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An Overview of Results on the Existence or Nonexistence and the Error Term of Gauss-Kronrod Quadrature Formulae

Sotirios E. Notaris*

Dedicated to Walter Gautschi on the occasion of his 65th birthday

Abstract. Kronrod in 1964, trying to estimate economically the error of the n-point Gauss-Legendre quadrature formula, 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 the zeros of a polynomial orthogonal with respect to a variable-sign weight function. This polynomial was considered for the first time by Stieltjes in 1894. Important for the new formula, now appropriately called the Gauss-Kronrod quadrature formula, are properties such as the interlacing of the Gauss nodes with the new nodes, the inclusion of all nodes in the interior of the interval of integration, and the positivity of all quadrature weights. We review, for classical and nonclassical weight functions, the existence or nonexistence and the error term of Gauss-Kronrod formulae having one or more of the aforementioned properties.

1 INTRODUCTION

The Gauss quadrature formula for the Legendre weight function $w(t) = 1$ on $[-1,1]$ has the form

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

where $\tau_\nu = \tau_\nu^{(n)}$ are the zeros of the nth-degree (monic) Legendre polynomial π_n, and $\gamma_\nu = \gamma_\nu^{(n)}$ are the Christoffel numbers. It is known that (1.1) has degree of exactness $d_n^G = 2n-1$, i.e., $R_n^G(f) = 0$ for all $f \in \mathbf{P}_{2n-1}$.

Let $Q_n^G(f) = \sum_{\nu=1}^{n} \gamma_\nu f(\tau_\nu)$. A practical way to estimate the error of (1.1) is the following. Consider two formulae, one with n points and another with m, where $m > n$. Then

$$|R_n^G(f)| \simeq |Q_n^G(f) - Q_m^G(f)|. \tag{1.2}$$

The disadvantage of this method lies in the number of function evaluations required in order to obtain a reasonable estimate for $R_n^G(f)$. For example, with $m = n+1$

*Department of Mathematics, University of Missouri-Columbia, Columbia, MO 65211, USA; *Current address:* 1 Xenokratous St., 10675 Athens, Greece

additional evaluations of the function f (at the new nodes $\tau_\nu^{(n+1)}$), the degree of exactness goes from $2n-1$ to $2n+1$, only a slight improvement.

Motivated by this, Kronrod in 1964 (cf. [15, 16]) started with the n Gauss nodes τ_ν and added $n+1$ new ones, obtaining what is now called the Gauss-Kronrod quadrature formula,

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

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 (1.3) has maximum degree of exactness. Since there are $3n+2$ degrees of freedom, one expects to get $d_n^K = 3n+1$ (at least). The advantage of using $Q_n^K(f) = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*)$ instead of $Q_m^G(f) = Q_{n+1}^G(f)$ in (1.2) is clear. With the same number of additional evaluations of the function (i.e., $n+1$, at the new nodes τ_μ^*) the degree of exactness goes much higher than $2n+1$.

Let $\pi_{n+1}^*(t) = \prod_{\mu=1}^{n+1}(t-\tau_\mu^*)$. It can be shown (see [8, Corollary]) that (1.3) has degree of exactness $3n+1$ if and only if π_{n+1}^* satisfies the orthogonality condition

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

that is, π_{n+1}^* is orthogonal to all polynomials of lower degree relative to the variable-sign "weight function" $w^*(t) = \pi_n(t)$. This kind of orthogonality was first considered by Stieltjes in 1894, through his work on continued fractions. It goes without saying that the theory of orthogonal polynomials relative to a (nonnegative) weight function cannot be applied here. In particular, there are no general results about the reality of the τ_μ^*, not to mention their inclusion in $(-1,1)$, both of which are important for the practical application of (1.3). Nevertheless, Stieltjes conjectured that π_{n+1}^* has $n+1$ real and simple zeros, all contained in $(-1,1)$, and interlacing with the zeros of π_n (cf. [2, v. 2, pp. 439-441]).

The connection between the Gauss-Kronrod formula (1.3) and the polynomial π_{n+1}^*, now appropriately called Stieltjes polynomial, was first noticed by Mysovskih in [24], and independently by Barrucand in [3].

In recent years, Gauss-Kronrod formulae have attracted considerable interest from both the computational and the mathematical point of view, the former in view of their potential use in packages for automatic integration, and the latter because of the mathematical problems they pose. It is therefore both useful and interesting to examine questions which relate to the computational feasibility of these formulae, such as the interlacing of the nodes τ_ν, τ_μ^*, the inclusion of all nodes in the interior of the interval of integration, and the positivity of all quadrature weights. The present paper summarizes, for classical and nonclassical weight functions, results on the existence and nonexistence of Gauss-Kronrod formulae having one or more of the interlacing, inclusion and positivity properties. Moreover, the error terms of these formulae are reviewed. Previous surveys on the subject can be found in [8, 22].

2 EXISTENCE AND NONEXISTENCE RESULTS

Consider the Gauss-Kronrod formula for the (nonnegative) weight function w on $[a,b]$,

$$\int_a^b f(t)w(t)dt = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*) + R_n^K(f), \tag{2.1}$$

where $\tau_\nu = \tau_\nu^{(n)}$ are the zeros of the nth-degree (monic) orthogonal polynomial $\pi_n(\cdot) = \pi_n(\cdot; w)$ relative to w, and, as in (1.3), $\tau_\mu^* = \tau_\mu^{*(n)}$, $\sigma_\nu = \sigma_\nu^{(n)}$, $\sigma_\mu^* = \sigma_\mu^{*(n)}$ are chosen such that (2.1) has maximum degree of exactness $d_n^K = 3n+1$ (at least). In this case, the orthogonality condition (1.4) takes the form

$$\int_a^b \pi_{n+1}^*(t) t^k \pi_n(t) w(t) dt = 0, \quad k = 0, 1, \ldots, n, \tag{2.2}$$

where $\pi_{n+1}^*(\cdot) = \pi_{n+1}^*(\cdot; w)$ is defined the same way as before. We say that the nodes τ_ν, τ_μ^* in (2.1) interlace if they are all real and, when ordered decreasingly, satisfy

$$\tau_{n+1}^* < \tau_n < \tau_n^* < \cdots < \tau_2^* < \tau_1 < \tau_1^*. \tag{2.3}$$

The weights in (2.1) are given by

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

where $\gamma_\nu = \gamma_\nu^{(n)}$ are the Christoffel numbers in the Gauss formula for the weight function w, and $\|\cdot\|$ is the weighted L_2-norm. Moreover, the interlacing property (2.3) is equivalent to $\sigma_\mu^* > 0$, $\mu = 1, 2, \ldots, n+1$ (see [18, Thms. 1 and 2]). For each $n \geq 1$, we consider the following properties for the formula (2.1).

(a) The nodes τ_ν, τ_μ^* interlace.

(b) All nodes τ_ν, τ_μ^* are contained in (a,b).

(c) All weights σ_ν, σ_μ^* are positive.

(d) All nodes τ_ν, τ_μ^*, without necessarily satisfying (a) and/or (b), are real.

In the following we review, for various weight functions, what has been proved, disproved, or conjectured with regard to the corresponding Gauss-Kronrod formulae having one or more of these properties.

2.1 Classical Weight Functions

The first existence result relates to the Legendre weight function $w(t) = 1$ on $[-1,1]$. Szegö in 1935 (cf. [35]), following Stieltjes's conjectures (see the introduction), expanded the Stieltjes polynomial in a Chebyshev series, and, using some results from the theory of reciprocal power series, proved 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. This allowed him to conclude properties (a) and (b) for all $n \geq 1$. Much later, Monegato, relying on Szegö's work, added property (c) for each $n \geq 1$ (see [19]).

Szegö extended his analysis to the case of the Gegenbauer weight function $w_\lambda(t) = (1-t^2)^{\lambda-1/2}$ on $[-1,1]$, $\lambda > -1/2$, whose special case, with $\lambda = 1/2$, is the Legendre weight. He showed that properties (a) and (b) hold for all $n \geq 1$, when $0 < \lambda \leq 2$ (cf. [35, §3]). Monegato noted in [19] that, as in the Legendre case, property (c) is true for each $n \geq 1$, when $0 \leq \lambda \leq 1$. Szegö was unable to determine what happens for $\lambda > 2$, while for $\lambda \leq 0$, already for $n = 2$, two of the τ_μ^* are outside of $(-1,1)$.

Gautschi and Notaris in [9] tried to close these gaps. Given n, one can compute the precise interval $(\lambda_n^p, \Lambda_n^p)$ of λ such that property (p) is valid, where $p =$ a,b,c,d. This can be done by varying λ and monitoring the motion of the nodes and weights in (2.1). Property (a) breaks down when a node τ_ν collides with a node τ_μ^*. This can be detected from the vanishing of the resultant of $\pi_n^{(\lambda)}(\cdot) = \pi_n(\cdot; w_\lambda)$ and $\pi_{n+1}^{*(\lambda)}(\cdot) = \pi_{n+1}^*(\cdot; w_\lambda)$. Similarly, property (d) ceases to hold when two nodes τ_μ^* collide and split to a pair of conjugate complex nodes, or equivalently, when the discriminant of $\pi_{n+1}^{*(\lambda)}$ vanishes. For properties (b) and (c) things are simpler. Assuming the interlacing property, the former amounts to finding when $\tau_1^* = 1$ and $\tau_{n+1}^* = -1$, while for the latter it suffices to find a $\sigma_\nu = 0$ (the interlacing property is equivalent to the positivity of the σ_μ^*; cf. [18, Thm. 1]). Gautschi and Notaris carried out this project analytically for $n = 1(1)4$, and numerically for $n = 5(1)20(4)40$. The corresponding values of λ_n^p, Λ_n^p, $p =$ a,b,c,d, are given in [9, Tables 2.1 and A.1].

Nonexistence results have been obtained by Monegato, and also by Notaris. Monegato proved (cf. [21, Thm. 1]) that the Gauss-Kronrod formula for the weight function w_λ, having properties (c) and (d), and degree of exactness $[2rn + l]$, where $r > 1$ and l is an integer, does not exist for all $n \geq 1$ when λ is sufficiently large.†

On the other hand, Notaris started from the limit formula that connects the Gegenbauer and Hermite orthogonal polynomials, and showed (cf. [26, §2]) that the corresponding Stieltjes polynomials $\pi_{n+1}^{*(\lambda)}$ and π_{n+1}^{*H} satisfy an analogous formula, namely, $\lim_{\lambda\to\infty} \lambda^{(n+1)/2}\pi_{n+1}^{*(\lambda)}(\lambda^{-1/2}t) = \pi_{n+1}^{*H}(t)$, $n \geq 1$. Then, based on this formula and a nonexistence result of Kahaner and Monegato for the Hermite weight function (cf. [14, Corollary]), he proved that the Gauss-Kronrod formula for the weight function w_λ and $n \neq 1,2,4$, having properties (c) and (d), does not exist if $\lambda > \lambda_n$, where λ_n is a constant sufficiently large.

Regarding the Jacobi weight function $w^{(\alpha,\beta)}(t) = (1-t)^\alpha(1+t)^\beta$ on $[-1,1]$, $\alpha > -1$, $\beta > -1$, the only results that have been proved concern (besides the Chebyshev weights, which are discussed below) the special cases $w^{(\alpha,1/2)}$ and

†The proof has an error, but can be repaired.

$w^{(-1/2,\beta)}$. For the first it can be shown that $\pi_{n+1}^{*(\alpha,1/2)}(2t^2-1) = 2^{n+1}\pi_{2n+2}^{*(\alpha,\alpha)}(t)$, $n \geq 1$ (see [22, Eq. (32)]). Then the nodes and weights in the Gauss-Kronrod formula for $w^{(\alpha,1/2)}$ can be expressed in terms of the corresponding ones for $w^{(\alpha,\alpha)}$, i.e., the Gegenbauer weight (see [9, Thm. 5.1]). Therefore, all results of the previous paragraphs, concerning $w^{(\alpha,\alpha)}$, can be applied to arrive at conclusions for $w^{(\alpha,1/2)}$. On the other hand, for the weight function $w^{(-1/2,\beta)}$, Rabinowitz has shown (cf. [32, pp. 74-75]‡) 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. Moreover, since interchanging α and β in $w^{(\alpha,\beta)}$ causes only a change in the sign of the nodes of the respective Gauss-Kronrod formula, the weights corresponding to nodes symmetric with respect to the origin being the same, one can derive for $w^{(1/2,\beta)}$ and $w^{(\alpha,-1/2)}$ results analogous to those obtained for $w^{(\alpha,1/2)}$ and $w^{(-1/2,\beta)}$.

Gautschi and Notaris in [9] extended their investigations to the Jacobi weight function, and using the same methods as for the Gegenbauer weight, they delineated, for a given n, areas in the (α,β)-plane where each of the properties (a), (b) and (c) (and also (d) when $n = 1$) holds. Their findings, explicitly for $n = 1$ and in the form of graphs for $n = 2(1)10$, are given in [9, p. 239 and Figure 4.1].

Also, Notaris obtained a nonexistence result. First, starting from the limit formula that connects the Jacobi and Laguerre orthogonal polynomials, he showed (cf. [26, §3]) that an analogous formula holds for the corresponding Stieltjes polynomials $\pi_{n+1}^{*(\alpha,\beta)}$ and $\pi_{n+1}^{*(\alpha)}$, namely,

$$\lim_{\beta\to\infty} (\beta/2)^{n+1}\pi_{n+1}^{*(\alpha,\beta)}(1 - 2\beta^{-1}t) = (-1)^{n+1}\pi_{n+1}^{*(\alpha)}(t), \; n \geq 1.$$

This formula, together with a nonexistence result of Kahaner and Monegato for the Laguerre weight function (cf. [14, Theorem]), led him to conclude that the Gauss-Kronrod formula for the weight function $w^{(\alpha,\beta)}$, α 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 sufficiently large.

When $|\alpha| = |\beta| = 1/2$ in $w^{(\alpha,\beta)}$, we obtain the Chebyshev weight functions of the four kinds, for which the Gauss-Kronrod formula has a special form. Specifically, for $\alpha = \beta = -1/2$, i.e., the Chebyshev weight of the first kind, the Gauss-Kronrod formula is the three-point Gauss formula when $n = 1$, and the $(2n + 1)$-point Gauss-Lobatto formula when $n \geq 2$, for the same weight. For $\alpha = \beta = 1/2$, i.e., the Chebyshev weight of the second kind, we get 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 the preassigned node at 1 and -1, respectively. Furthermore, the degree of exactness for each of these formulae is higher than the expected $3n + 1$, 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

‡The superscript $\mu + 1/2$ in Eq. (68) and in the discussion following Eq. (69) should read $\mu - 1/2$.

$\alpha = \mp 1/2$, $\beta = \pm 1/2$. All this has been noted first by Mysovskih in [24], and later on by Monegato in [18, §4], and [22, pp. 152-153]. In addition, Monegato in [18, §4] showed that in the cases $\alpha = \beta = \pm 1/2$, Kronrod's idea can be iterated to produce a sequence of quadrature formulae, in which the nodes and weights are explicitly known.

Very little yet has been proved for the Hermite weight function $w_H(t) = \mathrm{e}^{-t^2}$ on $(-\infty, \infty)$ and the Laguerre weight function $w^{(\alpha)}(t) = t^\alpha \mathrm{e}^{-t}$ on $[0, \infty)$, $\alpha > -1$. Both have been examined numerically for n up to 20. For the former, it has been found (cf. [18, §3], [34]) that the Gauss-Kronrod formula has property (d) only for $n = 1, 2, 4$. On the other hand, for the Laguerre weight, with $\alpha = 0$, numerical calculations indicate that the Gauss-Kronrod formula has real nodes, but one is negative, when $n = 1$, and has some complex nodes for $2 \leq n \leq 20$ (see [18, §3]).

A nonexistence result has been obtained by Kahaner and Monegato in [14]. 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 $\alpha = 0$). As a consequence of this, they concluded that the corresponding formula for the weight function w_H, having properties (c) and (d), does not exist if $n \neq 1, 2, 4$.[§] The nonexistence result for the Laguerre weight remains true for n sufficiently large, even if the degree of the Gauss-Kronrod formula is lowered to $[2rn + l]$, where $r > 1$ and l is an integer (see [21, Thm. 2]).

2.2 Nonclassical Weight Functions

A class of weight functions for which the Gauss-Kronrod formulae have been extensively studied by several authors are the so-called Bernstein-Szegö weight functions defined by $w^{(\pm 1/2)}(t) = (1-t^2)^{\pm 1/2}/\rho(t)$, $w^{(\pm 1/2, \mp 1/2)}(t) = (1-t)^{\pm 1/2}(1+t)^{\mp 1/2}/\rho(t)$ on $[-1, 1]$, where $\rho(t)$ is a polynomial of arbitrary degree that remains positive on $[-1, 1]$. The associated orthogonal and Stieltjes polynomials are linear combinations of Chebyshev polynomials of the four kinds. As a result of this, the corresponding Gauss-Kronrod formulae have properties (a), (b) and (c) for almost all n, exceptions occurring only for n below a specific value. In addition, the degree of exactness of these formulae is of the order $O(4n)$ instead of the usual $O(3n)$. To be precise, for the weight function $w_0^{(1/2)}(t) = (1+\gamma)^2(1-t^2)^{1/2}/[(1+\gamma)^2 - 4\gamma t^2]$ on $[-1, 1]$, $-1 < \gamma \leq 1$, which appeared for the first time in work of Geronimus (cf. [12]) and belongs to the above class of weight functions, property (b) was shown by Monegato in [22, p. 146], and properties (a) and (c) by Gautschi and Rivlin in [11], for all $n \geq 1$. (Property (b) for $n = 1$ is not shown in [22, p. 146], but can easily be verified.) Similarly, for the weight function $w^{(1/2)}$, with ρ a quadratic polynomial, the orthogonal and Stieltjes polynomials have been studied by Monegato and Palamara Orsi (cf. [23]). All four weights $w^{(\pm 1/2)}$, $w^{(\pm 1/2, \mp 1/2)}$, with ρ a

[§]This nonexistence result is stated in [14, Corollary] as follows: "Extended Gauss-Hermite rules with positive weights (and real nodes) only exist for $n = 1, 2, 4$". This is not quite accurate, since for $n = 4$ two of the σ_ν's in (2.1), relative to w_H, are negative.

quadratic polynomial, have been considered by Gautschi and Notaris in [10]. Properties (a), (b) and (c) have been established for almost all n, and the exceptions, which occur for $n \leq 3$, have been carefully identified. Also, the precise degree of exactness of the quadrature formulae in question has been determined. The general case of the weights $w^{(\pm 1/2)}$, $w^{(\pm 1/2, \mp 1/2)}$, with ρ a polynomial of arbitrary degree l, has been treated by Notaris in [25]. It was shown that properties (a), (b) 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 $w = w^{(\pm 1/2, \mp 1/2)}$. The corresponding degrees of exactness are respectively $4n-l-1, 4n-l+1$, and $4n-l$. For the weight $w^{(1/2)}$, with ρ a polynomial of arbitrary degree, Peherstorfer in [28] constructed a sequence of quadrature formulae by iterating Kronrod's idea. More precisely, he considered an n-point interpolatory quadrature formula whose nodes are the zeros of $\pi_n(\cdot; w^{(1/2)}(t)/q(t))$, where $q(t)$ is a polynomial of arbitrary degree m that remains positive on $[-1,1]$. If N^* is a natural number satisfying $2^{N^*-1}(n+1) \geq 2^{N^*}(l+m)+1-l$, then Peherstorfer showed that the quadrature formula in question admits N^* Kronrod extensions, all having properties (b) and (c). In addition, the nodes of the Nth Kronrod extension interlace with those of the $(N-1)$st extension, and the Nth Kronrod extension has degree of exactness $2^N[2(n+1)-(l+m)]+l-3$,† $N = 1, 2, \ldots, N^*$.

Peherstorfer in [29] extended his work to 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. He begins with an analysis of the asymptotic behavior of the associated functions of the second kind, which subsequently is used, in view of the connection between functions of the second kind and Stieltjes polynomials, to show that the corresponding Gauss-Kronrod formula has properties (a), (b) and (c) for all $n \geq n_0$, where n_0 is a constant not explicitly specified. The weight function in consideration includes as a special case the Bernstein-Szegö weight $w^{(1/2)}$, with ρ a polynomial of arbitrary degree, for which the same results were obtained in [25, 28], with the addition that n_0 was specified there.

Going even further, Peherstorfer in [30] considered polynomials orthogonal on the unit circle, and studied the asymptotic behavior of the associated functions of the second kind. This allowed him to arrive at conclusions for the asymptotic behavior of functions of the second kind associated with polynomials orthogonal on 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 $\pi_{n+1}(\cdot; w)$. In addition, he proved that the Gauss-Kronrod formula for the weight function w^* has properties (a), (b) and (c) for all $n \geq n_0$, where n_0 is a constant not explicitly specified.‡

For the weight function ${}^\gamma w^{(\alpha)}(t) = |t|^\gamma(1-t^2)^\alpha$ on $[-1,1]$, $\alpha > -1$, $\gamma > -1$,

†In [28, Theorem(c)], the 4 in the subscript of the displayed inclusion relation should be replaced by 3.

‡In [30, Theorem 4.2(a)], the subscript μ extends up to $n+1$.

Gautschi and Notaris have shown (cf. [9, Thm. 5.2]) that the corresponding Gauss-Kronrod formula with n odd can be obtained from the one for the Jacobi weight $w^{(\alpha,(1+\gamma)/2)}$. Therefore, whatever is known for the latter can be applied to arrive at conclusions for the former.

Numerical computations of Caliò, Gautschi and Marchetti in [4, 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 $n \geq 1$, with the exception of the weight with $\alpha = -1/2$ and n odd, for which property (b) (but not (d)) seems to be false. However, none of this has been proved yet.

3 ERROR TERM

The Gauss-Kronrod formula (2.1) can be obtained by applying the idea of Markov (cf. [17]). To be precise, we interpolate the function f at the simple nodes τ_{ν} and the double nodes τ_{μ}^{*}, and then integrate the resulting Hermite interpolation polynomial $p_{3n+1}(\cdot; f; \tau_{\nu}, \tau_{\mu}^{*}, \tau_{\mu}^{*})$ of degree at most $3n+1$. Evidently, the quadrature formula derived that way contains the values $f'(\tau_{\mu}^{*})$. To arrive at formula (2.1), we require that the weights corresponding to these values be all 0, and this requirement leads to the orthogonality condition (2.2).

Integrating the interpolation error yields an expression for the error term of formula (2.1),

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

assuming that $f \in C^{3n+2}[a,b]$. This formula was applied by Monegato in the case of the Gegenbauer weight function $w_{\lambda}(t) = (1-t^2)^{\lambda-1/2}$ on $[-1,1]$, $0 < \lambda < 1$ (see [20, §3]), in conjunction with $|\pi_{n+1}^{*(\lambda)}(t)| < 2^{-(n-1)}$, $-1 \leq t \leq 1$ (which follows directly from the work of Szegö in [35]) and bounds for $|\pi_n^{(\lambda)}(t)|$ (cf. [36, Eqs. (4.7.9) and (7.33.1)]), in order to derive a bound for $|R_n^K(f)|$ in terms of $\|f^{(3n+2+k)}\|_{\infty}$, where $k = 0$ for n even and $k = 1$ for n odd. This bound was improved and extended to the case $1 < \lambda < 2$ by Rabinowitz in [31, §4]. In the same paper, Rabinowitz proved that the Gauss-Kronrod formula for w_{λ}, $0 < \lambda \leq 2$, $\lambda \neq 1$, 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, as already stated in the previous section, the degree of exactness is $4n-1$ (5 for $n=1$) and $4n+1$, respectively. Also, Rabinowitz, based on a result of Akrivis and Förster in [1] and work of Szegö in [35], showed that the Gauss-Kronrod formula for the weight w_{λ}, $0 < \lambda < 1$, and $n \geq 2$, is nondefinite (see [33]).

Ehrich in [5] considers the Gauss-Kronrod formula for the Legendre weight function $w(t) = 1$ on $[-1,1]$ and is concerned with bounds for the error term of the form $|R_n^K(f)| \leq c_s(R_n^K)\|f^{(s)}\|_{\infty}$, where $c_s(R_n^K) = \sup_{\substack{f \in C^s[-1,1] \\ \|f^{(s)}\|_{\infty} \leq 1}} |R_n^K(f)|$. In particular, using results of Szegö in [35] and Rabinowitz in [31], he computes an upper bound for $c_{3n+2+k}(R_n^K)$, where $k = 0$ for n even and $k = 1$ for n odd, and examines its quality. Subsequently, he shows that there are better quadrature formulae using the same number of nodes, by comparing $c_{3n+2+k}(R_n^K)$ with $c_{3n+2+k}(R_{2n+1}^G)$ of the corresponding Gauss formula with $2n + 1$ points. Going further, he obtains in [6] upper bounds for c_s, $s < 3n + 2 + k$, useful for classes of functions of lower continuity. In the same paper, he extends the results in [5] to the case of the Gegenbauer weight function w_λ, $0 < \lambda < 1$. The quality of the bounds obtained in both cases is examined as well.

Also, Ehrich uses the results in [5] in order to derive bounds for the error term appropriate for analytic functions (cf. [7]). Specifically, if f is analytic in a simply connected region containing a closed contour C in its interior which surrounds $[-1, 1]$, he obtains bounds for R_n^K of the form $|R_n^K(f)| \le l(C)c(n, \delta) \max_{z \in C} |f(z)|$, where $l(C)$ is the length of C and $\delta > 0$ is a lower bound for the distance between any point on C and any point in $[-1, 1]$. In the same paper, he studies the behavior of R_n^K when applied to Chebyshev polynomials of the first and second kind.

A different approach to the error term of the Gauss-Kronrod formula relative to the Legendre weight function is taken by Notaris in [27]. Let f be a holomorphic function in $C_r = \{z \in \mathrm{C} : |z| < r\}$, $r > 1$. Then $f(z) = \sum_{k=0}^{\infty} a_k z^k$, $z \in C_r$. Define $|f|_r = \sup\{|a_k| r^k : k \in \mathbb{N}_0 \text{ and } R_n^K(t^k) \neq 0\}$, and set $X_r = \{f : f \text{ holomorphic in } C_r \text{ and } |f|_r < \infty\}$. It is easy to show that $|\cdot|_r$ is a seminorm on X_r, and that the error term R_n^K of the Gauss-Kronrod formula for the Legendre weight function is a continuous linear functional on $(X_r, |\cdot|_r)$. This leads to bounds for R_n^K of the form $|R_n^K(f)| \le \|R_n^K\|_r |f|_r$, the right-hand side of which can be optimized as a function of r, that is, if $f \in X_R$, then $|R_n^K(f)| \le \inf_{1<r\le R}(\|R_n^K\|_r |f|_r)$. Another bound for R_n^K can be obtained if $|f|_r$ is estimated by $\max_{|z|=r} |f(z)|$ (cf. [13, Eq. (4.2)]). Notaris, following the analysis of Hämmerlin in [13] for the error term of the Gauss-Legendre formula, gives an upper bound for $\|R_n^K\|_r$, $2 \le n \le 30$. (When $n = 1$, the Gauss-Kronrod formula for the Legendre weight function is the 3-point Gauss formula for the same weight function.) Notaris's method can also be extended to $n > 30$, after the computation of appropriate constants.

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