x)$ and from it the higher accuracy of $K_{2n+1}(f)$ over that of $G_n(f)$. For instance, in the QUADPACK adaptive routines using the Gauss–Kronrod basic rules (see [64]), the following device has been used.

The mean value of the integrand function $f(x)$ on a local interval of integration $[a_i, b_i]$ is computed numerically:

$$M(f; a_i, b_i) = \frac{1}{b_i - a_i} K_{2n+1}(f).$$

Then, the quantity $K_{2n+1}(|f-M|)$ is the discretization of an upper bound for $|R_{2n+1}^K(f)|$. Indeed, we have

$$\left|R_{2n+1}^K(f)\right| = \left|R_{2n+1}^K(f-M)\right| = \left|K_{2n+1}(f-M)\right| \leqslant K_{2n+1}\big(|f-M|\big).$$

This bound holds also for non smooth functions, but it is not sensitive to the smoothness of f. In particular, when f is smooth this estimate is too pessimistic. The error estimate $|G_n(f) - K_{2n+1}(f)|$ is thus compared with $K_{2n+1}(|f-M|)$. If this ratio is small then both rules $G_n(f)$ and $K_{2n+1}(f)$ give a sufficiently high accuracy in relation to the smoothness of f, and, in particular, $K_{2n+1}(f)$ is expected to yield a better approximation than $G_n(f)$. By assuming that our function f is sufficiently smooth so that the following behaviours hold:

$$R_n^G(f) = c_1 h^{2n} + \mathrm{O}\big(h^{2n+1}\big),$$
$$R_{2n+1}^K(f) = c_2 h^{3n+2+k} + \mathrm{O}\big(h^{3n+3+k}\big),$$

where $h = b_i - a_i$, the error estimate finally used to test the accuracy of $K_{2n+1}(f)$ is:

$$\left|R^K_{2n+1}(f)\right| \approx \min\left\{ K_{2n+1}\big(|f-M|\big), \left(200^{3/2}\left|\frac{G_n(f)-K_{2n+1}(f)}{K_{2n+1}(|f-M|)}\right|^{1/2}\right)\left|G_n(f)-K_{2n+1}(f)\right| \right\}$$

that is,

$$\left|R^K_{2n+1}(f)\right| \approx K_{2n+1}\big(|f-M|\big) \times \min\left\{1, \left(200\frac{|G_n(f)-K_{2n+1}(f)|}{K_{2n+1}(|f-M|)}\right)^{3/2}\right\}.$$

In QUADPACK the couples (G_7, K_{15}), (G_{10}, K_{21}), (G_{20}, K_{41}), (G_{25}, K_{51}), (G_{30}, K_{61}) are used, together with this error estimate, as local integration rules for adaptive automatic integration.

Since the usual application for error estimates occurs during adaptive integration processes, where the typical step is the bisection of the interval with the largest error estimate, some authors (see, for example, the introduction in [39]) have proposed to detect the higher accuracy of $K_{2n+1}(f)$ by using some extrapolation technique combined with some heuristics. Here we mention the attempt associated with the concept of "null rule".

In [6], starting from the remark that the error functional $G_n(f) - K_{2n+1}(f)$ is a null rule of degree $2n-1$ on the points of $K_{2n+1}(f)$, to detect the smoothness of the integrand f a sequence of $2n$ null rules of increasing degree $0, 1, \ldots, 2n-1$, using the same function values of $K_{2n+1}(f)$, is considered. The smoothness of f is related to the existence of an asymptotic behaviour of this sequence. In the case of positive answer, the error estimate given by $|G_n(f) - K_{2n+1}(f)|$ is improved by extrapolation. As in the previous case, a safety factor is inserted into the extrapolated estimate.

In the quadpack case, as well as in the latter, the final formula, which is used to define the error estimate, is obtained also with the aid of a substantial amount of numerical experimentation.

4. Generalizations and applications

Besides an intensive investigation on the existence and non existence of Kronrod extensions of Gaussian rules with more general weight functions (see [28,47,50,60]), including the case of non bounded intervals of integration, since the first appearance of Kronrod's work Patterson (see [52,53]) iterated the original idea of (1.6) by constructing a sequence of embedded rules of maximum degree of exactness. More precisely (see [52,55]), starting from $G_3(f)$ and $K_7(f)$, he constructed a new rule $KP_{15}(f)$, which includes among its 15 nodes the 7 ones of $K_7(f)$, where all the 23 free parameters (the 8 new nodes and all the coefficients) are chosen so that $KP_{15}(f)$ has maximum degree of exactness, that is, at least 23. Then he constructed

$KP_{31}(f)$, $KP_{63}(f)$, $KP_{127}(f)$, $KP_{255}(f)$ and $KP_{511}(f)$. These rules were then inserted in an automatic integrator [53]. In general, given a $(2m+1)$-point *KP* rule, of the form

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \approx \sum_{i=1}^{m} A_i^{P_1}\big(x_i^P\big) + \sum_{j=1}^{m+1} B_j^{P_1}\big(y_j^P\big) \tag{4.1}$$

and degree of exactness at least $3m+1$, he constructed a $(4m+3)$-point optimal extension of it

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \approx \sum_{i=1}^{m} A_i^{P_2}\big(x_i^P\big) + \sum_{j=1}^{m+1} B_j^{P_2}\big(y_j^P\big) + \sum_{l=1}^{2m+2} C_l^{P_2} f\big(z_l^P\big), \tag{4.2}$$

where $\{A_i^{P_2}\}, \{B_j^{P_2}\}, \{C_l^{P_2}\}, \{z_l^P\}$ are chosen so that the degree of exactness is at least $6m+4$.

Krogh and Van Snyder in [34] reduce the number of coefficients necessary to represent Patterson's sequence of rules. Their version of the method also reduces the amount of storage necessary for storing the function values and produces slightly smaller errors in evaluating the quadrature sums when the integrand has a singular behaviour at the endpoints of the interval of integration.

In QUADPACK, the analogous sequence $G_{10}(f)$, $K_{21}(f)$, $KP_{43}(f)$, $KP_{87}(f)$ is used to build a non adaptive integrator.

All these new rules share the properties of Kronrod's rules: real, distinct and symmetric nodes in $(-1, 1)$, positivity of all coefficients. These properties, as well as the existence of any number of Patterson's extensions, or the existence of these extensions for other starting Gauss–Legendre rules, have not been yet proved, although numerical evidences show that they certainly do not exist for all values of the initial n. For instance (see [54]), the sequence starting with $G_2(f)$ gives only the rules $K_5(f)$, $KP_{11}(f)$, $KP_{23}(f)$ and $KP_{47}(f)$, after that any further extension (with real nodes) becomes impossible. Notice that in four remarkable cases (see, however, also [58]) these repeated extensions always exist, for any starting value of n; moreover they coincide with classical Gaussian formulas (see [48]). These are associated with integrals of the form

$$\int_{-1}^{1} (1-x)^{\alpha}(1+x)^{\beta} f(x)\,\mathrm{d}x, \quad |\alpha| = |\beta| = \frac{1}{2}.$$

For the construction of these sequences see [54]. The proposed algorithm is not as efficient and elegant as those proposed for the Kronrod rules; it is however quite general, in the sense that it allows, in principle since there is no guarantee that the new nodes are real, the optimal extension of any n-point (interpolatory) quadrature rule by a $(n+m)$-point (interpolatory) new rule. Here we present a description of its main ingredients.

Denoting by $x_1, \ldots, x_n$ the preassigned nodes, and by $x_{n+1}, \ldots, x_{n+m}$ the additional ones, the new rule for an integral of type (1.11) has the form

$$\int_a^b w(x) f(x)\,\mathrm{d}x \approx \sum_{i=1}^{n} A_i f(x_i) + \sum_{i=1}^{m} A_{n+i} f(x_{n+i}). \tag{4.3}$$

The m free nodes $x_{n+1}, \ldots, x_{n+m}$ ought to be chosen to achieve degree of exactness at least $n + 2m - 1$. This necessarily implies the orthogonality relationship

$$\int_a^b w(x) H_n(x) E_m(x) x^k\,\mathrm{d}x = 0, \quad k = 0, 1, \ldots, m-1, \tag{4.4}$$

where $H_n(x)$ and $E_m(x)$ are the polynomials whose zeros coincide with the nodes $\{x_i\}_{i=1}^n$ and $\{x_{n+i}\}_{i=1}^m$, respectively.

Denoting by $\{p_i^*(x)\}$ the orthonormal set associated with (2.5), we write

$$H_n(x) = \sum_{i=m_0}^{n} \tau_i p_i^*(x), \quad \text{for some } m_0 \geqslant 0, \tag{4.5}$$

and

$$E_m(x) = \sum_{i=0}^{m} \varepsilon_i p_i^*(x). \tag{4.6}$$

Setting

$$H_{n+m}(x) = H_n(x) E_m(x) = \sum_{j=0}^{n+m} \gamma_i p_i^*(x),$$

relation (4.4) implies

$$\gamma_j = 0, \quad j = 0, \ldots, m-1, \tag{4.7}$$

hence,

$$H_{n+m}(x) = \sum_{j=m}^{n+m} \gamma_j p_j^*(x). \tag{4.8}$$

To obtain an explicit expression for the coefficients γ_j it is sufficient to multiply (4.6) by $w(x) p_k^*(x)$ and integrate over (a, b). Thus, we have

$$\gamma_k = \sum_{j=0}^{m} \varepsilon_j \sum_{i=m_0}^{n} \tau_i a_i^{(k,j)},$$

where

$$a_i^{(k,j)} = \int_a^b w(x) p_i^*(x) p_j^*(x) p_k^*(x)\,\mathrm{d}x$$

are the coefficients of the expansion of $p_k^* p_j^*$ in terms of the p_i^*'s, i.e.,

$$p_k^*(x)p_j^*(x) = \sum_{i=|k-j|}^{k+j} a_i^{(k,j)} p_i^*(x).$$

Expressions for $a_i^{(k,j)}$ are either known or can be generated using the 3-term recurrence relation associated with the system $\{p_i^*\}$.

In particular, condition (4.7) implies

$$\sum_{j=0}^{m} \varepsilon_j \sum_{i=m_0}^{n} \tau_i a_i^{(k,j)} = 0, \quad k = 0, \ldots, m-1. \tag{4.9}$$

From this, taking $\varepsilon_m = 1$, we obtain a symmetric linear system of m equations in the m unknowns $\varepsilon_0, \varepsilon_1, \ldots, \varepsilon_{m-1}$. Once $E_m(x)$ is known, the coefficients $\gamma_m, \ldots, \gamma_{n+m}$ can be calculated and another extension can be generated with $n + m$ replacing n and m replacing m_0.

Actually, (4.9) can be rewritten in the simpler form

$$\sum_{j=0}^{m} \varepsilon_j \sum_{i=\max\{m_0,|k-j|\}}^{\min\{n,|k+j|\}} \tau_i a_i^{(k,j)} = 0, \quad k = 0, \ldots, m-1. \tag{4.10}$$

The zeros of $E_m(x)$ are computed using a generalization of Bairstow's method. The corresponding weights A_j of (4.3) are determined using a known representation which springs directly from the interpolatory nature of the rule.

The algorithm can be used to produce specific individual quadrature rules or sequences of rules by iterative application.

The Kronrod and Patterson optimal extended rules have given rise to several proposals of alternative embedded sequences of rules, all having the main goal of defining an efficient strategy for the numerical evaluation of integrals, with required accuracy.

In [26] Favati et al., stimulated by the quadpack routines based on Kronrod's rules, defined a sequence of embedded interpolatory quadrature formulas with positive weights and increasing degree of precision, that they called "recursive monotone stable formulas". To test these formulas, they took two automatic adaptive integrators from the quadpack package and replaced the Gauss–Kronrod rules by some of their formulas (see [27]).

An interesting variation of the concept of embeeded or nested rules has been proposed by Laurie in [38]. These new rules are termed "stratified nested rules" and have the property that the weights associated with the nodes of a particular rule are a prescribed fraction of the weights for those same nodes in its successor. More precisely, denoting

by $Q^{(m-1)}$ and $Q^{(m)}$ two consecutive rules, with $n_{m-1} = 2^{m-1} - 1$ and $n_m = 2^m - 1$ nodes, respectively, we have

$$Q^{(m)} f = \theta Q^{(m-1)} f + \sum_{i=0}^{n_{m-1}} w_{i,m} f(x_{i,m}),$$

where the parameter θ and the quantities $\{w_{i,m}\}$ and $\{x_{i,m}\}$ are chosen so that the degree of exactness of the rule is maximized. In particular, they are determined by requiring that $Q^{(m)}$ integrates exactly all polynomials of degree $\leqslant n_m$. Therefore, they are at least of interpolatory type, but their degree of exactness (n_m) is much less than that of the corresponding *KP* rule having the same number of nodes, which is $(3n_m + 1)/2$. In [38] Laurie listed the rules with $1, 3, 7, \ldots, 255$ nodes, corresponding to $Q_1, Q_2, Q_3, \ldots, Q_8$. A quite severe loss of precision was noticed during the determination of these rules.

Following the general procedure discussed in [54], Patterson examined a variant of Laurie's approach, which combines the ideas of stratified nested sequence of rules and the optimal KP extension. Assuming that a given quadrature rule has n nodes $x_1, x_2, \ldots, x_n$, the subsequent rule will have $n + m$ nodes, with $m > n$, obtained by adding to the previous n nodes m new ones, chosen according to the following strategy.

Let

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \approx \sum_{i=1}^{n} w_i f(x_i)$$

be the first rule, and

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \approx \sum_{i=1}^{n} w_i^I f(x_i) + \sum_{j=1}^{m} w_j^{II} f(y_j)$$

the next one. Given a positive integer $l < n$, we pre-assign the first l weights

$$w_i^I = \theta_i w_i, \quad i = 1, \ldots, l.$$

Then the additional $n+2m-l$ conditions, nedeed to define (hopefully) a unique solution, are provided by requiring maximum degree of exactness to the rule. This turns out to be $d = n + 2m - l - 1$ ($d + 1$ if d is even).

Notice that $l = 0$ gives the *KP* rules, while for $l = n$ we have Laurie's rules. For other values of l we get a hybridization of Laurie and Patterson rules, with intermediate degree of exactness. These new rules are termed "hybrid rules". Various hybrid extensions were then generated. As for Laurie's rules, the linear systems one has to solve to generate these new formulas is very ill-conditioned, and, moreover, errors propagate very rapidly from the computation of one rule to that of the next one.

The rarity of extensions of Kronrod type, associated with general Gaussian rules, has suggested several authors to relax the requirements of maximum degree of exactness. This allows to introduce some degree of freedom in choosing the additional nodes, so that, if possible, the new (suboptimal) extension exists with all real nodes and positive weights.

In particular, Begumisa and Robinson in [5] have proposed to require to the polynomial $E_{n+1}(x) = \sum_{j=0}^{n+1} a_j P_j(x)$, $a_{n+1} = 1$, whose zeros define the additional nodes, to satisfy the weaker orthogonality condition

$$\int_a^b w(x) P_n(x) E_{n+1}(x) x^k \, \mathrm{d}x = 0, \quad k = 0, \ldots, n - r,$$

for some (possibly small) positive integer r. This relation determines (uniquely) only the leading $n+1-r$ coefficients $a_n, a_{n-1}, \ldots, a_r$. Their strategy is then to increase r, starting from $r = 1$, and for each value of r trying to choose the r free trailing coefficients of $E_{n+1}(x)$ so that all the zeros of E_{n+1} are real, distinct and in (a, b). The procedure is not automatic and fairly complex. However, in some cases where the (optimal) Kronrod extensions do not exist, such as the Gauss–Laguerre, the Gauss–Hermite and certain Gauss–Gegenbauer ones, they produce (suboptimal) extensions which have a degree of exactness only slightly less than the optimal one.

Patterson in [55] simplified the above approach by noticing that the above construction is equivalent to appending r arbitrary nodes $x_{n+1}, \ldots, x_{n+r}$ to the original n Gaussian nodes, thus giving a total of $n + r$ fixed abscissas, and define the additional $n + 1 - r$ free nodes $y_1, y_2, \ldots, y_{n+1-r}$ so that

$$\int_a^b w(x) \left[P_n(x) \prod_{i=n+1}^{n+r} (x - x_i) \right] E^*_{n+1-r}(x) x^k \, \mathrm{d}x = 0, \quad k = 0, 1, \ldots, n - r,$$

where $E^*_{n+1-r}(x) = \prod_{j=1}^{n+1-r} (x - y_j)$. The r arbitrary nodes hopefully can be chosen to make the new optimal extension successful. A reasonable guess is required for the positions of these nodes. This alternative approach can be applied using the general algorithm presented in [53].

Kahaner et al. in [32] looked for nonminimal extensions in the particular case of Gauss–Laguerre rules. They extended this Gaussian formulas by adding $m > n + 1$ new nodes, chosen so that the new rule has maximum degree of exactness, i.e., at least $n + 2m - 1$. Their results appear to indicate that in this case the value m should be around $2n$.

Finally, Patterson in [55] proposed to construct the extended rule by replacing in the starting Gaussian formula one or more nodes with "judiciously" chosen values. The modified rule hopefully can be extended with optimal degree of exactness in the usual way. Examples of this new approach are given for the classical Gauss–Laguerre and Gauss–Hermite cases.

The non existence of Kronrod rules has also suggested Laurie (see [40]) to associate with a n-point (weighted) Gaussian rule $G_n f$ a particular suboptimal $(2n+1)$-point extension, whose existence with real nodes and positive weights is always guaranteed. This is obtained by considering first a new $(n + 1)$-point formula $H_{n+1} f$, which is designed to have an error precisely opposite to that of $G_n f$ whenever f is a polynomial of degree $\leqslant 2n + 1$. The extended rule is then $L_{2n+1} f = \frac{1}{2}(G_n f + H_{n+1} f)$, and the

corresponding error estimate is given by $L_{2n+1}f - G_nF = \frac{1}{2}(H_{n+1}f - G_nf)$. The construction of $H_{n+1}f$ is quite simple.

The most important and successful application of Kronrod's rules is certainly the error estimation of a Gauss–Legendre formula and the construction of an (automatic) adaptive integrator (see [53,62,64]). A byproduct of it, examined by Rabinowitz in [63] and in our opinion minor from the practical point of view, is the natural use of Gaussian and Kronrod rules for the evaluation of a Cauchy principal value integral of the form

$$\int_a^b \frac{f(x)}{x-y}\,\mathrm{d}x.$$

This can be reformulated in the new form

$$\int_a^b w(x)\frac{f(x)-f(y)}{x-y}\,\mathrm{d}x + f(y)\int_a^b \frac{w(x)}{x-y}\,\mathrm{d}x,$$

where the first integral, which is defined in the usual sense, can be approximated by a Gaussian rule, hence, also by its Kronrod extension whenever the latter exists. Non-minimal extensions with $n+2$ additional nodes, to avoid the presence of a derivative when y coincides with one of the nodes of $E_{n+1}(x)$, have also been examined. See also [11].

One of the first variants of Kronrod's original idea has been proposed by Piessens in [61]. In this paper he constructed Kronrod type rules for the evaluation of the Bromwich inversion formula

$$f(t) = \frac{1}{2\pi\mathrm{i}}\int_L \mathrm{e}^{pt}F(p)\,\mathrm{d}p,$$

where L is defined as the line $\{p\colon \Re(p) = c\}$ in the complex plane, and c is chosen so that L lies to the right of all the singularities of $F(p)$.

A very recent variation on the theme has been proposed by Gautschi. In [29] he considers the construction of Kronrod type rules which provide exact answers for a mixture of rational functions and polynomials. These new formulas are called rational Gauss–Kronrod rules, whenever they exist. This idea has been developped in the context of quadrature problems involving functions that have poles outside the interval of integration which make less efficient the use of standard rules.

Since Padé approximants can be considered as formal Gaussian quadrature formulas, in [9,10] Brezinski has extended Kronrod's procedure to Padé approximation to obtain estimates of the error. In this particular application only the knowledge of the polynomials $P_n(x)$ and $E_{n+1}(x)$ is needed. Their zeros are of no use and it does not matter if they are all real or not.

For further extensions of Kronrod's idea see [43,44,68].

Finally, we recall that Ehrich in [22] has considered the construction of product integration rules for integrals containing a nonsmooth kernel, of the form

$$\int_{-1}^{1} k(x, y) f(x)\,\mathrm{d}x = \sum_{i=1}^{n} w_{1,i}(k) f(x_i) + \sum_{j=1}^{n+1} w_{2,j}(k) f(y_j) + R_{2n+1}^{K}(k; f).$$

These rules are obtained by interpolating $f(x)$ at the $2n+1$ nodes of (1.6). They have stability and convergence properties which are very similar to those of the corresponding product rules based on Clenshaw–Curtis abscissas.

In particular, Ehrich has proved that when $k \in L^p$ for some $p > 1$, then $R_{2n+1}^{K}(k; f)$ converges to zero for all Riemann-integrable functions f. Moreover,

$$\lim_{n\to\infty} \sum_{i=1}^{n} \big|w_{1,i}(k)\big| f(x_i) + \sum_{j=1}^{n+1} \big|w_{2,j}(k)\big| f(y_j) = \int_{-1}^{1} \big|k(x)\big| f(x)\,\mathrm{d}x$$

for all $f \in C[-1, 1]$. Uniform convergence is then proved when these rules are used to solve weakly singular integral equations of the second kind.

Acknowledgement

The author is grateful to Sven Ehrich and Dirk Laurie for reading a preliminary version of the paper and for their useful comments.

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