

## GAUSS-KRONROD QUADRATURE FORMULAE — A SURVEY OF FIFTY YEARS OF RESEARCH\*

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**Abstract.** Kronrod in 1964, trying to estimate economically the error of the  $n$ -point Gauss quadrature formula for the Legendre weight function, developed a new formula by adding to the  $n$  Gauss nodes  $n + 1$  new ones, which are determined, together with all weights, such that the new formula has maximum degree of exactness. It turns out that the new nodes are zeros of a polynomial orthogonal with respect to a variable-sign weight function, considered by Stieltjes in 1894, without though making any reference to quadrature. We survey the considerable research work that has been emerged on this subject, during the past fifty years, after Kronrod’s original idea.

**Key words.** Gauss quadrature formula, Gauss-Kronrod quadrature formula, Stieltjes polynomials

**AMS subject classifications.** 65D32, 33C45

**1. Introduction.** One of the most useful and widely used integration rules is the Gauss quadrature formula for the Legendre weight function  $w(t) = 1$  on  $[-1, 1]$ ,

$$(1.1) \quad \int_{-1}^1 f(t)dt = \sum_{\nu=1}^n \gamma_{\nu} f(\tau_{\nu}) + R_n^G(f),$$

where  $\tau_{\nu} = \tau_{\nu}^{(n)}$  are the zeros of the  $n$ th degree Legendre polynomial and  $\gamma_{\nu} = \gamma_{\nu}^{(n)}$  are the so-called Christoffel numbers. It is well known that formula (1.1) has precise degree of exactness  $d_n^G = 2n - 1$ , i.e.,  $R_n^G(f) = 0$  for all  $f \in \mathbb{P}_{2n-1}$ , where  $\mathbb{P}_{2n-1}$  denotes the space of polynomials of degree at most  $2n - 1$  (cf. [81]).

The error term of the Gauss formula has been extensively studied for more than a century and continues to be an active topic of research (cf. [81, Section 4]). Nevertheless, a simple error estimator is the following: Let  $Q_n^G = \sum_{\nu=1}^n \gamma_{\nu} f(\tau_{\nu})$ , and consider formula (1.1) with  $m$  points, where  $m > n$ . Then we write

$$(1.2) \quad |R_n^G(f)| \simeq |Q_n^G - Q_m^G|,$$

i.e.,  $Q_m^G$  plays the role of the “true” value of the integral  $\int_{-1}^1 f(t)dt$ . Although effective, a disadvantage of this method lies in the number of function evaluations in order to obtain an accurate assessment for  $R_n^G(f)$ . For example, if we take  $m = n + 1$ , then  $n + 1$  additional evaluations of the function (at the zeros of the  $(n + 1)$ st degree Legendre polynomial) raise the degree of exactness from  $d_n^G = 2n - 1$  to  $d_{n+1}^G = 2n + 1$  — a minor improvement. Furthermore, estimating  $R_n^G(f)$  by means of  $Q_n^G - Q_{n+1}^G$  could be unreliable (cf. [30, p. 199]).

Motivated probably from the latter, Kronrod introduced, in 1964 (cf. [119, 120]), what is now called the Gauss-Kronrod quadrature formula for the Legendre weight function,

$$(1.3) \quad \int_{-1}^1 f(t)dt = \sum_{\nu=1}^n \sigma_{\nu} f(\tau_{\nu}) + \sum_{\mu=1}^{n+1} \sigma_{\mu}^* f(\tau_{\mu}^*) + R_n^K(f),$$

where  $\tau_{\nu}$  are the Gauss nodes, while the new nodes  $\tau_{\mu}^* = \tau_{\mu}^{*(n)}$  and all weights  $\sigma_{\nu} = \sigma_{\nu}^{(n)}$ ,  $\sigma_{\mu}^* = \sigma_{\mu}^{*(n)}$  are chosen such that formula (1.3) has maximum degree of exactness (at least)

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$d_n^K = 3n + 1$ . The advantage of using  $Q_n^K = \sum_{\nu=1}^n \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*)$  instead of  $Q_{n+1}^G$  in (1.2) is rather obvious: With  $n + 1$  additional evaluations of the function (at the new nodes  $\tau_\mu^*$ ), the degree of exactness rises from  $d_n^G = 2n - 1$  to at least  $d_n^K = 3n + 1$  — a substantial improvement.

Kronrod computed the new formula for  $n$  up to 40 (cf. [120]) showing that in these cases the  $\tau_\mu^*$  are all in  $(-1, 1)$  and the  $\sigma_\nu, \sigma_\mu^*$  are all positive. For general  $n$ , clearly of paramount importance is the behavior of the polynomial having as zeros the  $\tau_\mu^*$ . Hence, denoting by  $\pi_n$  the  $n$ th degree (monic) Legendre polynomial, setting  $\pi_{n+1}^*(t) = \prod_{\mu=1}^{n+1} (t - \tau_\mu^*)$ , and applying a well-known result of Jacobi (cf. [105]), one can show that formula (1.3) has degree of exactness  $d_n^K = 3n + 1$  if

$$(1.4) \quad \int_{-1}^1 \pi_{n+1}^*(t) t^k \pi_n(t) dt = 0, \quad k = 0, 1, \dots, n$$

(cf. [82, Corollary]). Two things must be noted here. First, the polynomial  $\pi_{n+1}^*$  can be uniquely defined by means of (1.4). Furthermore, Equation (1.4) can be viewed as an orthogonality condition, i.e., the polynomial  $\pi_{n+1}^*$  is orthogonal to all polynomials of lower degree relative to the weight function  $w^*(t) = \pi_n(t)$  on  $[-1, 1]$ ; however, as this is a variable-sign weight function, the usual theory of orthogonal polynomials cannot be applied in this case.

Now, interestingly enough, the polynomial  $\pi_{n+1}^*$  had emerged in a different context some 70 years earlier. 1894 was the year that Stieltjes published his monumental work on continued fractions and the moment problem. Trying to extend his major theory to the case of oscillatory measures, in particular,  $d\mu(t) = P_n(t)dt$  on  $[-1, 1]$ , where  $P_n$  is the  $n$ th degree (non-monic) Legendre polynomial, by analyzing the Legendre function of the second kind, he came up with a polynomial that, apart from the leading coefficient, is precisely  $\pi_{n+1}^*$  (cf. [82, Section 1]). Stieltjes reported all this to Hermite in a letter dated November 8, 1894 (which was the last letter in a life-long correspondence with Hermite; see [3, v. 2, pp. 439–441]).

Stieltjes proceeded further conjecturing (a) that  $\pi_{n+1}^*$  has  $n + 1$  real and simple zeros, all contained in  $(-1, 1)$ , and (b) that these zeros separate those of  $\pi_n$ ; he even presented a numerical example for  $n = 4$  that verified his conjectures. Furthermore, he expressed the belief (apparently stronger in the case of reality and simplicity of zeros, and less so for the separation property) that this is a special case of “a much more general theorem”.

In his reply, on November 10, 1894 (see [3, v. 2, pp. 441–443]), Hermite was delighted with the new polynomial and the conjectured “beautiful properties”, and he suggested Stieltjes to look for a differential equation that could help proving them. As Stieltjes passed away at the end of that same year, he might have been too weak, by the time he got Hermite’s reply, in order to further pursue this matter. Hence, his conjectures remained unanswered for 40 years, until Szegő proved and even generalized them in 1935 (cf. [214]), without though following Hermite’s suggestion.

The connection between Gauss-Kronrod formulae and the polynomial  $\pi_{n+1}^*$ , now appropriately called Stieltjes polynomial, has first been pointed out by Mysovskih (cf. [153]) and independently, in the Western literature, by Barrucand (cf. [5]).

Previous reviews on the subject can be found, chronologically, in [150, 82, 160, 60, 151].

**2. Existence and nonexistence results.** Let  $d\sigma$  be a (nonnegative) measure on the interval  $[a, b]$ . If  $\sigma(t)$  is absolutely continuous, then  $d\sigma(t) = w(t)dt$  with  $w$  being a (nonnegative) weight function on  $[a, b]$ , and consider the Gauss quadrature formula associated with it,

$$(2.1) \quad \int_a^b f(t)w(t)dt = \sum_{\nu=1}^n \gamma_\nu f(\tau_\nu) + R_n^G(f),$$

where  $\tau_\nu = \tau_\nu^{(n)}$  are the zeros of the  $n$ th degree (monic) orthogonal polynomial  $\pi_n(\cdot) = \pi_n(\cdot; w)$  relative to the weight function  $w$  on  $[a, b]$ . It is well-known that the weights  $\gamma_\nu = \gamma_\nu^{(n)}$  are all positive, and formula (2.1) has precise degree of exactness  $d_n^G = 2n - 1$  (cf. [81]).

The Gauss-Kronrod quadrature formula, extending formula (2.1), has the form

$$(2.2) \quad \int_a^b f(t)w(t)dt = \sum_{\nu=1}^n \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*) + R_n^K(f),$$

where  $\tau_\nu$  are the Gauss nodes, while the new nodes  $\tau_\mu^* = \tau_\mu^{*(n)}$ , referred to as the Kronrod nodes, and all weights  $\sigma_\nu = \sigma_\nu^{(n)}$ ,  $\sigma_\mu^* = \sigma_\mu^{*(n)}$  are chosen such that formula (2.2) has maximum degree of exactness (at least)  $d_n^K = 3n + 1$ .

It should be noted that for formula (2.2) to improve on the degree of exactness of formula (2.1), i.e.,  $d_n^K > 2n - 1$ , the number of additional nodes  $\tau_\mu^*$  has to be at least  $n + 1$  (cf. [147, Introduction, in particular, Lemma 1]).

It turns out that the nodes  $\tau_\mu^*$  are zeros of a (monic) polynomial  $\pi_{n+1}^*(\cdot) = \pi_{n+1}^*(\cdot; w)$  satisfying the orthogonality condition

$$(2.3) \quad \int_a^b \pi_{n+1}^*(t)t^k \pi_n(t)w(t)dt = 0, \quad k = 0, 1, \dots, n,$$

i.e.,  $\pi_{n+1}^*$  is orthogonal to all polynomials of lower degree relative to the variable-sign weight function  $w^*(t) = \pi_n(t)w(t)$  on  $[a, b]$ . We call  $\pi_{n+1}^*$  the Stieltjes polynomial relative to the weight function  $w$  on  $[a, b]$ .

The weights of formula (2.2) are given by

$$(2.4) \quad \begin{aligned} \sigma_\nu &= \gamma_\nu + \frac{\|\pi_n\|^2}{\pi_n'(\tau_\nu)\pi_{n+1}^*(\tau_\nu)}, & \nu &= 1, 2, \dots, n, \\ \sigma_\mu^* &= \frac{\|\pi_n\|^2}{\pi_n(\tau_\mu^*)\pi_{n+1}^{*'}(\tau_\mu^*)}, & \mu &= 1, 2, \dots, n + 1, \end{aligned}$$

where  $\|\cdot\|$  is the  $L_2$ -norm for the weight function  $w$  on  $[a, b]$ . Furthermore, all  $\sigma_\mu^*$  are positive if and only if the nodes  $\tau_\nu$  and  $\tau_\mu^*$  interlace, i.e.,

$$\tau_{n+1}^* < \tau_n < \tau_n^* < \dots < \tau_2^* < \tau_1 < \tau_1^*$$

(cf. [144, Theorems 1 and 2]).

Of interest are the following properties of formula (2.2):

- (a) The nodes  $\tau_\nu$  and  $\tau_\mu^*$  interlace.
- (b) All nodes  $\tau_\nu, \tau_\mu^*$  are contained in  $(a, b)$ .
- (c) All weights  $\sigma_\nu, \sigma_\mu^*$  are positive.
- (d) All nodes  $\tau_\nu, \tau_\mu^*$ , without necessarily satisfying (a) and/or (b), are real.

Clearly, the validity of properties (a)–(d) depends on the behavior of the polynomial  $\pi_{n+1}^*$ , which is orthogonal relative to a variable-sign weight function, and therefore it does not follow the usual theory of orthogonal polynomials. So, whatever results are known have been derived for specific classical or nonclassical weight functions.

**2.1. Classical weight functions.** During the past 80 years, quite a bit has been unveiled for the polynomials  $\pi_{n+1}^*$  and the corresponding Gauss-Kronrod formulae for the Gegenbauer and the Jacobi weight functions.

**2.1.1. Gegenbauer weight function.** In 1935 (cf. [214]), Szegő turned his interest to Stieltjes's conjectures (see the introduction) for the Legendre weight function. He expanded the polynomial  $\pi_{n+1}^*$  into a Chebyshev series, and, using results from the theory of the reciprocal power series (cf. [115]), he showed that all the expansion coefficients are negative, except for the first one which is positive, and also that the sum of these coefficients is zero. That way he was able to conclude properties (a) and (b) for all  $n \geq 1$ . In 1978, Monegato, relying on Szegő's work, proved property (c) for all  $n \geq 1$  (cf. [145]).

Szegő's analysis was not peculiar only to the Legendre weight, but it was extended to the Gegenbauer weight function  $w_\lambda(t) = (1 - t^2)^{\lambda-1/2}$  on  $[-1, 1]$ ,  $\lambda > -1/2$ . He showed properties (a) and (b) for all  $n \geq 1$  when  $0 < \lambda \leq 2$  (cf. [214, §3]); for  $\lambda = 0$ , i.e., the Chebyshev weight of the first kind, see Section 2.1.3 below). Moreover, Monegato proved property (c) for all  $n \geq 1$  when  $0 \leq \lambda \leq 1$  (cf. [145]).

Unfortunately, Szegő was unable to determine what happens for  $\lambda > 2$ , while, when  $\lambda \leq 0$ , already for  $n = 2$ , two of the  $\tau_\mu^*$  are outside of  $(-1, 1)$ . This gap had been left unanswered until 1988, when Gautschi and Notaris tried to close it (cf. [90]). Their idea was, for a given  $n$ , to compute precise intervals  $(\lambda_n^p, \Lambda_n^p)$  of  $\lambda$  such that property (p) is valid, where  $p = a, b, c, d$ . This was done by varying  $\lambda$  and monitoring the motion of the nodes in formula (2.2), through the vanishing of the resultant of  $\pi_n^{(\lambda)}(\cdot) = \pi_n(\cdot; w_\lambda)$  and  $\pi_{n+1}^{*(\lambda)}(\cdot) = \pi_{n+1}^*(\cdot; w_\lambda)$  or the discriminant of  $\pi_{n+1}^{*(\lambda)}(\cdot)$  for properties (a) or (d), respectively, and more directly for properties (b) and (c). The project was undertaken analytically for  $n = 1(1)4$  and computationally for  $n = 5(1)20(4)40$ . The values of  $\lambda_n^p, \Lambda_n^p, p = a, b, c, d$ , are given in [90, Tables 2.1 and A.1].

Also, of interest are two nonexistence results. The first one by Monegato in 1979 (cf. [147, Theorem 1]), who proved that the Gauss-Kronrod formula for the weight function  $w_\lambda$ , having properties (c) and (d), and degree of exactness  $[2rn + l]$ , where  $r > 1$  and  $l$  is an integer, i.e.,  $d_n^K$  can be lower than  $3n + 1$ , does not exist for all  $n \geq 1$  when  $\lambda$  is sufficiently large.<sup>1</sup> The second nonexistence result was obtained by Notaris in 1991 (cf. [157, Section 2]). First, starting from a well-known limit formula that connects the Gegenbauer and the Hermite orthogonal polynomials (cf. [157, Equation (2.3)]), he showed that an analogous formula holds for the corresponding Stieltjes polynomials, in particular,

$$(2.5) \quad \lim_{\lambda \rightarrow \infty} \lambda^{(n+1)/2} \pi_{n+1}^{*(\lambda)}(\lambda^{-1/2}t) = \pi_{n+1}^{*H}(t), \quad n \geq 1,$$

where  $w^H(t) = e^{-t^2}$  on  $(-\infty, \infty)$  is the Hermite weight function and  $\pi_{n+1}^{*H}(\cdot) = \pi_{n+1}^*(\cdot; w^H)$ . Then, combining (2.5) with a nonexistence result of Kahaner and Monegato for the Hermite weight function (cf. [112, Corollary]), he proved that the Gauss-Kronrod formula for the weight function  $w_\lambda$  and  $n \neq 1, 2, 4$ , having properties (c) and (d), does not exist if  $\lambda > \lambda_n$ , where  $\lambda_n$  is a constant.

From all the results presented so far, it appears that, for  $n \neq 1, 2, 4$ , the intervals  $(\lambda_n^p, \Lambda_n^p)$ ,  $p = a, b, c, d$ , are finite. Two questions still remain open (cf. also [93]):

- (i) What is  $\lim_{n \rightarrow \infty} \Lambda_n^p$ , for  $p = a, b, c, d$ ?
- (ii) What about the validity of property (p),  $p = a, b, c, d$ , when  $-1/2 < \lambda < 0$ ?

An attempt to answer these questions was made by Peherstorfer, Petras, and de la Calle Ysern. The first two proved that property (d) cannot be true, i.e., the Gauss-Kronrod formula cannot exist, for  $\lambda > 3$  and  $n$  sufficiently large, while properties (a), (b), and (c) hold true for  $\lambda = 3$  and  $n$  sufficiently large (cf. [177, Theorems 1 and 2] and [179, Theorem]). Their proof is based on a new representation for the associated Stieltjes polynomials and the use of Bessel

<sup>1</sup>The proof contains an error, but it can be repaired (cf. [82, p. 53]).

functions. Furthermore, fairly recently, de la Calle Ysern and Peherstorfer showed that, for  $-1/2 < \lambda < 0$  and all  $n \geq 1$ , the zeros of  $\pi_{n+1}^{*(\lambda)}$  are real, simple, and, except for the smallest and the largest ones, lie inside  $(-1, 1)$ ; hence, property (b) is false, but properties (a), (d), and also (c) remain true (cf. [45, Theorem 2.1 and Corollary 2.2]). A key point in their proof is a result on the coefficients of the reciprocal power series analogous to that of Kaluza (cf. [115]) used by Szegő in [214]. It should also be noted that the two zeros of  $\pi_{n+1}^{*(\lambda)}$  lying outside of  $[-1, 1]$  approach the end of the interval as  $n$  increases (cf. [45, p. 772]), while, for  $\lambda = 0$ , i.e., for the Chebyshev weight function of the first kind, these two zeros become  $\pm 1$  for all  $n \geq 2$  (cf. Section 2.1.3 below). Moreover, two asymptotic representations of the respective Stieltjes polynomials, holding uniformly, the first one on the whole interval  $[-1, 1]$  and a second, sharper one, on compact subintervals of  $(-1, 1)$ , as well as an asymptotic representation of the Stieltjes polynomials in terms of Chebyshev polynomials of the first kind are given.

In addition to the previous existence and nonexistence results, some properties of the Gauss-Kronrod formulae for the Gegenbauer weight function  $w_\lambda$ ,  $0 \leq \lambda \leq 2$ , have been established by Ehrich. First, for  $0 \leq \lambda \leq 1$ , relying on Szegő's work in [214], he proved (cf. [54]) an asymptotic representation for the associated Stieltjes polynomials and their derivatives, which hold uniformly on compact subintervals of  $(-1, 1)$ . This was subsequently used to derive results for the distribution of the zeros of the Stieltjes polynomials as well as for the interlacing of the zeros of successive Stieltjes polynomials, thus proving conjectures of Monegato (cf. [147, p. 235] and [150, Section I.5]) and Peherstorfer (cf. [175, p. 186]). Furthermore, he obtained asymptotic representations for the weights and a precise asymptotic value for the variance of the Gauss-Kronrod formulae in question. If  $Q_n^K$  is the quadrature sum in (2.2), then the variance of the Gauss-Kronrod formula is defined by  $\text{Var}Q_n^K = \sum_{\nu=1}^n \sigma_\nu^2 + \sum_{\mu=1}^{n+1} (\sigma_\mu^*)^2$ . It is a measure of the sensitivity of  $Q_n^K$  to random errors, and in that sense it should be as small as possible (cf. [16, Chapter 9]). On the other hand, Ehrich extended in [55], for  $1 < \lambda \leq 2$ , most of his findings in [54], in particular, the asymptotic representation for the Stieltjes polynomials, the distribution of their zeros, and the asymptotic representation for the weights  $\sigma_\nu$  of the respective Gauss-Kronrod formulae. The latter allowed him to prove (cf. [55, Corollary 2.2]) that the weights  $\sigma_\nu$  corresponding to nodes in compact subintervals of  $(-1, 1)$  are positive for  $n$  sufficiently large, thus answering, partially, a question posed earlier by Monegato (cf. [150, p. 157]).

Finally, using Szegő's and Kaluza's results (cf. [214, 115]), Rabinowitz has shown (cf. [187]) that the Gauss-Kronrod formula for the Gegenbauer weight function  $w_\lambda$ ,  $0 < \lambda \leq 2$ ,  $\lambda \neq 1$ , has precise degree of exactness  $3n + 1$  for  $n$  even and  $3n + 2$  for  $n$  odd. When  $\lambda = 0$  or  $\lambda = 1$ , i.e., for the Chebyshev weight of the first or second kind, the degree of exactness grows like  $4n$  (cf. Section 2.1.3 below).

**2.1.2. Jacobi weight function.** With regard to the Jacobi weight function  $w^{(\alpha, \beta)}(t) = (1-t)^\alpha(1+t)^\beta$  on  $[-1, 1]$ ,  $\alpha > -1$ ,  $\beta > -1$ , the first results concern the special cases  $w^{(\alpha, 1/2)}$  and  $w^{(-1/2, \beta)}$  (the Chebyshev weights are discussed separately in Section 2.1.3 below). For the former, the associated orthogonal polynomials are given in terms of the respective polynomials for the weight  $w^{(\alpha, \alpha)}$  (cf. [215, Theorem 4.1]). Then, setting  $\pi_{n+1}^{*(\alpha, \beta)}(\cdot) = \pi_{n+1}^*(\cdot; w^{(\alpha, \beta)})$ , Monegato notes that

$$\pi_{n+1}^{*(\alpha, 1/2)}(2t^2 - 1) = 2^{n+1} \pi_{2n+2}^{*(\alpha, \alpha)}(t), \quad n \geq 1$$

(cf. [150, Equation (32)]). Hence, the Gauss-Kronrod formula for the weight function  $w^{(\alpha, 1/2)}$  can be expressed in terms of the corresponding formula for the weight  $w^{(\alpha, \alpha)}$  (cf. [90, Section 5.1]), which is of Gegenbauer type with  $\lambda = \alpha + 1/2$ , and therefore one can apply

the results of Section 2.1.1; in particular, in view of the conclusions in [177], the Gauss-Kronrod formula cannot exist for  $\alpha > 5/2$ ,  $\beta = 1/2$ , and  $n$  sufficiently large. On the other hand, for the weight function  $w^{(-1/2, \beta)}$ , Rabinowitz has shown that property (b) is false for  $-1/2 < \beta < 1/2$  when  $n$  is even and for  $1/2 < \beta \leq 3/2$  when  $n$  is odd (cf. [188, pp. 74–75]<sup>2</sup>). By symmetry (cf. [90, Equations (4.1) and (4.2)]), one can derive for the weight functions  $w^{(1/2, \beta)}$  and  $w^{(\alpha, -1/2)}$  results analogous to those obtained for the weights  $w^{(\alpha, 1/2)}$  and  $w^{(-1/2, \beta)}$ .

Gautschi and Notaris in [90] also considered the case of the Jacobi weight function. Using the same methods as for the Gegenbauer weight, they delineated, for a given  $n$ , areas in the  $(\alpha, \beta)$ -plane such that each of the properties (a), (b), and (c) (and also (d) when  $n = 1$ ) holds. Their findings, explicitly for  $n = 1$  and numerically for  $n = 2(1)10$ , are given in [90, p. 239 and Figure 4.1].

Also, a nonexistence result was obtained by Notaris (cf. [157, Section 3]). Starting from a well-known limit formula that connects the Jacobi and the Laguerre orthogonal polynomials (cf. [157, Equation (3.3)]), he derived an analogous formula for the corresponding Stieltjes polynomials,

$$(2.6) \quad \lim_{\beta \rightarrow \infty} (\beta/2)^{n+1} \pi_{n+1}^{*(\alpha, \beta)}(1 - 2\beta^{-1}t) = (-1)^{n+1} \pi_{n+1}^{*(\alpha)}(t), \quad n \geq 1,$$

where  $w^{(\alpha)}(t) = t^\alpha e^{-t}$  on  $(0, \infty)$ ,  $\alpha > -1$ , is the Laguerre weight function and  $\pi_{n+1}^{*(\alpha)}(\cdot) = \pi_{n+1}^*(\cdot; w^{(\alpha)})$ . Then, combining (2.6) with a nonexistence result of Kahaner and Monegato for the Laguerre weight function (cf. [112, Theorem]), he proved that the Gauss-Kronrod formula for the weight function  $w^{(\alpha, \beta)}$ ,  $\alpha$  fixed,  $-1 < \alpha \leq 1$ , and  $n \geq 23$  ( $n > 1$  when  $\alpha = 0$ ), having properties (c) and (d), does not exist if  $\beta > \beta_{\alpha, n}$ , where  $\beta_{\alpha, n}$  is a constant.

All the previous results led Peherstorfer and Petras to examine the Gauss-Kronrod formula for the Jacobi weight function more closely (cf. [178]). First of all, for  $0 \leq \alpha, \beta < 5/2$ , they showed that on compact subintervals of  $(-1, 1)$  the associated Stieltjes polynomials and their derivatives are asymptotically equal to certain Jacobi polynomials. That way they obtained asymptotic representations for the weights of the respective Gauss-Kronrod formulae corresponding to nodes in compact subintervals of  $(-1, 1)$ , and they proved that these weights are positive for  $n$  sufficiently large. Finally, they concluded that property (d) cannot be true, i.e., the Gauss-Kronrod formula does not exist, when  $\min(\alpha, \beta) \geq 0$  and  $\max(\alpha, \beta) > 5/2$  and  $n$  is sufficiently large, which is a more precise version of what had been proved earlier by Notaris in [157].

In 1961, Davis and Rabinowitz (cf. [41]) formulated the so-called “circle theorem” for the Gauss and the Gauss-Lobatto quadrature formulae with respect to the Jacobi weight function. They showed that the Gaussian weights, suitably normalized and plotted against the Gaussian nodes, lie asymptotically for large orders on the upper half of the unit circle centered at the origin. For a much more restricted class of Jacobi weights, Gautschi proved the circle theorem for the Gauss-Kronrod formula (cf. [87]).

**2.1.3. Chebyshev weight functions.** A particular mention should be made about the four Chebyshev weights, which are special cases of the Jacobi weight function with  $|\alpha| = |\beta| = 1/2$ , as for each one of them the corresponding Gauss-Kronrod formula has a special form with explicitly known nodes and weights. More specifically, for  $\alpha = \beta = -1/2$ , i.e., the Chebyshev weight of the first kind, the Gauss-Kronrod formula is the 3-point Gauss

<sup>2</sup>The superscript  $\mu + 1/2$  twice in Equation (68) and twice on line 11 should read  $\mu - 1/2$  (cf. [188, second erratum]).

formula when  $n = 1$  and the  $(2n + 1)$ -point Gauss-Lobatto formula when  $n \geq 2$  for the same weight; in the latter case,  $\tau_1^* = 1$  and  $\tau_{n+1}^* = -1$ . For  $\alpha = \beta = 1/2$ , i.e., the Chebyshev weight of the second kind, the Gauss-Kronrod formula is the  $(2n + 1)$ -point Gauss formula for that weight. Finally, for  $\alpha = \mp 1/2$ ,  $\beta = \pm 1/2$ , i.e., the Chebyshev weight of the third or fourth kind, the Gauss-Kronrod formula is the  $(2n + 1)$ -point Gauss-Radau formula for the same weight, with additional node at 1 or  $-1$ , respectively. As a result, these formulae have elevated degree of exactness, in particular, 5 for  $n = 1$  and  $4n - 1$  for  $n \geq 2$  when  $\alpha = \beta = -1/2$ ,  $4n + 1$  when  $\alpha = \beta = 1/2$ , and  $4n$  when  $\alpha = \mp 1/2$ ,  $\beta = \pm 1/2$  (cf. [153], [144, Section 4], and [150, pp. 152–153]). Moreover, Monegato noted (cf. [144, Section 4]) that in the cases  $\alpha = \beta = \pm 1/2$  the idea of Kronrod can be iterated, producing a sequence of quadrature formulae with explicitly known nodes and weights.

**2.1.4. Hermite and Laguerre weight functions.** Very little has been proved for the Gauss-Kronrod formula relative to each of these two weights, probably because an early numerical investigation for up to  $n = 20$  led to negative results; in particular, property (d) is true for the Hermite weight function  $w^H$  only for  $n = 1, 2, 4$  and for the Laguerre weight  $w^{(0)}$  only for  $n = 1$  (although one of the nodes is negative) (cf. [195] and [144, Section 3]).

Nonetheless, Kahaner and Monegato obtained some nonexistence results (cf. [112, Theorem and Corollary]). They proved that the Gauss-Kronrod formula for the weight function  $w^{(\alpha)}$ ,  $-1 < \alpha \leq 1$ , having properties (c) and (d), does not exist if  $n \geq 23$  ( $n > 1$  when  $\alpha = 0$ ). Subsequently, they concluded that the corresponding formula for the Hermite weight function  $w^H$ , having properties (c) and (d), does not exist if  $n \neq 1, 2, 4$ .<sup>3</sup> The nonexistence result for the Laguerre weight remains true for  $n$  sufficiently large even if the degree of exactness is lowered to  $[2rn + l]$ , where  $r > 1$  and  $l$  is an integer (cf. [147, Theorem 2]).

**2.2. Nonclassical weight functions.** During the past 25 years, quite a bit of progress has been made regarding the Stieltjes polynomials and the corresponding Gauss-Kronrod formulae for a variety of nonclassical weights.

**2.2.1. Bernstein-Szegö weight functions.** These weight functions have been studied by several authors. They are defined by

$$(2.7) \quad \begin{aligned} w^{(\pm 1/2)}(t) &= \frac{(1 - t^2)^{\pm 1/2}}{\rho(t)}, & -1 < t < 1, \\ w^{(\pm 1/2, \mp 1/2)}(t) &= \frac{(1 - t)^{\pm 1/2}(1 + t)^{\mp 1/2}}{\rho(t)}, & -1 < t < 1, \end{aligned}$$

where  $\rho$  is an arbitrary polynomial that remains positive on  $[-1, 1]$ . The associated orthogonal and Stieltjes polynomials are linear combinations of Chebyshev polynomials of the four kinds, and this allows examining the validity of properties (a), (b), and (c). Furthermore, the corresponding Gauss-Kronrod formulae have elevated degree of exactness.

Already in 1930, the weight  $w^{(1/2)}$ , with  $\rho(t) = 1 - \frac{4\gamma}{(1+\gamma)^2}t^2$ ,  $-1 < \gamma \leq 1$ , on  $[-1, 1]$ , appeared in work of Geronimus (cf. [99] and [150, Section I.2]). For this weight, property (b) has been proved by Monegato (cf. [150, p. 146]) and properties (a) and (c), with quadrature weights representable by semiexplicit formulae, by Gautschi and Rivlin (cf. [95]), for all  $n \geq 1$ . (Property (b), for  $n = 1$ , is not shown in [150, p. 146], but it can easily be verified.) Furthermore, the degree of exactness of the quadrature formulae in question has been precisely determined and found to grow like  $4n$  rather than the usual  $3n + 1$  (cf. [150, p. 146]).

<sup>3</sup>The nonexistence result is stated in [112, Corollary] as following: “Extended Gauss-Hermite rules with positive weights (and real nodes) only exist for  $n = 1, 2, 4$ ”. This is not quite accurate, as for  $n = 4$  two of the  $\sigma_\nu$ 's in (2.2) relative to  $w^H$  are negative.

Monegato and Palamara Orsi, motivated by the work of Geronimus, have computed explicitly the orthogonal and Stieltjes polynomials for the weight  $w^{(1/2)}$  when  $\rho$  is an arbitrary quadratic polynomial (cf. [152]). All four weights  $w^{(\pm 1/2)}$ ,  $w^{(\pm 1/2, \mp 1/2)}$ , with  $\rho$  being an arbitrary quadratic polynomial, have been considered by Gautschi and Notaris (cf. [92]). They have computed explicitly the orthogonal and Stieltjes polynomials and have established properties (a), (b) (on the closed interval  $[-1, 1]$ ), and (c), with quadrature weights representable by semiexplicit formulae, for almost all  $n$ , with the exceptions in the case  $n \leq 3$  being carefully identified. Furthermore, the degree of exactness of the quadrature formulae in question has been precisely determined and found to grow like  $4n$  rather than the usual  $3n + 1$ . At the end of [92], the results are specialized to weight functions (2.7) in which the divisor polynomial is linear rather than quadratic.

The general case of the weights  $w^{(\pm 1/2)}$ ,  $w^{(\pm 1/2, \mp 1/2)}$ , with  $\rho$  an arbitrary polynomial of degree  $l$ , has been treated by Notaris (cf. [156]). He computed explicitly the respective orthogonal and Stieltjes polynomials and showed that properties (a), (b) (on the closed interval  $[-1, 1]$ ), and (c) hold for all  $n \geq l + 2$  if  $w = w^{(-1/2)}$ , for all  $n \geq l$  if  $w = w^{(1/2)}$ , and for all  $n \geq l + 1$  if  $w = w^{(\pm 1/2, \mp 1/2)}$ ; while, the corresponding degrees of exactness are  $4n - l - 1$ ,  $4n - l + 1$ , and  $4n - l$ . On the other hand, Peherstorfer, as part of a more general result, proved that Kronrod's idea can be iterated for the weight  $w^{(1/2)}$  (cf. [173]). If  $N^* \in \mathbb{N}$  satisfies  $2^{N^*-1}(n+1) \geq 2^{N^*}l + 1 - l$ , then he showed that the Gauss formula (2.1) with  $w = w^{(1/2)}$  admits  $N^*$  Kronrod extensions, all having properties (b) and (c). Furthermore, the Kronrod nodes of the  $N$ th extension interlace with those of the  $(N - 1)$ st Kronrod extension, which in a way implies property (a), and the  $N$ th Kronrod extension has degree of exactness  $2^N[2(n+1) - l] + l - 3$ ,  $N = 1, 2, \dots, N^*$ .<sup>4</sup>

**2.2.2. Various weight functions.** In [174], Peherstorfer extended his work in [173], by considering weight functions of the form  $w(t) = (1 - t^2)^{1/2} |D(e^{i\theta})|^2$ ,  $t = \cos \theta$ ,  $\theta \in [0, \pi]$ , where  $D(z)$  is analytic,  $D(z) \neq 0$  for  $|z| \leq 1$ , and  $D$  takes on real values for real  $z$ . By analyzing the asymptotic behavior of the associated functions of the second kind, and using their connection with Stieltjes polynomials, he showed that the corresponding Gauss-Kronrod formula has properties (a), (b), and (c) for  $n \geq n_0$ ,  $n_0$  sufficiently large. Clearly, the weight function in consideration includes as a special case the Bernstein-Szegő weight  $w^{(1/2)}$ , examined by the author in [173], except that the constant  $n_0 = l$  obtained in [173] cannot be derived by the general approach of [174].

Moreover, in [175], Peherstorfer went a step further by considering orthogonal polynomials on the unit circle and studying the asymptotic behavior of the associated functions of the second kind, paying particular attention to the interval  $[-1, 1]$ . Subsequently, using the connection between functions of the second kind and Stieltjes polynomials, he showed that if a weight function  $w$  on  $[-1, 1]$  satisfies  $\sqrt{1 - t^2}w(t) > 0$  for  $-1 \leq t \leq 1$  and  $\sqrt{1 - t^2}w(t) \in C^2[-1, 1]$ , then the Stieltjes polynomial  $\pi_{n+1}^*(\cdot; w^*)$ , where  $w^*(t) = (1 - t^2)w(t)$ , is asymptotically equal to  $\pi_{n+1}(\cdot; w)$ .<sup>5</sup> In addition, he proved that the Gauss-Kronrod formula for the weight function  $w^*$  has properties (a), (b), and (c) for  $n$  sufficiently large.<sup>6</sup> Moreover, several interlacing properties were established for sufficiently large  $n$ , among which the interlacing property for the zeros of two consecutive Stieltjes polynomials.

For the weight function  $\gamma w^{(\alpha)}(t) = |t|^\gamma (1 - t^2)^\alpha$  on  $(-1, 1)$ ,  $\alpha > -1$ ,  $\gamma > -1$ , Gautschi and Notaris have shown in [90, Subsection 5.2] that the corresponding Gauss-Kronrod formula with  $n$  odd can be expressed in terms of the respective formula for the Jacobi

<sup>4</sup>In [173, Theorem (c)], the 4 in the subscript of the displayed inclusion relation should be replaced by 3.

<sup>5</sup>Theorem 4.1(b) in [175] is incorrect, and it has to be replaced by Corollary 12 in [176] (cf. [176, Remark 13]).

<sup>6</sup>In [175, Theorem 4.2(a)], the subscript  $\mu$  extends up to  $n + 1$ .

weight  $w^{(\alpha, (1+\gamma)/2)}$ . Hence, whatever results are known for the latter can be applied to arrive at conclusions for the former.

Finally, numerical experiments of Calì, Gautschi, and Marchetti in [22, Examples 5.2 and 5.3] indicate that the Gauss-Kronrod formulae for the weight functions  $w(t) = t^\alpha \ln(1/t)$  on  $[0, 1]$ ,  $\alpha = 0, \pm 1/2$ , have properties (a), (b), and (c) for all  $n \geq 1$ , except for the weight with  $\alpha = -1/2$  and  $n$  odd, for which property (b) (but not also (d)) appears to be false ( $\pi_{n+1}^*$  has exactly one negative zero). However, nothing has been proved yet.

**2.3. Miscellaneous measures.** We now consider the Gauss-Kronrod formula relative to a (nonnegative) measure  $d\sigma$  on the interval  $[a, b]$ ,

$$\int_a^b f(t) d\sigma(t) = \sum_{\nu=1}^n \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*) + R_n^K(f),$$

defined the same way as formula (2.2).

**2.3.1. Measures with constant recurrence coefficients.** Consider a (nonnegative) measure  $d\sigma$  with support on the interval  $[a, b]$ , such that the respective (monic) orthogonal polynomials  $\pi_n(\cdot) = \pi_n(\cdot; d\sigma)$  satisfy a three-term recurrence relation

$$(2.8) \quad \begin{aligned} \pi_{n+1}(t) &= (t - \alpha_n)\pi_n(t) - \beta_n\pi_{n-1}(t), & n = 0, 1, 2, \dots, \\ \alpha_n &= \alpha, \quad \beta_n = \beta & \text{for all } n \geq l, \end{aligned}$$

where  $\alpha_n \in \mathbb{R}$ ,  $\beta_n > 0$ ,  $l \in \mathbb{N}$ , and  $\pi_0(t) = 1$ ,  $\pi_{-1}(t) = 0$ . Thus, the coefficients  $\alpha_n$  and  $\beta_n$  are constant equal, respectively, to some  $\alpha \in \mathbb{R}$  and  $\beta > 0$  for all  $n \geq l$ . Among the many orthogonal polynomials satisfying a recurrence relation of this kind we mention the four Chebyshev-type polynomials and their modifications discussed in Allaway's thesis (cf. [1, Chapter 4]) as well as the Bernstein-Szegő polynomials.

For measures satisfying (2.8), Gautschi and Notaris obtained in [94] for the respective Stieltjes polynomials  $\pi_{n+1}^*(\cdot) = \pi_{n+1}^*(\cdot; d\sigma)$  the following simple and useful representation

$$(2.9) \quad \pi_{n+1}^*(t) = \pi_{n+1}(t) - \beta\pi_{n-1}(t) \quad \text{for all } n \geq 2l - 1.$$

A key point in the proof of (2.9) is the expansion of  $t^k\pi_n(t)$  for  $k = 0, 1, \dots, n$  in terms of the  $\pi_m$ 's and the study of the relations between the expansion coefficients. Subsequently, (2.9) was used to show that the corresponding Gauss-Kronrod formula has properties (a), (b) (on the closed interval  $[a, b]$  under an additional assumption on  $d\sigma$ ), and (c) for all  $n \geq 2l - 1$ , while its degree of exactness is at least  $4n - 2l + 2$  if  $n \geq 2l - 1$ . Moreover, it is proved that the interpolatory quadrature formula based on the zeros of  $\pi_{n+1}^*$  only has positive weights and degree of exactness  $2n - 1$  for all  $n \geq 2l - 1$ , verifying that way a conjecture posed earlier by Monegato for the Legendre weight function (cf. [150, Section II.1]).

**2.3.2. Measures induced by a given orthogonal polynomial.** Stieltjes polynomials and Gauss-Kronrod formulae for a different kind of measures were investigated by Notaris (cf. [161]). Given a positive measure  $d\sigma$  on the interval  $[a, b]$ , a fixed  $n \geq 1$ , and  $\pi_n(\cdot) = \pi_n(\cdot; d\sigma)$ , one can define the nonnegative measure  $d\hat{\sigma}_n(t) = \pi_n^2(t)d\sigma(t)$  on  $[a, b]$ . The coefficients in the three-term recurrence relation of the respective (monic) orthogonal polynomials  $\hat{\pi}_{m,n}(\cdot) = \pi_m(\cdot; d\hat{\sigma}_n)$ ,  $m = 0, 1, 2, \dots$ , when  $d\sigma$  is a Chebyshev measure of any one of the four kinds, have been obtained analytically in closed form by Gautschi and Li (cf. [89]). In [161], Notaris gave explicit formulae for the Stieltjes polynomials  $\hat{\pi}_{n+1,n}^*(\cdot) = \pi_{n+1}^*(\cdot; d\hat{\sigma}_n)$  when  $d\sigma$  is any one of the four Chebyshev measures. In addition, he showed that the corresponding Gauss-Kronrod formulae for each of these  $d\hat{\sigma}_n$ , based on

the zeros of  $\hat{\pi}_{n,n}$  and  $\hat{\pi}_{n+1,n}^*$ , have properties (a), (b), and (c), with two noted exceptions: When  $d\sigma$  is the Chebyshev measure of the first kind, then  $\tau_{1,n}^* = 1$  and  $\tau_{n+1,n}^* = -1$ ; and when  $d\sigma$  is the Chebyshev measure of the third or fourth kind and  $n$  is even, then  $\tau_{1,n}^* > 1$  and  $\tau_{n+1,n}^* < -1$ , respectively, although  $\tau_{1,n}^*$  and  $\tau_{n+1,n}^*$  approach 1 and  $-1$  as  $n$  increases. Furthermore, the precise degree of exactness of the quadrature formulae in question has been determined, and, when  $d\sigma$  is the Chebyshev measure of the first kind, it was found to grow like  $4n$  rather than the usual  $3n + 1$ .

**2.4. Gauss-Kronrod formulae of Chebyshev type.** An  $n$ -point quadrature formula relative to the positive measure  $d\sigma$  on the interval  $(a, b)$  with equal weights is called a Chebyshev quadrature formula if all its nodes are real and the formula has degree of exactness (at least)  $n$ . It is well known that the only Gauss formula that is also a Chebyshev formula is the one relative to the Chebyshev measure of the first kind  $d\sigma(t) = (1 - t^2)^{-1/2} dt$  on  $(-1, 1)$  (see, e.g., [80, Section 4]). Notaris (cf. [158]), using the method of Geronimus (cf. [100]), proved that there is no positive measure  $d\sigma$  on the interval  $(a, b)$  such that the corresponding Gauss-Kronrod formula is also a Chebyshev formula. The same is true for measures of the form  $d\sigma(t) = \omega(t)dt$ , where  $\omega$  is even with symmetric support, and the Gauss-Kronrod formula is required to have equal weights only for  $n$  even. Furthermore, it was shown that the only positive and even measure  $d\sigma$  on  $(-1, 1)$ , for which the Gauss-Kronrod formula has all weights equal if  $n = 1$  and is almost of Chebyshev type

$$\int_{-1}^1 f(t)d\sigma(t) = w \sum_{\nu=1}^n f(\tau_\nu) + w_1 f(1) + w \sum_{\mu=2}^n f(\tau_\mu^*) + w_1 f(-1) + R_n^K(f) \quad \text{for all } n \geq 2,$$

is the Chebyshev measure of the first kind.

An extension of the results in [158] was given by Förster in [78, Corollary 2].

**3. Error term.** The Gauss-Kronrod formula (2.2) can be obtained by a Markov type argument (cf. [135]): Interpolate the function  $f$  at the Gauss nodes  $\tau_\nu$  and the double Stieltjes nodes  $\tau_\mu^*$ , integrate the derived Hermite interpolation polynomial  $p_{3n+1}(\cdot; f; \tau_\nu, \tau_\mu^*, \tau_\mu^*)$  of degree at most  $3n + 1$ , and then require that in the resulting quadrature formula the weights corresponding to the values  $f'(\tau_\mu^*)$  are all 0. This requirement will yield formula (2.2), under the assumption that the Stieltjes polynomial  $\pi_{n+1}^*$  satisfies the orthogonality condition (2.3).

Integrating the interpolation error, we get, as a by-product, an expression for the error term of formula (2.2),

$$(3.1) \quad R_n^K(f) = \frac{1}{(3n+2)!} \int_a^b \pi_n(t) [\pi_{n+1}^*(t)]^2 f^{(3n+2)}(\xi(t)) w(t) dt, \quad a < \xi(t) < b,$$

assuming that  $f \in C^{3n+2}[a, b]$ . Obviously, if formula (2.2) has degree of exactness higher than  $3n + 1$ , then (3.1) has to be modified accordingly.

The convergence theory for Gauss-Kronrod formulae is particularly simple if the interval of integration  $[a, b]$  is finite. By the well-known result of Pólya (cf. [185]) and Steklov (cf. [212]), formula (2.2) converges,

$$\lim_{n \rightarrow \infty} R_n^K(f) = 0, \quad f \in C[a, b],$$

i.e., the quadrature sum on the right-hand side of (2.2) converges to the integral on the left as  $n \rightarrow \infty$ , precisely if

$$\sum_{\nu=1}^n |\sigma_\nu| + \sum_{\mu=1}^{n+1} |\sigma_\mu^*| \leq K \quad \text{for all } n = 1, 2, \dots,$$

where  $K > 0$  is a constant not depending on  $n$  (cf. [215, Theorem 15.2.1]). In fact, by the result of Steklov (cf. [212]) and Fejér (cf. [76]), the convergence is immediate for those weight functions  $w$  for which the  $\sigma_\nu$  and the  $\sigma_\mu^*$  are all positive, as in this case

$$\sum_{\nu=1}^n |\sigma_\nu| + \sum_{\mu=1}^{n+1} |\sigma_\mu^*| = \sum_{\nu=1}^n \sigma_\nu + \sum_{\mu=1}^{n+1} \sigma_\mu^* = \int_a^b w(t) dt$$

(cf. [215, Theorem 15.2.2]). The sum of the absolute values of the quadrature weights is known as the absolute condition number of a quadrature formula. The connection between the convergence of a quadrature formula and its absolute condition number is reviewed for several interpolatory formulae, among which the Gauss-Kronrod formula, by Cuomo and Galletti (cf. [34]).

**3.1. Early results.** The first error estimate for the Gauss-Kronrod formula relative to the Gegenbauer weight function  $w_\lambda$ ,  $0 < \lambda < 1$ , was given by Monegato in [146, Section 3]. Applying (3.1), using a bound for  $|\pi_{n+1}^{*(\lambda)}(t)|$ , which follows directly from Szegő's work in [214], and bounds for  $|\pi_n^{(\lambda)}(t)|$  (cf. [215, Equations (4.7.9) and (7.33.1)]), and taking into account that the formula has degree of exactness  $d = 3n + 1 + k$  where  $k = 0$  for  $n$  even and  $k = 1$  for  $n$  odd, he obtained

$$(3.2) \quad |R_n^K(f)| \leq c_{3n+2+k}^{(\lambda)}(R_n^K) \max_{-1 \leq t \leq 1} |f^{(3n+2+k)}(t)|,$$

with

$$c_{3n+2+k}^{(\lambda)}(R_n^K) \leq C^{(\lambda)} \frac{2^{-3n} n^\lambda}{(3n + 2 + k)!},$$

where  $C^{(\lambda)}$  is an explicit constant independent of  $n$ .

This bound, using again Szegő's results in [214], was slightly improved and extended to the case  $1 < \lambda < 2$  by Rabinowitz in [187, Section 4].

Furthermore, Rabinowitz showed in [190] that the Gauss-Kronrod formula for the Gegenbauer weight function  $w_\lambda$ ,  $0 < \lambda < 1$ , and  $n \geq 2$ , is nondefinite, i.e., its error term cannot be written in the form

$$R_n^K(f) = \bar{c}_{3n+2+k}^{(\lambda)}(R_n^K) f^{(3n+2+k)}(\xi_{3n+2+k}), \quad -1 < \xi_{3n+2+k} < 1$$

(cf. (3.4) below).

**3.2. Peano kernel error bounds.** If the error functional  $R_n$  of a quadrature formula over the interval  $[a, b]$  satisfies  $R_n(p) = 0$  for all  $p \in \mathbb{P}_{s-1}$  and  $f$  has a piecewise continuous derivative of order  $s$  on  $[a, b]$  (or, less restrictively,  $f^{(s-1)}$  is absolutely continuous on  $[a, b]$ ), then

$$(3.3) \quad R_n(f) = \int_a^b K_s(t) f^{(s)}(t) dt,$$

where

$$K_s(t) = R_n \left[ \frac{(\cdot - t)_+^{s-1}}{(s-1)!} \right]$$

is the  $s$ -th Peano kernel of  $R_n$ , with the plus sign on the right-hand side indicating that the function on which it acts is to be equal to zero if the argument is negative. If  $K_s$  does not change sign on  $[a, b]$ , then

$$(3.4) \quad R_n(f) = \bar{c}_s(R_n) f^{(s)}(\xi_s), \quad \bar{c}_s(R_n) = \int_a^b K_s(t) dt = R_n\left(\frac{t^s}{s!}\right), \quad a < \xi_s < b,$$

in which case the quadrature formula is called definite, in particular, positive definite if  $K_s \geq 0$  and negative definite if  $K_s \leq 0$ .

Obviously, a quadrature formula having precise degree of exactness  $d$  generates exactly  $d + 1$  Peano kernels  $K_1, K_2, \dots, K_{d+1}$ . Then, from (3.3), we derive

$$(3.5) \quad |R_n(f)| \leq c_s(R_n) \max_{a \leq t \leq b} |f^{(s)}(t)|,$$

where

$$(3.6) \quad c_s(R_n) = \int_a^b |K_s(t)| dt, \quad s = 1, 2, \dots, d + 1,$$

are the so-called Peano constants of  $R_n$  (cf. [81, Section 4.2]). Clearly, Monegato's bound (3.2) is of the type (3.5).

For the Gauss-Kronrod formula relative to the Legendre weight function (which is a special case of the Gegenbauer weight with  $\lambda = 1/2$ ), Brass and Förster (cf. [15, Section 5]), using expansions of Chebyshev polynomials of the first kind, obtained an estimate of the form (3.5) with

$$c_{3n+2+k}^{(1/2)}(R_n^K) \leq \bar{C}^{(1/2)} \frac{2^{-3n}}{(3n+2+k)!},$$

where  $\bar{C}^{(1/2)}$  is an explicit constant independent of  $n$ , thus improving Monegato's bound by a factor of  $O(n^{-1/2})$ .

A further improvement in the case of the Gauss-Kronrod formula for the Legendre weight was made by Ehrich in [51], who, using results of Szegő in [214] and Rabinowitz in [187], obtained both upper and lower bounds for  $c_{3n+2+k}^{(1/2)}(R_n^K)$ ,  $n \geq 4$ ,

$$C_1^{(1/2)} \frac{2^{-3n} n^{-11/2}}{(3n+2+k)!} \leq c_{3n+2+k}^{(1/2)}(R_n^K) \leq C_2^{(1/2)} \frac{2^{-3n} n^{-1/2}}{(3n+2+k)!},$$

where  $C_1^{(1/2)}$  and  $C_2^{(1/2)}$  are explicit constants independent of  $n$ . The latter estimate raises the question of the precise order of  $c_{3n+2+k}^{(1/2)}(R_n^K)$ . This was answered by Ehrich in [57], who computed the error of the quadrature formula in question at the Chebyshev polynomials of the first kind and then used it to show that

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

where  $a_n \sim b_n$  if  $\lim_{n \rightarrow \infty} (|a_n|/|b_n|) = C$ ,  $C > 0$  a constant.

Ehrich extended his investigations to the Gauss-Kronrod formula for the Gegenbauer weight function  $w_\lambda$ ,  $0 < \lambda < 1$  (cf. [51, Section 3] and [49, Section 3]). Using results from [15, 187, 214], he obtained

$$C_1^{(\lambda)} \frac{2^{-3n} n^{-(3+\lambda+1/\lambda)}}{(3n+2+k)!} \leq c_{3n+2+k}^{(\lambda)}(R_n^K) \leq C_2^{(\lambda)} \frac{2^{-3n} n^{-\lambda}}{(3n+2+k)!},$$

where the lower bound holds for  $n \geq 5$  and  $C_1^{(\lambda)}$  and  $C_2^{(\lambda)}$  are explicit constants independent of  $n$ .

Error constants (3.6) of lower order are studied in [49, Section 2]. In the case of the Gauss-Kronrod formula for the Legendre weight, Ehrich derived upper and lower bounds for  $c_{3n+2+k-s}^{(1/2)}(R_n^K)$ , where  $s = s(n) < 3n + 2 + k$  is chosen such that  $\lim_{n \rightarrow \infty} \frac{3n+2+k-s}{n} = A$ ,  $A > 0$ ; for constant  $s$ , see [49, Section 2] and [57, Theorem 2]. His investigations were extended to the Gauss-Kronrod formula for the Gegenbauer weight in [51, Section 3].

Finally, a Peano stopping functional for the Gauss-Kronrod formula relative to the Legendre weight function is given by Ehrich (cf. [58]). For definitions and descriptions of Peano stopping functionals and stopping functionals in general, including those for Gauss-Kronrod formulae and Patterson extensions, see [77] and [61], respectively.

**3.3. Error bounds for analytic functions.** There are two approaches for estimating the error term  $R_n^K(f)$  in (2.2) when  $f$  is a holomorphic function, either by contour integration techniques or by Hilbert space methods, although the results are often comparable or even identical.

**3.3.1. Bounds based on contour integration.** Let  $f$  be an analytic function in a simply connected region containing a closed contour  $C$  in its interior which surrounds the interval  $[-1, 1]$ . For the error term of the Gauss-Kronrod formula for the Legendre weight function, Ehrich in [52], using the results in [51], obtained

$$(3.7) \quad |R_n^K(f)| \leq \left\{ \frac{17}{10\sqrt{3n-3(2+k)}} + \frac{4\sqrt{2}}{\sqrt{(6n+3+k)(6n+5+2k)}} \right\} \frac{L(C) \max_{z \in C} |f(z)|}{\pi 2^{3n+2+k} \delta^{3n+3+k}},$$

where  $\delta > 0$  is a lower bound for the distance of any point on  $C$  to any point in  $[-1, 1]$ . The bound (3.7) takes on a special form when  $C$  is a circle or an ellipse centered at the origin. In addition, the behavior of  $R_n^K$  for Chebyshev polynomials of the first or second kind is analyzed.

Moreover, Bello Hernández, de la Calle Ysern, Guadalupe Hernández, and López Lagomasino studied in [11], for general measures, among which the so-called regular, Blumenthal-Nevai, and Szegő classes of measures, the asymptotic behavior of the Stieltjes polynomials outside of the support of the measure. This allowed them to estimate the rate of convergence of Gauss-Kronrod formulae based on interpolating rational functions with prescribed poles, referred to as rational Gauss-Kronrod formulae, when  $f$  is an analytic function in a neighborhood of the support of the measure. All this was further generalized in [10]; special cases of the measures studied in [10] are those considered in [156, 173].

**3.3.2. Bounds based on Hilbert space norms.** The idea of using Hilbert space techniques to estimate the error functional  $R_n(f)$  of a quadrature formula can be traced back to Davis in 1953 (cf. [40]). The particular method presented here was introduced by Hämmerlin (cf. [102]) to estimate the error of the Gauss formula for the Legendre weight function. If  $f$  is a holomorphic function in the disk  $C_r = \{z \in \mathbb{C} : |z| < r\}$ ,  $r > 1$ , then it can be written in the form  $f(z) = \sum_{k=0}^{\infty} a_k z^k$ ,  $z \in C_r$ . Define

$$|f|_r = \sup \{ |a_k| r^k : k \in \mathbb{N}_0 \text{ and } R_n^K(t^k) \neq 0 \},$$

which is a seminorm in the space  $X_r = \{f : f \text{ holomorphic in } C_r \text{ and } |f|_r < \infty\}$ . Then the error term  $R_n^K(f)$  in (2.2) is a continuous, and therefore bounded, linear functional in  $(X_r, |\cdot|_r)$ , and its norm is given by

$$(3.8) \quad \|R_n^K\| = \sum_{k=0}^{\infty} \frac{|R_n^K(t^k)|}{r^k}.$$

The norm leads to bounds for the error functional itself; if  $f \in X_R$ , then

$$(3.9) \quad |R_n^K(f)| \leq \inf_{1 < r \leq R} (\|R_n^K\| |f|_r),$$

while another bound can be derived if  $|f|_r$  is estimated by  $\max_{|z|=r} |f(z)|$  (cf. [163, Section 2]).

For the error term of the Gauss-Kronrod formula for the Legendre weight function, Notaris (cf. [159]), using (3.8) and following a process similar to that of Hämmerlin, obtained

$$|R_n^K(f)| \leq \frac{(n!)^2(3n+2+k-i_n)!}{2^{n-2}(2n)!(3n+2+k)!} \times \inf_{1 < r \leq R} \left\{ \left[ \frac{r}{(r-1)^{3n+3+k-i_n}} + (-1)^{i_n} \frac{r}{(r+1)^{3n+3+k-i_n}} \right] |f|_r \right\},$$

where  $i_n = i_n(n)$  is a constant that has been computed and tabulated for  $2 \leq n \leq 30$ . (When  $n = 1$ , the Gauss-Kronrod formula for the Legendre weight is the 3-point Gauss formula for the same weight.) These bounds can be extended to  $n > 30$ , after the computation of the constants  $i_n$ .

If, for  $\epsilon \in \{-1, 1\}$ ,  $\epsilon R_n^K(t^k) \geq 0$  or  $\epsilon(-1)^k R_n^K(t^k) \geq 0$  for all  $k \geq 0$ , then  $\|R_n^K\|$  can be computed explicitly by means of specific formulae in terms of  $\pi_n(\cdot; w)$  and  $\pi_{n+1}^*(\cdot; w)$ . This was done in [162] by Notaris when  $w$  is one of the Bernstein-Szegö weight functions (2.7) with  $\rho(t) = 1 - \frac{4\gamma}{(1+\gamma)^2}t^2$ ,  $-1 < \gamma \leq 0$ , on  $[-1, 1]$ . If  $\tau = r - \sqrt{r^2 - 1}$ , then he obtained, e.g., for the weight  $w^{(1/2)}$ ,

$$\|R_n^{K(1/2)}\| = \frac{2\pi(1+\gamma)^2 r \tau^{4n+2} (\tau^2 - \gamma) \sqrt{\tau^2 - 1}}{(1 - \gamma\tau^2)[1 - \tau^{4n+4} - 2\gamma\tau^2(1 - \tau^{4n}) + \gamma^2\tau^4(1 - \tau^{4n-4})]}, \quad n \geq 2,$$

and similar results for the remaining Bernstein-Szegö weights. As  $\|R_n^K\|$  is explicitly computed, the bounds (3.9) are optimal and cannot be further improved. Moreover, it is shown that the Gauss-Kronrod formulae for the aforementioned Bernstein-Szegö weights with  $0 < \gamma < 1$  are nondefinite for almost all  $n$  (cf. [162, Proposition 3.4]).

**3.4. Error bounds for functions of low-order continuity and for nonsmooth functions.** For both classes of functions, the existing error bounds are either of Peano type or derived by Peano's Theorem.

**3.4.1. Bounds for functions of low-order continuity.** Let  $s \in \mathbb{N}$  be fixed with increasing  $n$ , and thus independent of it. For the Gauss-Kronrod formula relative to the Legendre weight function, the precise asymptotic limit of the low-order Peano constants  $c_s^{(1/2)}(R_n^K)$  in (3.5) was given by Ehrich in [56],

$$\lim_{n \rightarrow \infty} (2n+1)^s c_s^{(1/2)}(R_n^K) = \pi^s B\left(\frac{1}{2}s+1, \frac{1}{2}\right) \int_0^1 |B_s(x)| dx,$$

where  $B(x, y) = \int_0^1 t^{x-1}(1-t)^{y-1} dt = \Gamma(x)\Gamma(y)/\Gamma(x+y)$  is the Beta function and  $B_s$  is the  $s$ th Bernoulli polynomial.

**3.4.2. Bounds for nonsmooth functions.** If  $f$  is not necessarily differentiable but only of bounded variation, then, instead of (3.5), one can study, for the error functional  $R_n(f)$  of a quadrature formula over the interval  $[a, b]$ , estimates of the form

$$(3.10) \quad |R_n(f)| \leq \rho_V(R_n) \text{Var}(f),$$

where

$$\rho_V(R_n) = \sup_{a \leq t \leq b} |K_1(t)|,$$

with  $K_1$  being the first Peano kernel of  $R_n$  and  $\text{Var}(f)$  is the total variation of  $f$  on  $[a, b]$ . For the Gauss-Kronrod formula (2.2) relative to the Legendre weight function, the precise asymptotic limit of  $\rho_V(R_n^K)$  in (3.10) was given by Ehrich in [53],

$$\lim_{n \rightarrow \infty} (2n + 1)\rho_V(R_n^K) = \frac{\pi}{2}.$$

**3.5. Comparison of Gauss-Kronrod formulae with other quadrature formulae.** Several comparisons have been made, mainly, between the Gauss-Kronrod and the Gauss formulae for the Legendre weight function, all based on Peano constants (cf. Section 3.2, in particular, Equations (3.5)–(3.6)).

As mentioned in the introduction,  $|Q_n^K - Q_n^G|$  is used as an error estimator for  $Q_n^G$ , and this goes under the assumption that  $Q_n^K$  gives a better approximation than  $Q_n^G$ . Brass and Förster have shown in [15, Section 5] that this is true for functions that are arbitrarily differentiable, in particular,

$$\frac{c_{2n}^{(1/2)}(R_n^K)}{c_{2n}^{(1/2)}(R_n^G)} \leq C \sqrt[4]{n} \left( \frac{16}{25\sqrt{5}} \right)^n = C \sqrt[4]{n} \left( \frac{1}{3.493\dots} \right)^n,$$

where  $C$  is a constant independent of  $n$ . However, the superiority of  $Q_n^K$  over  $Q_n^G$  depends on the degree of smoothness of  $f$ ; for every fixed  $s \in \mathbb{N}$  independent of  $n$  and  $f \in C^s[-1, 1]$ , Ehrich proved in [56, Corollary 1] that

$$\lim_{n \rightarrow \infty} \frac{c_s^{(1/2)}(R_n^K)}{c_s^{(1/2)}(R_n^G)} = 2^{-s}.$$

Now, although one would believe that the superiority of  $Q_n^K$  over  $Q_n^G$  would diminish for less smooth functions, Ehrich has shown in [53, Corollary 1.8] that

$$\lim_{n \rightarrow \infty} \frac{\rho_V(R_n^K)}{\rho_V(R_n^G)} = \frac{1}{2},$$

i.e.,  $Q_n^K$  continues to be twice as good as  $Q_n^G$  for functions of bounded variation.

On the other hand, as the Gauss-Kronrod formula is used in packages of automatic integration (cf. [199, 154, 184, 220]), it is important to know if there are any  $(2n + 1)$ -point quadrature formulae better than the Gauss-Kronrod formula, and, in particular, how the  $(2n + 1)$ -point Gauss formula compares to the Gauss-Kronrod formula. Ehrich has shown in [51, Corollary] that, for  $n \geq 1$ ,  $c_{3n+2+k}^{(1/2)}(R_{2n+1}^G) \leq c_{3n+2+k}^{(1/2)}(R_n^K)$ , while, for  $n \geq 15$ ,

$$\frac{c_{3n+2+k}^{(1/2)}(R_{2n+1}^G)}{c_{3n+2+k}^{(1/2)}(R_n^K)} \leq 3^{-n+1}.$$

Asymptotically, we have

$$\lim_{n \rightarrow \infty} \sqrt[n]{\frac{c_{3n+2+k}^{(1/2)}(R_{2n+1}^G)}{c_{3n+2+k}^{(1/2)}(R_n^K)}} = \sqrt{\frac{6^6}{7^7}} = \frac{1}{4.2013\dots}$$

i.e., the  $(2n + 1)$ -point Gauss formula is substantially better than the Gauss-Kronrod formula. Comparisons based on lower error constants are studied in [49, Section 2]. The advantage of the  $(2n + 1)$ -point Gauss formula essentially disappears for functions of low-order continuity or of bounded variation; Ehrich proved that, for fixed  $s \in \mathbb{N}$  independent of  $n$ ,

$$\lim_{n \rightarrow \infty} \frac{c_s^{(1/2)}(R_{2n+1}^G)}{c_s^{(1/2)}(R_n^K)} = 1, \quad \lim_{n \rightarrow \infty} \frac{\rho_V(R_{2n+1}^G)}{\rho_V(R_n^K)} = 1$$

(cf. [56, Corollary 2] and [60, Corollary 3.12]). Furthermore, it was also shown that among all quadrature formulae using the  $n$  Gaussian nodes (zeros of the  $n$ th degree Legendre polynomial) and  $n+1$  additional nodes which interlace with the Gaussian nodes, the Gauss-Kronrod formula is asymptotically optimal in the class of functions of bounded variation (i.e., with respect to  $\rho_V$ ) (cf. [53, Corollary 1.7] and [60, Theorem 3.8]).

Finally, if the nesting of nodes in the Gauss-Kronrod formula a la Patterson (cf. [166] and Section 5) is of importance, as is the case in routines of automatic integration packages [154] and [184], then the only other known quadrature formula enjoying this nesting property is the  $(2n + 1)$ -point Clenshaw-Curtis formula (cf. [30]). Although the nodes and weights of the latter are given explicitly, and therefore they can easily be computed, the Clenshaw-Curtis formula error functional  $R_{2n+1}^{CC}$  behaves significantly worse than that of the Gauss-Kronrod formula for infinitely differentiable functions, in particular,

$$\lim_{n \rightarrow \infty} \sqrt[n]{\frac{c_{2n+1}^{(1/2)}(R_n^K)}{c_{2n+1}(R_{2n+1}^{CC})}} \leq \frac{16}{25\sqrt{5}}$$

(cf. [60, pp. 69–70]; for a comparison of the error behavior and the performance between the Gauss formula and the Clenshaw-Curtis formula, see [218, 216, 47]).

**4. Computational methods.** Since their presentation in 1964, several methods have been developed for the computation of Gauss-Kronrod formulae.

**4.1. Separate computation of nodes and weights.** Naturally, the first one who computed the Gauss-Kronrod formula (1.3) was Kronrod himself (cf. [120]). He first calculated the polynomial  $\pi_{n+1}^*$  in power form by means of (1.4), i.e., by constructing and solving a linear system. The zeros  $\tau_\mu^*$  of  $\pi_{n+1}^*$  were found by a rootfinding procedure, while the weights  $\sigma_\nu, \sigma_\mu^*$  were computed from a linear system expressing the exactness of formula (1.3) for the first  $2n + 1$  monomials. (Of course, symmetry was utilized throughout the whole process.) Kronrod noticed that his method suffers from severe loss of accuracy, and he therefore had to use extended precision up to 65 digits in order to produce results correct to 16 decimal digits for  $n \leq 40$ .

Patterson tried to alleviate the loss of accuracy by expanding  $\pi_{n+1}^*$  in terms of Legendre polynomials (cf. [166]), and that way he obtained a stable algorithm. The stability was further enhanced, and the method became even simpler, by expansion of  $\pi_{n+1}^*$  in terms of Chebyshev polynomials. This was demonstrated by Piessens and Branders (cf. [183]), although the idea existed in the work of Szegő (cf. [214], of which Piessens and Branders were apparently unaware), as it was pointed out by Monegato (cf. [146]). Szegő's algorithm is somewhat simpler, and it can even be applied to the case of the Gauss-Kronrod formula (2.2) for the Gegenbauer weight function.

It should be noted that the computation of the polynomial  $\pi_{n+1}^*(\cdot; w)$  by expansion in terms of the orthogonal polynomials  $\pi_m(\cdot; w)$ ,  $m = 0, 1, \dots, n + 1$ , can be applied to any weight function  $w$ . One has to use (2.3) and replace  $t^k$  by  $\pi_k(t)$ , whence, by orthogonality,

one obtains a lower triangular system of equations with a unique solution. The coefficients of the system can be computed effectively by Gauss-Christoffel quadrature relative to the weight function  $w$ , using  $[(3n + 3)/2]$  points (cf. [22, Section 4]); for another method, see [24] and [27].

An alternative iterative method was presented by Monegato in [151, pp. 178–179]. By first using the Clenshaw summation algorithm, one can compute efficiently the values of  $\pi_{n+1}^*(t)$ ,  $\pi_{n+1}'(t)$ , and  $\pi_{n+1}''(t)$ , which are then used in a third-order iterative method, such as the Laguerre algorithm, in order to compute the zeros of  $\pi_{n+1}^*$ . The weights in Monegato's method, as well as in those of Patterson and of Piessens and Branders, can always be computed by means of formulae (2.4). The method has complexity  $O(n^2)$ , and it can be generalized to the case of the Gauss-Kronrod formula (2.2) for the Gegenbauer weight function.

Also, a fixed point iterative method was given by Ehrich (cf. [50]). The method emanates from (1.4) with  $k = n$ , by setting  $\pi_{n+1}^*(t)/(t - \tau_\mu^*)$  in place of  $t^n$  and then solving for  $\tau_\mu^*$ . The procedure is locally convergent of order two, and the involved arithmetical operations depend quadratically on the number of nodes. Furthermore, a posteriori error estimates are provided. As before, the weights can be computed by means of formulae (2.4). Ehrich compares his method with the hitherto known methods, and he shows that the method can be used to construct the Patterson sequence of quadrature formulae (cf. Section 5 below).

A quite different but rather natural approach is the one that generalizes the well-known Golub and Welsch algorithm (cf. [101]). It is known that the computation of the Gauss-Christoffel quadrature formula can be reduced to the solution of an eigenvalue problem for an  $n \times n$  symmetric tridiagonal matrix known as the Jacobi matrix. The first attempt to extend the Golub and Welsch algorithm to quadratures with fixed nodes, which contain among others the Gauss-Kronrod formula, was made by Kautsky and Elhay (cf. [117] and [67]). Their idea was to extend the concept of Jacobi matrices to weight functions that change sign within the interval of orthogonality, in which case only a few orthogonal polynomials may exist. That way, Kautsky and Elhay compute the nodes while for the weights they use their own methods and software for generating interpolatory quadrature formulae (cf. [116] and [68]).

**4.2. Simultaneous computation of nodes and weights.** In all methods of Section 4.1, the Gauss-Kronrod formula was computed piecemeal: First the underlying Stieltjes polynomial, then the nodes, and finally the weights. A more preferred method would be to compute nodes and weights simultaneously, by first constructing a nonlinear system expressing the exactness of formula (2.2) for some set of basis functions in  $\mathbb{P}_{3n+1}$ , and then solving the system by Newton's method. This idea was first investigated by Caliò, Gautschi, and Marchetti (cf. [22]), who also analyzed the condition of the underlying problem, i.e., the stability of the method. Although the latter performs quite well for the Gauss-Kronrod formula relative to the Legendre and logarithmic weight functions, it appears that it runs into severe ill-conditioning when it is applied to the case of repeated Kronrod extension (cf. [91]).

Another method for computing simultaneously the nodes and weights of the Gauss-Kronrod formula was obtained by a generalization of the Golub and Welsch algorithm. Although, as mentioned in Section 4.1, this was first initiated by Kautsky and Elhay, a true advancement in this direction was made by Laurie (cf. [127] and also [83, 151]). He showed that if the Gauss-Kronrod formula exists with real distinct nodes and positive weights, then we can associate with it a  $(2n + 1) \times (2n + 1)$  symmetric tridiagonal matrix, analogous to the Jacobi matrix, thus appropriately called Jacobi-Kronrod matrix. Laurie proved that the leading and trailing  $n \times n$  principal submatrices of the Jacobi-Kronrod matrix have the same eigenvalues. That way, the computation of the nodes and weights of the Gauss-Kronrod formula is reduced to an inverse eigenvalue problem, which is efficiently solved through a five-term recurrence relation of certain mixed moments.

An improvement of Laurie's algorithm was given by Calvetti, Golub, Gragg, and Reichel (cf. [29]; see also [129]). Their algorithm avoided to compute explicitly the Jacobi-Kronrod matrix, whose entries might be sensitive to round-off errors. This algorithm as well as that of Laurie can be implemented in  $O(n^2)$  arithmetic operations, while it can efficiently be applied on parallel computers.

Furthermore, Laurie's algorithm was modified by Ammar, Calvetti, and Reichel (cf. [2]) in order to cover cases of Gauss-Kronrod formulae with complex conjugate nodes and weights or with real nodes and positive and negative weights. This modified algorithm has two versions requiring either  $O(n^2)$  or  $O(n^3)$  arithmetic operations. The faster version computes the nodes and weights with sufficient accuracy for most problems; the slower version, on the other hand, is used to provide higher accuracy in certain difficult problems.

**4.3. Numerical tables and computer programs.** There are a number of places where the nodes and weights of Gauss-Kronrod formulae are tabulated; detailed information are given in [82, Sections 4.2 and 4.3]. For the Legendre weight function, nodes and weights can be found in Kronrod's original paper (cf. [120]), and also in the work of Patterson (cf. [166], on microfiche) and of Piessens (cf. [182]). The most accurate results of all though are tabulated in [184].

For logarithmic type weight functions  $w(t) = t^a \ln(1/t)$  on  $[0, 1]$ ,  $a = 0, \pm 1/2$ , nodes and weights for the respective Gauss-Kronrod formulae are given by Caliò, Gautschi, and Marchetti (cf. [22], in the supplement section of the issue) and also Caliò and Marchetti (cf. [24]).

Computer programs in Fortran for generating the Gauss-Kronrod formula for the Legendre weight function are given by Squire (cf. [211, p. 279]) and by Piessens and Branders (cf. [183], in the appendix and the supplement section of the issue). For the Gegenbauer weight function  $w_\lambda$ ,  $0 \leq \lambda \leq 2$ ,  $\lambda \neq 1$ , Dagnino and Fiorentino implemented the algorithm of Szegö as described by Monegato in [146] (see [39], although the Fortran code is given in [38]). For general weight functions, a Fortran program is given by Caliò and Marchetti (see [24], although again the Fortran code is given in [23]).

Furthermore, routines implementing Laurie's algorithm, described in the previous subsection, have been included in the MATLAB suite OPQ, which is a companion piece of [85]. Also, Gauss-Kronrod routines have been included in modern numerical software libraries such as IMSL (cf. [199]), NAG (cf. [154]), QUADPACK (cf. [184]), and Mathematica (cf. [220]).

**5. Applications.** There are several places where Kronrod's idea or the Gauss-Kronrod formulae have been applied. Typing "Gauss-Kronrod" on Google Scholar produces about 2,120 results, and going through them shows that Gauss-Kronrod formulae are widely used in all those scientific areas where the computation of integrals is required.

Kronrod's motivation originated from the need to estimate accurately the error of the Gauss formula, using the Gauss-Kronrod formula as a substitute for the exact value of the integral. This was utilized in the development of automatic integration schemes (cf. [33, 168, 182, 184]; see also [13], while an interesting interpretation of Kronrod's idea is actually given by Laurie in [124]). Also, Kronrod's idea has been used in adaptive integration schemes (see, e.g., [79] or [107]).

Kronrod's idea has been applied repeatedly by Patterson (cf. [166, 168]); it has already been mentioned in Sections 2.1.3 and 2.2.1 that Kronrod's idea can be iterated for the Chebyshev weight of the first and second kind and for the Bernstein-Szegö weight  $w^{(1/2)}$ . Starting from the 3-point Gauss formula for the Legendre weight function and constructing the 7-point Gauss-Kronrod formula, he added 8 new points deriving a 15-point formula, then 16 more points for a 31-point formula, and he continued that way up to a 255-point formula. Interestingly enough, it was found numerically that in each quadrature formula in this sequence, the new

nodes interlace with the old ones, all nodes are contained in  $(-1, 1)$ , and all weights are positive (these properties correspond to properties (a), (b), and (c) of Section 2). However, none of this has been proved theoretically; in fact, numerical results indicate that the Kronrod-Patterson sequence of quadrature formulae cannot exist, with real nodes and positive weights, for whatever initial  $n$ -point Gauss formula one starts with (cf. [151, p. 187]). Nonetheless, an algorithm for generating these formulae has been presented by Patterson (cf. [169, 170]; for a short description of it, see [151, pp. 187–189]). It is not as elegant and efficient as those of the previous section, yet it is quite general allowing the extension of any  $n$ -point interpolatory formula to a new  $(n + m)$ -point one.

An improvement of Patterson’s algorithm is given by Krogh and Van Snyder (cf. [118]); their method reduces the number of weights necessary to represent Patterson’s quadrature formulae as well as the amount of storage necessary for storing function values, while it produces slightly smaller error when the integrand has singular behavior at the end of the interval.

A generalization of Patterson’s method for the purpose of computing a multidimensional integral over the infinite integration region was given by Genz and Keister (cf. [96]). Also, a generalization of Patterson’s algorithm, which circumvents the use of the three-term recurrence relation and works instead directly with the moments of the underlying distribution, is presented by Mehrotra and Papp (cf. [136]).

The Kronrod-Patterson sequence of quadrature formulae has been used for the evaluation of improper integrals that arise in the solution of weakly singular integral equations. In one case, these formulae are employed together with the  $\epsilon$ -algorithm in order to accelerate the sequence of approximants (cf. [75]), and in another, in collaboration with appropriate polynomial transformations for alleviating the singularity (cf. [74]).

Rabinowitz, Elhay, and Kautsky start with the Gauss-Kronrod formula (2.2) for the weight function  $w$  and add  $m \geq n + 2$  new nodes, obtaining, in an optimal way, the so-called “first Patterson extension” of the Gauss-Kronrod formula, which is said to be minimal if  $m = n + 2$  and nonminimal if  $m > n + 2$ . They give some experimental results and make some conjectures for the minimal and nonminimal quadrature formulae when  $w$  is the Gegenbauer or the Jacobi weight functions (cf. [191]). For further investigations when  $w$  is the Laguerre and the Hermite weight functions, see [69, 70].

The Kronrod-Patterson quadrature formulae belong to the category of the so-called “nested quadrature rules” and are used, among other things, in adaptive quadrature schemes. Laurie, trying to improve on the amount of storage used, coined the term “stratified nested quadrature rules”. A nested sequence of quadrature rules is called stratified if it has the property that

$$Q_{k+1} = c_k Q_k + (1 - c_k) \bar{Q}_k,$$

where  $Q_k$  is the nested rule at stage  $k$  and  $\bar{Q}_k$  is the rule involving the new points only; hence, the function values used for  $Q_k$  need not to be stored for the computation of  $Q_{k+1}$ , but all that is needed instead is the value of  $Q_k$  (cf. [125]). Ehrich in [62] applied and generalized Laurie’s ideas in constructing stratified extensions of the Gauss formula for the Laguerre and the Hermite weight functions with higher degree of exactness (see also Section 7 below).

In Laurie’s stratified nested rules, implicit constraints are imposed on the nodes in order to achieve the relationships between the weights, and this in turn implies a constraint on the maximum achievable degree of exactness. To overcome this, Patterson, assisted by the work in [118], proposed (cf. [172]) the so-called “hybrid quadrature rules”, which combine the properties of Laurie’s stratified nested rules and of Kronrod-Patterson formulae.

As odd as it might look like, another idea for obtaining a sequence of nested quadrature formulae is by contraction (cf. [82, pp. 50–51]). Here, one starts with a base formula,

containing a sufficiently large number of nodes, and successively removes subsets of nodes, obtaining a sequence of quadrature formulae containing each time fewer and fewer nodes. The resulting sequence is then turned the other way around, obtaining that way a sequence of nested quadrature formulae. A number of authors have applied this technique (see [167, 192] and also [192, Appendix A]). The work in [192] has found an application in Bayesian analysis (cf. [46]).

Motivated by the nonexistence of Gauss-Kronrod formulae with real nodes and positive weights for several of the classical weight functions, a number of authors tried to relax some of the conditions necessary for maximum degree of exactness. Begumisa and Robinson in [6], writing the Stieltjes polynomial in the form  $\pi_{n+1}^*(t) = \sum_{\mu=0}^{n+1} a_{\mu} \pi_{\mu}(t)$ ,  $a_{n+1} = 1$ , require that the latter satisfies

$$\int_a^b \pi_{n+1}^*(t) t^k \pi_n(t) w(t) dt = 0, \quad k = 0, 1, \dots, n-r,$$

rather than (2.3). That way, they determine the coefficients  $a_n, a_{n-1}, \dots, a_r$ , while the remaining coefficients  $a_0, \dots, a_{r-1}$  are chosen such that the polynomial  $\pi_{n+1}^*$  has  $n+1$  real and distinct zeros in  $(a, b)$ . Furthermore, as the resulting Gauss-Kronrod formula has degree of exactness  $3n-r+1$ , an attempt was made to keep  $r$  as small as possible. Although their procedure is rather complicated, it was nonetheless successful in obtaining a nonoptimal Kronrod extension of the Gauss formula for the Hermite weight function, but less so for the Laguerre and the Gegenbauer weight functions.

Now, Patterson in [171] showed that the Begumisa and Robinson extension can alternatively be derived by appending  $r$  arbitrary nodes,  $\tau_{n+1}, \dots, \tau_{n+r}$ , to the  $n$  Gaussian ones, thus starting with a total of  $n+r$  fixed nodes, and obtaining the  $n-r+1$  new nodes,  $\tau_1^*, \dots, \tau_{n-r+1}^*$ , such that

$$\int_a^b \left[ \pi_n(t) \prod_{\nu=n+1}^{n+r} (t - \tau_{\nu}) \right] \pi_{n-r+1}^*(t) t^k w(t) dt = 0, \quad k = 0, 1, \dots, n-r,$$

where  $\pi_{n-r+1}^*(t) = \prod_{\mu=1}^{n-r+1} (t - \tau_{\mu}^*)$ . So, while Begumisa and Robinson adjusted the trailing coefficients of the Stieltjes polynomial, Patterson varied the  $r$  appended nodes. The benefit of his approach is that the new nodes can be computed with little effort by means of the general algorithm in [169, 170]. Patterson proceeded a step further, by showing that one can actually induce optimal extensibility, i.e., extensibility with the maximum attainable degree of exactness, if one or more nodes of the starting Gauss formula are replaced by judiciously chosen ones. There is some little extra work incurred, one integrand evaluation for each replaced node, but the new method is applied successfully in the extension of the Gauss formula for the Hermite and the Laguerre weight functions.

Kahaner, Wadvogel, and Fullerton, motivated by the nonexistence of the Gauss-Kronrod formula for the Laguerre weight function with positive nodes and weights, investigated the possibility of adding to the  $n$  Gauss nodes  $n+q$  new ones, where  $q > 1$  (cf. [113, 114]). They present a method for computing the new nodes and weights, and they report results for  $n = 1(1)10$  and various values of  $q$ . In a number of cases, the Kronrod extension was successful with nonnegative nodes and positive weights.

In certain integrals, the functions to be integrated happen to have poles outside of the interval of integration. In this case, it would be more natural to use a quadrature formula which is exact for a mixture of polynomials and rational functions having the same, or at least the more important, poles (those closest to the interval of integration). The implementation of this idea for Gauss-Kronrod formulae, appropriately called rational Gauss-Kronrod quadrature formulae, is given in [88, 84], while their error is studied in [11, 10, 42].

In Wilf-type quadrature formulae, the nodes and weights are computed by requiring that the average error be as small as possible over the family of the monomials (cf. [219]). Kronrod and Patterson extensions of Wilf-type formulae of a mixed rational-polynomial type were developed by Engels, Ley-Knieper, and Schwelm (cf. [73, 72]).

Extended product quadrature formulae, even subinterpolatory ones, i.e., having degree of exactness lower than that of interpolatory quadrature formulae, are studied by Dagnino in [36]; see also [37]. The degree of exactness is sacrificed and severe conditions are applied in the function and the kernel of the underlying integral such that the quadrature formulae in question converge and are stable. For the computation of product quadrature formulae and their Kronrod extension, see [165]. On the other hand, Gauss-Kronrod product quadrature formulae are studied by Ehrich in [59]. He considers quadrature formulae of the form

$$(5.1) \quad \int_{-1}^1 k(t)f(t)dt = \sum_{\nu=1}^n \sigma_{\nu}(k)f(\tau_{\nu}) + \sum_{\mu=1}^{n+1} \sigma_{\mu}^*(k)f(\tau_{\mu}^*) + R_n(k; f),$$

where  $k \in L^1$ , not necessarily of one sign,  $f$  is a (bounded) Riemann integrable function,  $\tau_{\nu}$  are the zeros of the  $n$ th degree Legendre polynomial  $P_n$ , and  $\tau_{\mu}^*$  are the zeros of the corresponding Stieltjes polynomial, i.e., formula (5.1) is based on the nodes of the original Gauss-Kronrod formula (1.3). Ehrich proved that, if  $k \in L^p$  for some  $p > 1$ , then the quadrature sum on the right-hand side of (5.1) converges to the integral on the left for all Riemann integrable functions  $f$ . Furthermore, under the same condition,

$$\lim_{n \rightarrow \infty} \left( \sum_{\nu=1}^n |\sigma_{\nu}(k)|f(\tau_{\nu}) + \sum_{\mu=1}^{n+1} |\sigma_{\mu}^*(k)|f(\tau_{\mu}^*) \right) = \int_{-1}^1 |k(t)|f(t)dt,$$

for all  $f \in C[-1, 1]$ . Similar results are shown for product quadrature formulae based on the  $\tau_{\mu}^*$  only. These results are then used for obtaining uniform convergence of the approximate solutions of weakly singular integral equations of the second kind.

Kronrod's idea has been applied to various types of integrals. In one case, to Cauchy principal value integrals (cf. [188]), where the stability of the underlying algorithm is examined in [189]; see also [164]. And in another case, to the evaluation of the Bromwich integral, which arises in the inversion of the Laplace transform (cf. [181]).

Complex Stieltjes polynomials  $\pi_{n+1}^*(z; w_{\lambda})$  for the Gegenbauer weight function  $w_{\lambda}$ , on the semicircle  $\Gamma = \{z \in \mathbb{C} : z = e^{i\theta}, 0 \leq \theta \leq \pi\}$ , were studied by Caliò and Marchetti (cf. [25]). In particular, for  $\lambda = 0$  or  $1$ , they showed that all zeros of  $\pi_{n+1}^*(z)$  are simple and located in the interior of the upper unit half disk, based on which they constructed the respective Gauss-Kronrod formulae. These formulae are subsequently used (cf. [26]) for the evaluation of certain Cauchy principal value integrals. For Gauss-Kronrod quadrature formulae on the unit circle, see [193].

For a derivation of the Gauss-Kronrod formula by means of a formula relating the quadrature weights to their approximations using the trapezoidal rule, see [194].

Since Padé approximants can be viewed as formal Gaussian quadrature (cf. [17]), Brezinski in [19] extended Kronrod's procedure to Padé approximation in order to obtain estimates of the error. Subsequently, a new interpretation was given in [20] (see also [21]), which led to new procedures for estimating the error. Brezinski's procedure has been extended to vector Padé approximants by Belantari (cf. [7]).

Gauss-Kronrod formulae are also used for computing Fourier coefficients in orthogonal expansions (cf. [82, p. 61]).

Moreover, Stieltjes polynomials and Gauss-Kronrod formulae have found an application in constructing space-localized bases for the wavelet space of band-limited functions on the sphere (cf. [121]).

Gauss-Kronrod formulae as well as the Kronrod extension of the Gauss-Radau and the Gauss-Lobatto quadrature formulae (cf. the following section) were utilized for the development of Runge-Kutta methods (cf. [221, 222, 223, 224, 225]). On the other hand, although numerical integration methods are frequently used in finite element and projection methods, Gauss-Kronrod formulae have not got much attention. However, Bellen applied them in the so-called “extended collocation-least squares method” (cf. [8]). Also, Rashidinia and Mahmoodi (cf. [196]) used them, together with a collocation method based on quintic B-splines, for the numerical solution of Fredholm and Volterra integral equations. Finally, Sinsbeck and Nowak succeeded to reproduce the Gauss-Kronrod formula by means of an optimized stochastic collocation method (cf. [201]).

Finally, Kronrod’s idea has been applied to cubature methods (cf. [12, 31, 32, 71, 96, 97, 98, 123, 133, 134, 155, 180, 217]).

**6. Kronrod extensions of other than the Gauss formulae.** Several authors have worked on the Kronrod extension of the Gauss-Radau, Gauss-Lobatto, and, particularly, Gauss-Turán and Chakalov-Popoviciu quadrature formulae; for definitions and descriptions on each of these formulae, see [81, Sections 2.1–2.2].

The Kronrod extension of the Gauss-Radau quadrature formula for the weight function  $w$  on the interval  $[a, b]$  and additional node at  $a$  (respectively  $b$ ) requires that the Gauss formula for the weight function  $(t - a)w(t)$  (respectively  $(b - t)w(t)$ ) admits a Kronrod extension, i.e., the Stieltjes polynomial  $\pi_{n+1}^*(\cdot; (t - a)w(t))$  (respectively  $\pi_{n+1}^*(\cdot; (b - t)w(t))$ ) has real and distinct zeros, all in  $(a, b)$ , and different from the zeros of  $\pi_n(\cdot; (t - a)w(t))$  (respectively  $\pi_n(\cdot; (b - t)w(t))$ ) (cf. [82, Example 2.2]). The Kronrod extension of the  $(n + 1)$ -point Gauss-Radau formula for the Legendre weight function is studied by Baratella in [4], where nodes and weights are given for  $n = 2(2)16$ . Also, the Kronrod extension of the Gauss-Radau formula for the Gegenbauer weight function  $w_\lambda$  is studied by Sismondi in [202], where the quadrature formulae are given for the case  $\lambda = 1$ , i.e., the Chebyshev weight of the second kind, and  $n = 1, 2, 4, 8$ , and 16.

In a like manner, the Kronrod extension of the Gauss-Lobatto quadrature formula for the weight function  $w$  on the interval  $[a, b]$  assumes that the Gauss formula for the weight function  $(t - a)(b - t)w(t)$  allows a Kronrod extension (cf. [82, Example 2.3]). That way, one can use existence and nonexistence results stated previously for the Gauss-Kronrod formulae in order to derive results for the Kronrod extension of the Gauss-Lobatto formula. In particular, the Kronrod extension of the  $(n + 2)$ -point Gauss-Lobatto formula for the Gegenbauer weight function  $w_\lambda$  has properties (a) and (b) for all  $n \geq 1$  when  $-1/2 < \lambda \leq 1$  (cf. [214, §3]), and if in addition  $\lambda \neq 0$ , then the precise degree of exactness is  $3n + 3$  for  $n$  even and  $3n + 4$  for  $n$  odd, while an error bound of type (3.2) is also given (cf. [187]). Furthermore, the Kronrod extension is not possible for  $\lambda > 2$  and  $n$  sufficiently large, while properties (a) and (b) hold true for  $\lambda = 2$  and  $n$  sufficiently large (cf. [177, Theorems 1 and 2]). For the positivity of the weights, partial results are derived, when  $-1/2 < \lambda \leq 0$ , by Monegato (cf. [145]) and, when  $0 < \lambda \leq 1$ , by Ehrich (cf. [55, Section 2]). In the same sense, the Kronrod extension of the Gauss-Lobatto formula for the Bernstein-Szegő weight function  $w^{(-1/2)}$ , with  $\rho(t) = 1 - \frac{4\gamma}{(1+\gamma)^2}t^2$ ,  $-1 < \gamma < 1$ , on  $[-1, 1]$ , has properties (a), (b), and (c) for all  $n \geq 1$  (cf. [95, p. 753]).

Laurie, generalizing the method of Baratella (cf. [4]), and using the software package OPQ of Gautschi (cf. [85]), showed how to calculate the Kronrod extension of the Gauss-Radau and the Gauss-Lobatto formulae (cf. [128]). On the other hand, the improvement of Laurie’s

algorithm given by Calvetti, Golub, Gragg, and Reichel for the Gauss-Kronrod formula can be applied to the Kronrod extension of the Gauss-Radau and the Gauss-Lobatto formulae (cf. [29]). The same is the case with the Dagnino and Fiorentino implementation of Szegő's algorithm in [39].

The Kronrod extension of the Gauss-Radau and the Gauss-Lobatto quadrature formulae with double end points for each of the four Chebyshev weight functions was studied by Li in [132], where the underlying Stieltjes polynomials are explicitly or computationally obtained, and the interlacing and inclusion of the nodes in  $(-1, 1)$  as well as the positivity of the weights (corresponding to properties (a), (b), and (c) of Section 2) are examined.

The Kronrod extension of the Gauss-Turán quadrature formulae has been investigated by several authors for a variety of weight functions. Bellen and Guerra worked on the case of the Legendre weight (cf. [9]). Li, on the other hand, considered the case of the Chebyshev weight of the first kind (cf. [130]), deriving the respective Stieltjes polynomials and, in a few special cases, the weights. Li's work has been generalized by Shi (cf. [200]). An interesting approach in constructing the Kronrod extension of the Gauss-Turán formula is presented by Cvetković and Spalević in [35].

The work of Li and Shi was taken a step further by Milovanović and Spalević in [139]. They studied the Kronrod extension of the Gauss-Turán formulae, including the underlying Stieltjes polynomials, for the generalized Chebyshev weight functions

$$\begin{aligned} w_1(t) &= (1-t^2)^{-1/2}, & w_2(s;t) &= (1-t^2)^{1/2+s}, & -1 < t < 1, \\ w_3(s;t) &= (1-t)^{-1/2}(1+t)^{1/2+s}, & w_4(s;t) &= (1-t)^{1/2+s}(1+t)^{-1/2}, & -1 < t < 1, \end{aligned}$$

where  $s \in \mathbb{N}_0$ . Furthermore, they obtained  $L^1$  estimates for the remainder term by contour integration techniques on confocal ellipses.

In [141], Milovanović, Spalević, and Galjak took the results of [139] a step further by considering the Chakalov-Popoviciu quadrature formula; the latter is a generalization of the Gauss-Turán formula in the sense that each node in the quadrature sum occurs with its own multiplicity. The Kronrod extension of the Chakalov-Popoviciu formula for some cases of the generalized Chebyshev and the Gori-Micchelli weight functions were derived. Furthermore, effective  $L^1$  estimates for the remainder term of the Gauss-Turán-Kronrod formula for the Gori-Micchelli weight function were obtained by contour integration techniques on confocal ellipses. These estimates were further improved in [142]<sup>7</sup>.

In [143], Milovanović, Spalević, and Pranić derived effective  $L^\infty$  error bounds for the remainder term of the Gauss-Turán-Kronrod formula for the generalized Chebyshev weight functions, by investigating the location on elliptic contours where the modulus of the underlying kernel attains its maximum value. Moreover, following Kronrod's idea (cf. the introduction), by using the modulus of the difference between the quadrature sums of the Gauss-Turán formula and its Kronrod extension, new error estimates were derived for the Gauss-Turán formula, which were compared with  $L^1$  error bounds obtained for that formula in [138].

Fairly recently, Milovanović and Spalević (cf. [140]) extended the work of Bojanov and Petrova (cf. [14]) for computing Fourier coefficients in orthogonal expansions. They examined the existence and, wherever possible, they determined real Kronrod extensions of Gaussian quadrature formulae with multiple nodes, in particular, for generalized Chebyshev and Gori-Micchelli weight functions, appropriate for the computation of Fourier coefficients. Moreover, Spalević and Cvetković (cf. [210]), trying to estimate effectively the error of Gaussian quadrature formulae by using their extensions with multiple nodes, obtained (optimal) Kronrod

<sup>7</sup>In [142, pp. 224–225], a mistake is corrected in the proof of Proposition 2.1 in [141].

extensions with multiple nodes for Gaussian quadrature formulae relative to generalized Chebyshev and Gori-Micchelli weight functions.

In [204], Smith considered the quadrature formula

$$(6.1) \quad \int_{-1}^1 f(t)w(t)dt = \sum_{\nu=1}^r \gamma_{r,\nu} f(\tau_{r,\nu}) + \sum_{k=0}^{n-r-1} (\gamma_{0,k} f^{(k)}(-1) + \gamma_{n,k} f^{(k)}(1)) + R_{r,n}(f),$$

where the Gaussian nodes  $\tau_{r,\nu}$  and all weights  $\gamma_{r,\nu}$ ,  $\gamma_{0,k}$ , and  $\gamma_{n,k}$  were determined so that the formula has maximum degree of exactness  $2n - 1$ . It was proved that this formula, which includes as special cases the Gauss and the Gauss-Lobatto formulae, has all weights positive except for  $\gamma_{n,k}$  whose signs depend on the parity of  $k$ . Subsequently, in [205], the Kronrod extension of formula (6.1) was defined, and it was shown that its weights satisfy formulae analogous to those obtained by Monegato for the original Gauss-Kronrod formula (cf. [144]). Furthermore, motivated by the work of Gautschi and Notaris (cf. [90]), Smith, when  $w$  is the Gegenbauer weight function  $w_\lambda$ , computed intervals of  $\lambda$  in which each of the properties (a)–(d) of Section 2 is true (cf. [206]). Going a step further, Smith and Hunter investigated (cf. [207]) the feasibility of the “first Patterson extension” (cf. [191]) of the Kronrod extension of formula (6.1) when  $w$  is the Gegenbauer weight function.

**7. Quadrature formulae inspired by Kronrod’s idea.** As already mentioned, Kronrod’s motivation came originally from his desire to estimate accurately the error of the Gauss formula. However, Gauss-Kronrod formulae fail to satisfy properties (a)–(d), i.e., do not exist with real and distinct nodes in the interval of integration and positive weights, for several of the classical weight functions; notable examples are the Hermite and the Laguerre weights, but the list also includes the Gegenbauer and the Jacobi weights for values of  $\lambda$  and  $(\alpha, \beta)$  above specific constants and regions, respectively, depending on  $n$  (cf. Section 2.1). The nonexistence of Gauss-Kronrod formulae inspired Laurie to develop the so-called anti-Gaussian quadrature formula, which led to the averaged Gaussian quadrature formula (cf. [126]). The latter is a special case of a stratified nested quadrature rule (cf. [125]) and enjoys nice properties: It always exists with real nodes, at most two of which are outside of the interval of integration, and all its weights are positive. Furthermore, the formula can easily be constructed.

As mentioned previously, Laurie’s ideas were generalized by Ehrich (cf. [62]) in an attempt to construct optimal, i.e., having the highest possible degree of exactness, anti-Gaussian and averaged Gaussian formulae for the Laguerre and the Hermite weight functions. Further work for generalized Hermite and Gegenbauer weight functions was done by Hascelik in [103, 104].

In [208], Spalević proposed a simple numerical method for constructing (optimal) generalized averaged Gaussian formulae, while, when the underlying weight function is the Jacobi weight, necessary and sufficient conditions on the parameters  $\alpha$  and  $\beta$  are provided such that all nodes of the quadrature formulae are in  $[-1, 1]$ . Proceeding further, Spalević investigated, in [209], conditions under which the degree of exactness of (optimal) generalized averaged Gaussian formulae can reach as high as  $3n + 1$ , in which case these formulae form a satisfactory alternative to Gauss-Kronrod formulae for estimating the error of the Gauss formula.

Calvetti and Reichel made a modification on Laurie’s anti-Gaussian formula, which that way was transformed into a symmetric Gauss-Lobatto formula (cf. [28]).

On the other hand, the generalized averaged extensions of Gauss-Turán formulae are studied in [35].

Moreover, the generalized averaged Gaussian formulae have already found an application in the approximation of matrix functions and matrix functionals (cf. [197, 198, 48]).

**8. Stieltjes polynomials.** From what was mentioned in the previous sections, it became clear that Stieltjes polynomials are strongly connected to Gauss-Kronrod formulae, as the zeros

of the former are the so-called Kronrod nodes. Hence, many authors have studied Stieltjes polynomials in order to prove certain properties of Gauss-Kronrod formulae. However, there is also a number of authors who were attracted by the intriguing nature of Stieltjes polynomials and the challenging mathematical problems they pose.

First of all, as already mentioned, the Stieltjes polynomial  $\pi_{n+1}^*$  in (2.3) is orthogonal to all polynomials of lower degree relative to the variable-sign weight function  $w^*(t) = \pi_n(t)w(t)$  on  $[a, b]$ , hence, the usual theory of orthogonal polynomials cannot be applied in this case. An attempt to develop a general theory for polynomials orthogonal relative to a weight function which changes sign on its support interval was made by Struble as well as by Monegato (see [213, 148] and the references therein). All results obtained, however, relate to specific weight functions.

Monegato, relying on an inequality that dominates Szegő's work (cf. [214] and [149, Equation 9]), derived in [149] bounds for the Gegenbauer polynomial  $\pi_n^{(\lambda)}$  as well as the derivatives of  $\pi_n^{(\lambda)}$  and the corresponding Stieltjes polynomial  $\pi_{n+1}^{*(\lambda)}$ .

Peherstorfer, in view of the close relation between Stieltjes polynomials and functions of the second kind, discussed in [176] known and new facts on the asymptotic behavior of Stieltjes polynomials and their close connection with the asymptotic behavior of the boundary values of functions of the second kind on  $[-1, 1]$ .

Brezinski defined a functional of the form

$$c(t^k) = \int_{-1}^1 t^k w(t) dt, \quad k = 0, 1, 2, \dots,$$

where  $w$  is an even weight function  $w(t) = w(-t)$ , and derived some properties for the class of orthogonal and the corresponding class of Stieltjes polynomials relative to this functional (cf. [18]).

As already mentioned in Section 3.3.1, the asymptotic behavior of Stieltjes polynomials relative to general measures, including the so-called regular, Blumenthal-Nevai, and Szegő classes of measures, was studied outside of the support of the measure by Bello Hernández, de la Calle Ysern, Guadalupe Hernández, and López Lagomasino in [11] and in a more general form in [10].

Jung and Sakai in [108, 110], for the Gegenbauer weight function  $w_\lambda$ ,  $0 < \lambda < 1$ , obtained several estimates and asymptotic properties for the first and second derivatives of  $\pi_{n+1}^{*(\lambda)}$  and  $\pi_n^{(\lambda)} \pi_{n+1}^{*(\lambda)}$ . These estimates play an important role in the so-called Hermite-Fejér interpolation based on the zeros of  $\pi_{n+1}^{*(\lambda)}$  or  $\pi_n^{(\lambda)} \pi_{n+1}^{*(\lambda)}$ .

Finally, zeros of Stieltjes polynomials were used as nodes in interpolation processes, either alone or in collaboration with the Gauss nodes. First, Li proved that Lagrange interpolation based on the zeros of  $\pi_n \pi_{n+1}^*$  relative to the Chebyshev weight function of the first, third, or fourth kind converges in the mean (cf. [131]). Moreover, Ehrich and Mastroianni proved bounds for the Stieltjes polynomial  $\pi_{n+1}^*$  relative to the Legendre weight function as well as lower bounds for the distances between consecutive zeros of  $\pi_{n+1}^*$  and  $\pi_n \pi_{n+1}^*$  (cf. [64]). Then, applying these results, they showed that Lagrange interpolation based either on the zeros of  $\pi_{n+1}^*$  or on those of  $\pi_n \pi_{n+1}^*$  in the uniform or the weighted  $L^p$  norm have Lebesgue constants of optimal order, i.e.,  $O(\log n)$  in the uniform norm; thus, Stieltjes polynomials have the property of improving the interpolation process based on the zeros of  $\pi_n$  only, which is known to have Lebesgue constants of order  $O(n^{1/2})$ . Further, convergence results in the weighted  $L^p$  norm are given in [66]. In [63], Ehrich and Mastroianni extended the results in [64] to the Gegenbauer weight function  $w_\lambda$ ,  $0 \leq \lambda \leq 1$ . They first proved bounds in the uniform norm for the Stieltjes polynomial  $\pi_{n+1}^{*(\lambda)}$  as well as lower bounds for the distances

between consecutive zeros of  $\pi_{n+1}^{*(\lambda)}$  and  $\pi_n^{(\lambda)}\pi_{n+1}^{*(\lambda)}$ , which were subsequently used in Lagrange interpolation based either on the zeros of  $\pi_{n+1}^{*(\lambda)}$  or on those of  $\pi_n^{(\lambda)}\pi_{n+1}^{*(\lambda)}$ ; in the second case, the process does not have optimal Lebesgue constants when  $1/2 < \lambda \leq 1$ . Convergence results in the weighted  $L^p$  norm with a generalized Jacobi weight were also obtained. On the other hand, Jung, in [109], studied convergence in the uniform norm of Hermite-Fejér interpolation for the Gegenbauer weight function  $w_\lambda$ ,  $0 \leq \lambda \leq 1$ , based on the zeros of  $\pi_{n+1}^{*(\lambda)}$  or on those of  $\pi_n^{(\lambda)}\pi_{n+1}^{*(\lambda)}$ ; he showed that, except for the second case when  $1/2 < \lambda \leq 1$ , the process has optimal Lebesgue constants. Furthermore, convergence results, when  $0 \leq \lambda \leq 1$ , for Hermite-Fejér interpolation and Hermite interpolation in the weighted  $L^p$  norm were also given. High-order Hermite-Fejér interpolation based either on the zeros of  $\pi_{n+1}^{*(\lambda)}$  or on those of  $\pi_n^{(\lambda)}\pi_{n+1}^{*(\lambda)}$ , when  $0 < \lambda < 1$ , has been studied by Jung and Sakai (cf. [111]).

Moreover, Marcinkiewicz inequalities based on the zeros of the Stieltjes polynomials  $\pi_{n+1}^{*(\lambda)}$  or on those of  $\pi_n^{(\lambda)}\pi_{n+1}^{*(\lambda)}$  relative to the Gegenbauer weight function  $w_\lambda$ ,  $0 < \lambda < 1$ , are studied by Ehrich and Mastroianni in [65].

Polynomials orthogonal on a circular arc, together with the associated functions of the second kind and the corresponding Stieltjes polynomials, have been studied by Milovanović and Rajković (cf. [137]).

Stieltjes-type polynomials have been considered in two instances. Prévost (cf. [186]) studied them with respect to a linear functional; these polynomials are important for the estimation of the error in Padé approximation. On the other hand, de la Calle Ysern, López Lagomasino, and Reichel (cf. [44]) defined Stieltjes-type polynomials on the unit circle; the nodes of these polynomials were used for the development of Szegő-Kronrod quadrature formulae, which are useful for the integration of periodic functions with known periodicity. An extension of the results in [44] can be found in [43], while Szegő-Kronrod quadrature is briefly mentioned in [106].

**9. Historical notes.** The subject of the present survey started with Kronrod in 1964, who developed, at least up to a point, the underlying theory of the quadrature formulae that bear his name, and he produced extensive numerical tables for the nodes and weights of these formulae (cf. [119, 120]).

As already mentioned, the Gauss-Kronrod formulae are closely connected with work that Stieltjes did some 70 years earlier. The  $n + 1$  new nodes that Kronrod added to the  $n$  Gauss nodes in order to construct his quadrature formula are zeros of a polynomial considered and named after Stieltjes, who used it in his study of continued fractions and the moment problem. As in all of Kronrod's exposition there is no mention of Stieltjes's work, it is safe to assume that the former was unaware of the work of the latter.

Now, fairly recently, Gautschi (cf. [86]) discovered that in the same year that Stieltjes presented his polynomials, Skutsch (cf. [203]) pointed out the possibility of obtaining a new quadrature formula, by inserting  $n + 1$  new nodes into the  $n$ -point Gauss formula for the Legendre weight function and choosing them and all quadrature weights in such a way that the resulting  $(2n + 1)$ -point formula has degree of exactness  $3n + 1$  for  $n$  even and  $3n + 2$  for  $n$  odd. He even noted that for improving the degree of exactness of the  $n$ -point Gauss formula, one cannot add fewer than  $n + 1$  points (cf. [203, p. 81]), a result proved later by Monegato (cf. [147, Lemma 1]). Skutsch also gave a numerical example, implementing the 7-point extension of the 3-point Gauss formula and comparing it with the 3-point and the 7-point Gauss formulae. Did Stieltjes know about Skutsch's paper? As his letter to Hermite (cf. [3, v. 2, pp. 439–441]) contains no reference to quadrature, most likely, he was unaware of Skutsch's work.

So, both Skutsch and Kronrod had the same idea, although the former did not pursue it further, while the latter did and received credit for it.

All this brings us to the natural question: Who was Kronrod? An answer to that was given only recently, when Gautschi discovered and edited the exposition *Remembering A.S. Kronrod* by Landis and Yaglom (cf. [122]). Alexander Semenovich “Sasha” Kronrod was born in 1921 and, by education, was a mathematician. He studied at Moscow State University, from where he received his Doctoral Degree. He started as a pure mathematician, having made important contributions to the theory of functions of two or more variables; in particular, he introduced the concept of a monotone function in two variables. Later on, though, his interests shifted to computational mathematics and computer science; he conceived and implemented, together with N. I. Bessonov, the idea of a universal program-controlled digital computer, and he was also interested in what is now called artificial intelligence (in those days known as heuristic programming). All this reflects one of Kronrod’s leading principles: An idea is nothing, its implementation everything; and it was for this reason that he generously gave away ideas that he had, being convinced that the ownership of an idea actually belongs to the one who implemented it. He also believed that a mathematician solving the mathematical aspect of a physical problem should understand the significance of the problem, realize how the results obtained are going to be used, work out the algorithm for the problem’s solution, write the program implementing the algorithm, and run it. Besides pure and computational mathematics and computer science, he also made contributions to economics, in particular, price formation. He was a great teacher, respected and appreciated by his students. The last part of his life was devoted to helping the terminally ill, by developing a medicine for cancer patients. He died of a stroke in 1986.

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