

A Survey of Gauss-Christoffel Quadrature Formulae

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We present a historical survey of Gauss-Christoffel quadrature formulae, beginning with Gauss' discovery of his well-known method of approximate integration and the early contributions of Jacobi and Christoffel, but emphasizing the more recent advances made after the emergence of powerful digital computing machinery. One group of inquiry concerns the development of the quadrature formula itself, e.g. the inclusion of preassigned nodes and the admission of multiple nodes, as well as other generalizations of the quadrature sum. Another is directed towards the widening of the class of integrals made accessible to Gauss-Christoffel quadrature. These include integrals with nonpositive measures of integration and singular principal value integrals. An account of the error and convergence theory will also be given, as well as a discussion of modern methods for generating Gauss-Christoffel formulae, and a survey of numerical tables.

Introduction

Gauss' famous method of approximate integration, almost immediately after its discovery and throughout the 19th century, attracted the attention of some of the leading mathematicians of the time. It first inspired Jacobi to provide an elegant alternative derivation. Christoffel then significantly generalized the method and subsequently extended it to arbitrary measures of integration. Stieltjes established the legitimacy of the method, by proving its convergence, while Markov endowed it with an error term. Thus, by the end of the 19th century, the Gauss-Christoffel integration method became firmly entrenched in the repertoire of numerical methods of approximation.

Whether or not the Gauss-Christoffel method had actually been widely used in practice is a matter of some doubt, since the method requires the evaluation of functions at irrational arguments, hence tedious interpolation. All this changed when powerful digital computers entered the scene, which generated a climate of renewed interest in Gauss-Christoffel quadrature. The formulae began to be routinely applied, and increased usage, in turn, led to important new theoretical developments. The state of the art, including applications and extensive numerical tables, has been summarized in the book by Stroud & Secrest [1966]. Here we wish to present an extensive historical survey of Gauss-Christoffel quadrature formulae, covering the period from the early beginnings to the most recent developments, emphasizing, however, the progress made in the last 10-15 years.

We begin in Section 1 with a brief outline of the discovery of Gauss and

the early contributions of Jacobi, Christoffel, and others. In Section 2 we describe how the Gauss–Christoffel quadrature rule has been extended in various directions, first by Christoffel, who introduced preassigned nodes, then much later by Turán and others, who introduced derivative values in addition to function values. Closely related to Christoffel’s work is Kronrod’s extension of Gauss–Christoffel quadrature rules, which leads to practical schemes of implementation. Further miscellaneous extensions of the idea of Gauss continue to be made. Section 3 is devoted to various efforts of extending the scope of applications of Gauss–Christoffel formulae. Thus, applications to more general types of integrals are considered, including integrals with nonpositive measures of integration and singular principal value type integrals. In Section 4 we review work on the remainder term and related questions of convergence. Section 5, finally, will deal with constructive methods of generating Gauss–Christoffel formulae and also contains a review of available numerical tables.

Although an effort has been made to make this survey reasonably complete, it was not possible to include all topics of interest. Perhaps the most important omission is the extension of Gauss–Christoffel quadrature formulae to multiple integrals. While it is not entirely clear what constitutes a Gauss–Christoffel formula for a multiple integral, various interpretations are possible. A full discussion of these, however, would go beyond the scope of this review. Indefinite integrals, likewise, have been omitted from consideration. Numerous applications of Gauss–Christoffel’s quadrature formula have been, and continue to be made, both within the fields of numerical analysis and outside of it. It was not feasible to survey them all, and we restricted ourselves to mentioning only a few selected applications, as the occasion permits. Special properties of zeros of orthogonal polynomials and of Christoffel numbers, and composite Gauss–Christoffel formulae, are additional topics left out from consideration.

1. Genesis of Gaussian Quadrature and Early History

The story of Gaussian quadrature begins with Newton and Cotes. Newton, in 1676, was the first to suggest a truly general method of approximate integration. Cotes, independently, arrived at similar methods, and brought them into workable form after learning of Newton’s ideas. In 1814, Gauss takes the work of Newton and Cotes as a point of departure, combines it with his own work on the hypergeometric series, and develops his famous new method of integration which significantly improves upon the earlier method of Newton and Cotes. Gauss’ work in turn was simplified by Jacobi and further developed through much of the 19th century by Mehler, Christoffel, and others. Eventu-

ally, there emerged a coherent theory which received its first systematic expositions by Christoffel [1877], Radau [1880], and Heine [1881] in his book on spherical functions.

In this section, we can only give a bare outline of the developments that took place in this period of approximately 200 years. A very detailed historical account can be found in Runge & Willers [1915], and a German edition of the four principal memoirs (of Newton, Cotes, Gauss and Jacobi) in Kowalewski [1917]. The important contribution of Christoffel [1858], which also falls in this period but points into new directions, will be discussed later in Section 2.1.1.

1.1. Newton–Cotes quadrature formulae

One of Newton's early accomplishments (which he already alluded to in a letter to Leibniz, dated October 24, 1676, and published later in 1687 as Lemma 5 in the third book of the "Principia") was his "... expeditious method of passing a parabolic curve through given points". In modern terminology, given a function f and n pairwise distinct points τ_ν , Newton constructs the unique polynomial $p_{n-1}(f; \cdot)$ of degree $\leq n - 1$ which at the points τ_ν assumes the same values as f ,

$$p_{n-1}(f; \tau_\nu) = f(\tau_\nu), \quad \nu = 1, 2, \dots, n, \quad p_{n-1} \in \mathbf{P}_{n-1}.$$

Newton ingeniously expresses this interpolation polynomial in terms of divided differences. Here we find it more convenient to express it in the form given much later (1795) by Lagrange,

$$(1.1) \quad p_{n-1}(f; t) = \sum_{\nu=1}^n l_\nu(t) f(\tau_\nu),$$

where $l_\nu \in \mathbf{P}_{n-1}$ are the special polynomials with $l_\nu(\tau_\nu) = 1$ and $l_\nu(\tau_\mu) = 0$, $\mu \neq \nu$. If we write

$$(1.2) \quad f(t) = p_{n-1}(f; t) + r_n(f; t),$$

where $r_n(f; \cdot)$ denotes the interpolation error, we then have, by the uniqueness of the interpolation polynomial,

$$(1.3) \quad r_n(f; \cdot) = 0, \quad \text{all } f \in \mathbf{P}_{n-1}.$$

Newton, in the "Principia", already hints at the possibility that "... the area under the curve can be found, since the quadrature of a parabolic curve can be effected". Indeed, if

$$(1.4) \quad I(f) = \int_a^b f(t) dt,$$

where $a < b$ are finite numbers, integration of (1.2) yields

$$(1.5) \quad I(f) = Q_n(f) + R_n(f), \quad Q_n(f) = \sum_{\nu=1}^n \lambda_\nu f(\tau_\nu)$$

where, by (1.1),

$$(1.6) \quad \lambda_\nu = I(l_\nu), \quad \nu = 1, 2, \dots, n, \quad R_n(f) = I(r_n(f; \cdot)).$$

(The quantities λ_ν , as well as the points τ_ν , depend on n ; for simplicity we suppress this dependence in our notation, both here and in subsequent discussions.) One calls (1.5) an n -point *quadrature formula*, $Q_n(f)$ the *quadrature sum*, and $R_n(f)$ the *remainder*. The points τ_ν are also referred to as *nodes*, while the numbers λ_ν are called the *weights* of the quadrature formula. The quadrature sum is expected to approximate the integral, the error being given by the remainder. The latter, by virtue of (1.3), satisfies

$$(1.7) \quad R_n(f) = 0, \quad \text{all } f \in \mathbf{P}_{n-1}.$$

Following Radau [1880], one expresses (1.7) by saying that the quadrature rule Q_n has *degree of exactness* $n - 1$, and we write $d(Q_n) = n - 1$. (Q_n then also has degree of exactness k for any integer k with $0 \leq k < n$.) It is easily seen that a quadrature formula Q_n has degree of exactness $n - 1$ if and only if it is obtained via interpolation, as described. Hence Q_n , for which (1.7) holds, is also called *interpolatory*.

In the case of equally spaced points τ_ν , the numbers λ_ν in (1.6) can be computed once and for all. They are called *Cotes numbers*, in recognition of Roger Cotes who first computed them for $n \leq 11$. (For a history of these numbers, see Johnson [1915].) In the case of arbitrary (distinct) nodes τ_ν , the Cotes numbers can be expressed in terms of the *node polynomial*

$$(1.8) \quad \omega_n(t) = \prod_{\nu=1}^n (t - \tau_\nu).$$

Indeed, from (1.6), using Lagrange's formula for l_ν , one gets

$$(1.9) \quad \lambda_\nu = I \left[\frac{\omega_n(\cdot)}{\omega_n'(\tau_\nu)(\cdot - \tau_\nu)} \right], \quad \nu = 1, 2, \dots, n.$$

The formula (1.5), with λ_ν given by (1.9), is called the *Newton-Cotes quadrature formula*. It includes as special cases the trapezoidal formula, Simpson's formula, and many other formulas that were known prior to Newton's time. It will serve here as a basis on which to build the more advanced quadrature formulae to be discussed later in this survey.

1.2. The discovery of Gauss

If we let the nodes τ_ν in the Newton-Cotes formula (1.5) vary freely, and for each set of (distinct) nodes compute the weights λ_ν in accordance with (1.9),

what is the maximum degree of exactness that can be achieved? And how are the nodes τ_ν to be selected in order to realize this optimum? These were questions raised by Gauss [1814], and answered most elegantly by means of his theory of continued fractions associated with hypergeometric series.

To begin with, one easily conjectures that $\max_{\tau_\nu, \lambda_\nu} d(Q_n) = 2n - 1$, since there are $2n$ unknowns to be found, and $2n$ conditions imposed. To verify the conjecture, Gauss starts from the characteristic function of the “monomial errors”,

$$R_n\left(\frac{1}{z-\cdot}\right) = \sum_{k=0}^{\infty} \frac{R_n(t^k)}{z^{k+1}},$$

where z is a formal parameter (intended to be large). The problem then amounts to determine τ_ν, λ_ν such that

$$R_n\left(\frac{1}{z-\cdot}\right) = O\left(\frac{1}{z^{2n+1}}\right), \quad z \rightarrow \infty.$$

Observe now that for the integral in (1.4), where $b = -a = 1$,

$$(1.10) \quad I\left(\frac{1}{z-\cdot}\right) = \ln \frac{1+1/z}{1-1/z} = \frac{2}{z} - \frac{1/3}{z^2} + \frac{2 \cdot 2/3 \cdot 5}{z^3} - \frac{3 \cdot 3/5 \cdot 7}{z^4} \dots$$

The continued fraction on the right was well known to Gauss, being a special case of his general continued fraction for ratios of hypergeometric functions (Gauss [1812]). He also knew well that the n -th convergent — a rational function $R_{n-1,n}$ with numerator degree $n - 1$ and denominator degree n — if expanded in reciprocal powers of z , approximates the function on the left up to terms of order z^{-2n-1} ,

$$I\left(\frac{1}{z-\cdot}\right) = R_{n-1,n}(z) + O\left(\frac{1}{z^{2n+1}}\right), \quad z \rightarrow \infty.$$

Gauss now decomposes $R_{n-1,n}$ in partial fractions and takes the residues and poles to be the weights and nodes in the quadrature formula (1.5),

$$R_{n-1,n}(z) = \sum_{\nu=1}^n \frac{\lambda_\nu}{z - \tau_\nu} =: Q_n\left(\frac{1}{z-\cdot}\right).$$

It then follows immediately that

$$\begin{aligned} R_n\left(\frac{1}{z-\cdot}\right) &= I\left(\frac{1}{z-\cdot}\right) - Q_n\left(\frac{1}{z-\cdot}\right) \\ &= I\left(\frac{1}{z-\cdot}\right) - R_{n-1,n}(z) = O\left(\frac{1}{z^{2n+1}}\right), \quad z \rightarrow \infty, \end{aligned}$$

hence $d(Q_n) = 2n - 1$, as desired. Gauss proceeds to express the denominator

and numerator polynomials of $R_{n-1,n}$ (now known as Legendre polynomials of the first and second kind) in terms of his hypergeometric series.

Gauss' discovery must be rated as one of the most significant events of the 19th century in the field of numerical integration and perhaps in all of numerical analysis. The result not only has great beauty and power, but also influenced many later developments in computing and approximation. It soon inspired contemporaries, such as Jacobi and Christoffel, to perfect Gauss' method and to develop it into new directions. Towards the end of the century, it inspired Heun [1900] to generalize Gauss' idea to ordinary differential equations, which in turn led to significant developments in the numerical solution of differential equations, notably the discovery of the Runge-Kutta method (Kutta [1901]). Gauss' influence continues into the 20th century and is still felt today, as we shall have ample occasion to document in subsequent chapters of this survey.

1.3. The contribution of Jacobi

The continued fraction (1.10) and its close association with the integral $I(1/(z - \cdot))$ is seen by Gauss to be the true source of his new method of integration. Jacobi [1826], on the other hand, with characteristic clarity and simplicity, derives Gauss' result purely on the basis of polynomial divisibility arguments. The central concept that emerges in Jacobi's work is *orthogonality*. (The name "orthogonal" for function systems came into use only later, probably first in E. Schmidt's 1905 Göttingen dissertation; see also Schmidt [1907, p. 439]. For polynomials, the term appears in the early writings of Szegö (Szegö [1918], [1919]. Murphy [1835] uses the term "reciprocal".) In effect, Jacobi shows that, *given any integer k , with $0 \leq k \leq n$, the quadrature rule Q_n in (1.5) has degree of exactness $d(Q_n) = n - 1 + k$ if and only if the following two conditions are satisfied:*

- (i) Q_n is interpolatory
- (ii) $I(\omega_n p) = 0$, all $p \in \mathbf{P}_{k-1}$.

Here ω_n is the node polynomial (1.8). Condition (ii) requires ω_n to be orthogonal to all polynomials of degree $\leq k - 1$. (If $k = 0$, a polynomial of degree -1 is understood to be identically zero.) It is seen, therefore, that each additional degree of exactness, over and beyond what is possible with the Newton-Cotes formula, requires orthogonality of ω_n to one additional power. In particular, $k \leq n$, since ω_n cannot be orthogonal to itself, so that the maximum possible degree of exactness is indeed $2n - 1$.

Jacobi's argumentation is extremely transparent; it goes as follows: Clearly, (i) is necessary. The necessity of (ii) is a consequence of $I(\omega_n p) = Q_n(\omega_n p) = 0$, the degree of exactness of Q_n being $n - 1 + k$ and ω_n vanishing at all the nodes τ_r . For the sufficiency, let p be an arbitrary polynomial of degree $\leq n - 1 + k$. Divide p by ω_n ,

$$p = q\omega_n + r, \quad q \in \mathbf{P}_{k-1}, \quad r \in \mathbf{P}_{n-1}.$$

Then

$$\begin{aligned} I(p) &= I(q\omega_n) + I(r) \\ &= I(r) \quad \text{[by (ii)]} \\ &= Q_n(r) \quad \text{[by (i)]} \\ &= Q_n(p) - Q_n(q\omega_n) = Q_n(p), \end{aligned}$$

i.e., Q_n has degree of exactness $n - 1 + k$.

The case $k = n$, of course, is of particular interest, as it leads to the Gauss formula of maximum degree of exactness. In this case, ω_n must be orthogonal to all lower degree polynomials, i.e. ω_n is the n -th degree Legendre polynomial (if the interval $[a, b]$ is standardized to $[-1, 1]$),

$$\omega_n(t) = \pi_n(t), \quad I(\pi_k \pi_l) = 0 \quad \text{for } k \neq l.$$

Jacobi then proceeds to obtain the "Rodrigues formula"

$$(1.11) \quad \pi_n(t) = \text{const} \cdot D^n (t^2 - 1)^n, \quad D = d/dt,$$

from which he concludes that all nodes τ_ν are real, simple, and contained in the interior of $[-1, 1]$. (The simplicity of the nodes is already pointed out by Gauss. The fact that all weights λ_ν are positive seems to have escaped both Gauss and Jacobi, although Jacobi's result $-1 < \tau_\nu < 1$, combined with an observation of Gauss (Gauss [1814, §21]) indeed yields positivity).

The analogue of (1.11) for general $0 \leq k \leq n$,

$$\omega_n(t) = \text{const} \cdot D^k [(t^2 - 1)^k p(t)], \quad p \in \mathbf{P}_{n-k},$$

where p has exact degree $n - k$, but is otherwise arbitrary, is due to Radau [1880].

1.4. Gauss-Christoffel quadrature formulae

After the work of Jacobi, the matter of Gaussian quadrature, except for Christoffel's 1858 memoir which we discuss later, remained dormant for nearly forty years. Then, in 1864, Mehler, and others after him, began to introduce weighted integrals, i.e. integrals over $[-1, 1]$ with respect to a measure $d\lambda(t) = \omega(t)dt$ with $\omega \neq 1$. This development soon led Posse [1875], and Christoffel [1877], to consider the case of a *general* (nonnegative and integrable) *weight function* ω on a finite interval $[a, b]$. Christoffel, in particular, systematically generalizes the Gauss-Jacobi theory to arbitrary weighted integrals, and in the process establishes (what is now called) the Christoffel-Darboux formula for an arbitrary weight function (anticipating

Darboux [1878, p. 413] by one year). Following Stieltjes [1894] we will consider, somewhat more generally, integrals of the form

$$(1.12) \quad I(f) = \int_a^b f(t) d\lambda(t),$$

where $d\lambda(t)$ is a (positive) Stieltjes measure on the finite or infinite interval $[a, b]$. We assume that $\lambda(t)$ has infinitely many points of increase, and $d\lambda(t)$ finite moments of all orders. It seems appropriate, then, in view of Christoffel's work, to call the n -point quadrature formula (1.5) for the weighted integral $I(f)$ in (1.12) a *Gauss-Christoffel quadrature formula*, if it has maximum degree of exactness $2n - 1$. The weights λ_ν , as has long been customary, will be called the *Christoffel numbers* for $d\lambda$.

With the measure $d\lambda$ there is associated a unique system of (monic) *orthogonal polynomials* $\pi_k(t) = \pi_k(t; d\lambda)$,

$$\begin{aligned} \deg \pi_k &= k, & k &= 0, 1, 2, \dots, \\ \int_a^b \pi_k(t) \pi_l(t) d\lambda(t) &= 0, & \text{all } k &\neq l. \end{aligned}$$

They are known to satisfy a three-term recurrence relation (Christoffel [1877], Darboux [1878], Stieltjes [1884a])

$$(1.13) \quad \begin{aligned} \pi_{k+1}(t) &= (t - \alpha_k) \pi_k(t) - \beta_k \pi_{k-1}(t), & k &= 0, 1, 2, \dots, \\ \pi_{-1}(t) &= 0, & \pi_0(t) &= 1, \end{aligned}$$

where the coefficients α_k, β_k are real, and $\beta_k > 0$ for $k > 0$. (β_0 is arbitrary.) The generalized Gauss-Jacobi theory rests precisely on these orthogonal polynomials.

To begin with, there is a verbatim extension of Jacobi's argument: The quadrature rule Q_n in (1.5) has degree of exactness $d(Q_n) = n - 1 + k$ if and only if λ_ν is given by (1.9) and the node polynomial ω_n is orthogonal (with respect to $d\lambda$) to all polynomials of degree $\leq k - 1$. The last condition can be expressed equivalently in the form

$$\omega_n(t) = \pi_n(t) - c_1 \pi_{n-1}(t) - \dots - c_{n-k} \pi_k(t),$$

where c_i are arbitrary real constants. If $k = n$, we get uniquely $\omega_n(t) = \pi_n(t; d\lambda)$, i.e. *the nodes τ_ν of the n -point Gauss-Christoffel formula are the zeros of the n -th degree orthogonal polynomial π_n* . They are all real, simple, contained in (a, b) , and separated by the zeros of π_{n-1} (Christoffel [1877]). Equally interesting is the case $k \geq n - 1$, which leads to "quasi-orthogonal" polynomials $\omega_n = \pi_n - c \pi_{n-1}$ with c arbitrary real. These were introduced by M. Riesz [1922/23] in connection with the moment problem, and were shown to have only real and simple zeros, at least $n - 1$ of which are in (a, b) . Combining this with a remark of Stieltjes [1884a, pp. 384-85], it follows that

$$(1.14) \quad \lambda_\nu = I(I_\nu^2) > 0, \quad \nu = 1, 2, \dots, n,$$

whenever (1.5) has degree of exactness $\geq 2n - 2$. In particular, *all Christoffel numbers are positive*. The case $k \geq n - 2$ is studied in detail by Micchelli & Rivlin [1973a].

To generalize the approach of Gauss, it is convenient to introduce the three functions

$$L(z) = \int_a^b \frac{d\lambda(t)}{z-t}, \quad \rho_n(z) = \int_a^b \frac{\pi_n(t)}{z-t} d\lambda(t), \quad z \notin [a, b],$$

$$\sigma_n(z) = \int_a^b \frac{\pi_n(z) - \pi_n(t)}{z-t} d\lambda(t),$$

which figure prominently in the work of Christoffel [1877], and have previously been used by Christoffel [1858] and Jacobi [1859] in special cases. Clearly,

$$\pi_n(z)L(z) = \sigma_n(z) + \rho_n(z).$$

Since σ_n is a polynomial of degree $n - 1$, it represents the “entire part” of $\pi_n L$, while ρ_n , containing only negative powers in its power series expansion, is the “remainder”. We have, in fact,

$$\rho_n(z) = \sum_{k=0}^{\infty} \frac{r_k}{z^{k+1}}, \quad r_k = \int_a^b t^k \pi_n(t) d\lambda(t),$$

which shows that $\rho_n(z) = O(z^{-n-1})$, by virtue of π_n being the orthogonal polynomial of degree n . Therefore,

$$(1.15) \quad L(z) - \frac{\sigma_n(z)}{\pi_n(z)} = \frac{\rho_n(z)}{\pi_n(z)} = O\left(\frac{1}{z^{2n+1}}\right), \quad z \rightarrow \infty.$$

One now defines the weights λ_ν and the nodes τ_ν of Q_n , as Gauss did previously in the case $d\lambda(t) = dt$, by means of the partial fraction decomposition of σ_n/π_n ,

$$\frac{\sigma_n(z)}{\pi_n(z)} = \sum_{\nu=1}^n \frac{\lambda_\nu}{z - \tau_\nu} =: Q_n\left(\frac{1}{z-\cdot}\right),$$

which, incidentally, yields

$$(1.16) \quad \lambda_\nu = \frac{\sigma_n(\tau_\nu)}{\pi_n'(\tau_\nu)}, \quad \nu = 1, 2, \dots, n.$$

It then follows that

$$L(z) - \frac{\sigma_n(z)}{\pi_n(z)} = I\left(\frac{1}{z-\cdot}\right) - Q_n\left(\frac{1}{z-\cdot}\right)$$

$$= R_n\left(\frac{1}{z-\cdot}\right) = \sum_{k=0}^{\infty} \frac{R_n(t^k)}{z^{k+1}},$$

which, combined with (1.15), shows that $R_n(t^k) = 0$ for $0 \leq k \leq 2n - 1$, i.e. (1.5) is the desired Gauss-Christoffel formula. At the same time we recognize

$$\frac{\rho_n(z)}{\pi_n(z)} = \sum_{k=2n}^{\infty} \frac{R_n(t^k)}{z^{k+1}}$$

to be the *generating function of the monomial errors*.

Eq. (1.15) gives rise to another important observation. If both L and σ_n/π_n are expanded in descending powers, the two expansions must agree through the first $2n$ terms. This identifies the rational function σ_n/π_n as the n -th convergent of the continued fraction associated with the integral L ,

$$(1.17) \quad L(z) \sim \frac{\beta_0}{z - \alpha_0} - \frac{\beta_1}{z - \alpha_1} - \frac{\beta_2}{z - \alpha_2} - \dots$$

The characterization of π_n as the denominator of this convergent indeed is the way orthogonal polynomials were generally viewed throughout the 19th century. (See, however, Murphy [1835].) The recurrence relation (1.13) (with $t = z$) is nothing but the recurrence relation that σ_n and π_n , as numerators and denominators of the continued fraction (1.17), must satisfy. The coefficients α_k, β_k in (1.13) are therefore the same as those in (1.17) (where $\beta_0 = \int_a^b d\lambda(t)$), and we now recognize σ_n as being a second solution of (1.13); its initial values are $\sigma_{-1} = -1, \sigma_0 = 0$.

Our developments up to this point already yielded several explicit formulas for the Christoffel numbers λ_ν ; cf. (1.9), (1.14), (1.16). Among the many others that are known, we mention only the elegant formula

$$\lambda_\nu = \frac{1}{\sum_{k=0}^{n-1} [\pi_k^*(\tau_\nu)]^2}, \quad \nu = 1, 2, \dots, n,$$

due to Shohat [1929], which expresses λ_ν in terms of the orthonormal polynomials $\pi_k^* = h_k^{-1/2} \pi_k, h_k = \int_a^b \pi_k^2(t) d\lambda(t)$. In principle, as has recently been observed (Billauer [1974]), one could dispense with Christoffel numbers altogether if one writes the Gauss-Christoffel quadrature sum in the form

$$Q_n(f) = \frac{[\tau_1, \tau_1, \dots, \tau_n](f/\pi_{n+1})}{[\tau_1, \tau_2, \dots, \tau_n](1/\pi_{n+1})} \int_a^b d\lambda(t),$$

where $[\tau_1, \tau_2, \dots, \tau_n]g$ denotes the $(n - 1)$ -st order divided difference of g , and $\pi_{n+1} = \pi_{n+1}(\cdot; d\lambda)$.

Still another approach to the Gauss-Christoffel formula, due to Markov [1885], is via Hermite interpolation. One replaces the integral over f by the integral over $q_{2n-1}(f; \cdot)$, the Hermite interpolation polynomial of degree $\leq 2n - 1$ interpolating both f and its derivative f' at the nodes τ_ν . By requiring the weights of the derivative terms $f'(\tau_\nu)$ in the quadrature sum to be all equal to zero, one again is led to choose τ_ν as the zeros of the orthogonal polynomial

$\pi_n(\cdot; d\lambda)$. Markov's derivation has the advantage of yielding, via the remainder term of Hermite interpolation, an explicit expression for the remainder R_n in (1.5), namely

$$R_n(f) = \int_a^b \pi_n^2(t) [\tau_1, \tau_1, \dots, \tau_n, \tau_n, t] f d\lambda(t),$$

where $[\tau_1, \tau_1, \dots, \tau_n, \tau_n, t]f$ denotes the $2n$ -th divided difference of f formed with the nodes τ_ν (each taken twice) and t . If $f \in C^{2n}[a, b]$, then, alternatively,

$$(1.18) \quad R_n(f) = \frac{h_n}{(2n)!} f^{(2n)}(\bar{t}_n), \quad h_n = \int_a^b \pi_n^2(t) d\lambda(t),$$

where $\bar{t}_n \in (a, b)$ is an (unknown) intermediate value.

The remainder in (1.18) can be further expanded in the manner of Euler–Maclaurin, as is proposed by Bilharz [1951] for the Gauss–Legendre formula and discussed in Krylov [1959, Ch. 11, §3] for arbitrary quadrature rules.

Another form of the remainder, valid for holomorphic functions f ,

$$(1.19) \quad R_n(f) = \frac{1}{2\pi i} \oint_{\Gamma} \frac{P_n(z)}{\pi_n(z)} f(z) dz,$$

where Γ is a contour encircling the interval $[a, b]$, follows from a contour integral representation of the error in polynomial interpolation, given by Darboux [1878] and Heine [1881].

The development of Gauss–Christoffel formulae, as already mentioned, began with Mehler [1864], who considered $d\lambda(t) = (1-t)^\alpha(1+t)^\beta dt$ on $[-1, 1]$ with arbitrary $\alpha > -1, \beta > -1$. The resulting quadrature formula is now named after Jacobi, who studied the corresponding orthogonal polynomials (Jacobi [1859]). Particularly noteworthy is the special case $\alpha = \beta = -1/2$, already discussed by Mehler, which yields as orthogonal polynomials the Chebyshev polynomials of the first kind, $\pi_n(\cos \theta) = 2^{1-n} \cos n\theta$. Its zeros τ_ν are given explicitly by $\tau_\nu = \cos((2\nu - 1)\pi/2n)$, and all weights λ_ν turn out to be equal, $\lambda_\nu = \pi/n$. Posse [1875] indeed proves that this Gauss–Chebyshev formula is the only Gauss–Christoffel formula having equal weights. Other Gauss–Christoffel formulae for which the nodes and weights can be expressed explicitly in terms of trigonometric functions are those for $d\lambda(t) = (1-t^2)^{1/2} dt$ and $d\lambda(t) = [(1-t)/(1+t)]^{1/2} dt$ on $[-1, 1]$, obtained independently by Posse [1875] and Stieltjes [1884b]. Gauss–Christoffel quadrature rules on infinite intervals appear first in Radau [1883], who considers $d\lambda(t) = e^{-t} dt$ on $[0, \infty]$, and in Gourier [1883], who considers $d\lambda(t) = e^{-t^2/2} dt$ on $[-\infty, \infty]$. The former are named after Laguerre, who earlier discussed the relevant orthogonal polynomials (Laguerre [1879]), the latter after Hermite [1864], who studied the orthogonal polynomials for $d\lambda(t) = e^{-t^2} dt$ on $[-\infty, \infty]$. (These attributions may

not be entirely justified, historically, as Laguerre polynomials were already used by Lagrange [1762–1765, pp. 534–539] and were treated in unpublished work, dated 1826, by Abel [Oeuvres 2, p. 284] and again, later, by Murphy [1835, pp. 146–148] and Chebyshev [1859b]. Likewise, Hermite polynomials were used by Laplace [1810/11] in his work on probability and studied by Chebyshev [1859b].) The more general orthogonal polynomials relative to the measure $d\lambda(t) = t^\alpha e^{-t} dt$ on $[0, \infty)$ occur in the work of Sochockiĭ [1873] and Sonin [1880, pp. 41–43], the corresponding Gauss-Christoffel formula in Deruyts [1886].

We remark that Gauss-Christoffel quadrature formulae can also be interpreted as quadrature rules of given degree of exactness and *minimal number of nodes* (Chakalov [1930/31]). Indeed, given an integer $d \geq 1$, any quadrature rule (1.5) of degree of exactness d , having distinct (real or complex) nodes τ_ν and (real or complex) weights λ_ν , must have more than $d/2$ nodes, i.e. $n > d/2$. If d is odd, the Gauss-Christoffel formula is the unique quadrature rule Q_n with $d(Q_n) = d$ having the minimum number $n = (d + 1)/2$ of nodes. If d is even, there are infinitely many Q_n with $d(Q_n) = d$ that have the minimum number $n = (d/2) + 1$ of nodes. They all can be obtained by taking as node polynomial ω_n any polynomial $\pi_n - c\pi_{n-1}$ having distinct zeros, and by defining λ_ν in the usual manner by (1.9).

2. Extensions of the Gauss-Christoffel Quadrature Formula

2.1. Gaussian quadrature with preassigned nodes

While in Gauss-Christoffel quadrature formulae there is no freedom in the choice of the nodes, all being uniquely determined by the measure $d\lambda$, there may be situations in which employment of certain preassigned nodes is highly desirable. The question then arises as to how the remaining (free) nodes, and all weights (including those for the preassigned nodes), are to be chosen in order to maximize the degree of exactness. Christoffel [1858] was the first to consider this problem and, in the case $d\lambda(t) = dt$ on $[-1, 1]$, to give a complete solution under the assumption that all preassigned nodes are *outside* the open interval $(-1, 1)$. An interesting case of preassigned nodes *inside* the interval of integration is considered only recently by Kronrod [1964 a, b] in connection with a practical implementation of the Gaussian integration scheme.

2.1.1. *Christoffel's work and related developments.* Although Christoffel, in his 1858 paper, considers only integrals with constant weight function and finite interval $[-1, 1]$, his work extends easily to general weighted integrals over a finite or half-infinite interval $[a, b]$,

$$(2.1) \quad I(f) = \int_a^b f(t) d\lambda(t), \quad d\lambda(t) \geq 0.$$

He proposes to approximate this integral by means of a quadrature formula of the form

$$(2.2) \quad I(f) = Q_n(f) + R_n(f), \quad Q_n(f) = \sum_{\nu=1}^n \lambda_\nu f(\tau_\nu) + \sum_{\lambda=1}^l \mu_\lambda f(u_\lambda),$$

where $l \geq 1$, and u_1, u_2, \dots, u_l are given real numbers not in the open interval (a, b) . We call u_λ the *fixed nodes* of Q_n , and τ_ν the *free nodes*. All weights λ_ν and μ_λ are assumed real and freely variable. We continue to use the notation ω_n for the node polynomial of the free nodes, and let u denote the one for the fixed nodes,

$$\omega_n(t) = \prod_{\nu=1}^n (t - \tau_\nu), \quad u(t) = \pm \prod_{\lambda=1}^l (t - u_\lambda).$$

By assumption, u preserves its sign on $[a, b]$, and the plus or minus sign is taken so as to render $u(t) \geq 0$ on $[a, b]$.

Following the approach of Newton-Cotes (cf. Section 1.1), it is clearly possible to make (2.2) *interpolatory*, i.e. to achieve degree of exactness $n - 1 + l$. On the other hand, by Jacobi's argument with obvious changes (replace ω_n by $u\omega_n$ in Section 1.3), one finds that $d(Q_n) = n - 1 + l + k, 0 \leq k \leq n$, if and only if Q_n is interpolatory and $I(u\omega_n p) = 0$ for all $p \in P_{k-1}$. Thus, ω_n must be orthogonal to all polynomials of degree $\leq k - 1$ with respect to the measure $d\sigma(t) = u(t)d\lambda(t)$. Since $d\sigma$ is a positive measure, we are back to the situation discussed in Section 1.4. In particular, the quadrature formula (2.2) will have maximum degree of exactness $d(Q_n) = 2n - 1 + l$ precisely if $\omega_n = \pi_n(\cdot; u\lambda)$ and the weights are obtained by interpolation,

$$(2.3) \quad \lambda_\nu = I \left[\frac{u(\cdot)\omega_n(\cdot)}{u(\tau_\nu)\omega'_n(\tau_\nu)(\cdot - \tau_\nu)} \right], \quad \mu_\lambda = I \left[\frac{u(\cdot)\omega_n(\cdot)}{u'(u_\lambda)\omega_n(u_\lambda)(\cdot - u_\lambda)} \right],$$

$$\nu = 1, 2, \dots, n, \quad \lambda = 1, 2, \dots, l.$$

The formula (2.2), with τ_ν the zeros of $\pi_n(\cdot; u\lambda)$, and λ_ν, μ_λ given by (2.3), is called the *Christoffel quadrature formula*. Christoffel proceeds to express $\pi_n(\cdot; u\lambda)$ explicitly in terms of the polynomials $p_r(\cdot; d\lambda)$ orthogonal with respect to $d\lambda$,

$$(2.4) \quad u(t)\pi_n(t; u\lambda) = \text{const} \cdot \begin{vmatrix} p_n(t) & p_{n+1}(t) & \cdots & p_{n+l}(t) \\ p_n(u_1) & p_{n+1}(u_1) & \cdots & p_{n+l}(u_1) \\ \dots & \dots & \dots & \dots \\ p_n(u_l) & p_{n+1}(u_l) & \cdots & p_{n+l}(u_l) \end{vmatrix}.$$

This is now commonly referred to as *Christoffel's theorem*. It shows that $u\pi_n$ is a linear combination of p_n, p_{n+1}, p_{n+l} . The theorem is useful in many applications, e.g. in the asymptotic theory of orthogonal polynomials (Shohat [1928])

and in studying the qualitative behavior of the zeros and weights of π_n (Bezikiović [1937]).

It is interesting to read how Christoffel motivates his formula (Christoffel [1858, p. 74]): "... Gegenwärtige Methode gewährt demnach die Möglichkeit, bei der angenäherten Integration einer *gegebenen* Funktion alle Vortheile zu vereinigen, welche einerseits aus der Berücksichtigung des numerischen Verlaufs dieser Funktion, und andererseits aus der Anwendung der Gaußischen Methode entspringen können. Man wird nämlich jene n willkürlichen Wurzeln so wählen, daß für sie die Funktion $F(x)$ besonders einfache, oder auch solche Werthe annimmt, von denen ein großer Einfluß auf den Werth des gesuchten Integrals zu erwarten ist." [His " F " is our " f ", and his " n " is our " l ".] One of the "... especially simple values" of f that Christoffel had in mind, undoubtedly, was $f(u_\lambda) = 0$, in which case the corresponding term $\mu_\lambda f(u_\lambda)$ in the quadrature sum $Q_n(f)$ disappears, and the high degree of accuracy is retained with one fewer quadrature node. In the extreme case where *all* u_λ are zeros of f , one effectively gets an n -point formula with degree of exactness $2n - 1 + l$.

Christoffel's new quadrature formula, and the companion theorem of Christoffel, is but one of several important discoveries contained in Christoffel's remarkable 1858 memoir. Among the others is the discrete orthogonality property for Legendre polynomials, obtained by Christoffel independently of Chebyshev, who introduced discrete orthogonal polynomials in his least-squares approximation method (Chebyshev [1855]). From the discrete orthogonality relation Christoffel then derives the "Christoffel-Darboux" summation formula for Legendre polynomials. Equally remarkable is the fact that Christoffel was already preoccupied with the question of convergence of Gaussian quadrature rules, and with the related question of convergence of series expansions in Legendre polynomials. Evidently convinced, but unable to prove, that his summation formula holds the key to convergence, he writes in a letter to Borchardt, dated December 3, 1857, that for convergence "... scheint nun die Formel 44. [his summation formula] wie geschaffen...".

Christoffel's quadrature formula (2.2), (2.3) allows an interesting alternative interpretation, already pointed out by Christoffel [1858, p. 76] and recently rediscovered (Esser [1971a], [1972]) in a more general context (multiple fixed nodes). Observe, first of all, that

$$Q_n^*(f) = \sum_{\nu=1}^n \lambda_\nu f(\tau_\nu)$$

is a quadrature rule in its own right. It has the property that $Q_n^*(up) = I(up)$ for all $p \in \mathbf{P}_{2n-1}$. Let P be the interpolation operator $Pf = p_{l-1}(f; \cdot)$, where $p_{l-1}(f; \cdot)$ is the polynomial of degree $\leq l-1$ interpolating f at the fixed nodes u_1, u_2, \dots, u_l . Then, with E denoting the identity operator, the quadrature sum in (2.2) can be written equivalently in the form

$$(2.5) \quad Q_n(f) = I(Pf) + Q_n^*((E - P)f).$$

Christoffel indeed interprets the interpolation term $I(Pf)$ on the right as a "first approximation" to $I(f)$, and the second term as "the correction to be applied in order to obtain a more accurate value". More importantly, (2.5) yields a new formula for the weights μ_λ ,

$$(2.6) \quad \mu_\lambda = (I - Q_n^*) \left[\frac{u(\cdot)}{u'(u_\lambda)(\cdot - u_\lambda)} \right], \quad \lambda = 1, 2, \dots, l,$$

which lends itself more easily for the study of convergence of Christoffel's quadrature rule (Esser [1971a], [1972]). The function on which $I - Q_n^*$ acts in (2.6) is just the elementary Lagrange polynomial l_λ for the nodes u_1, u_2, \dots, u_l (cf. Section 1.1).

Another interesting use of (2.5) is made by Krylov [1959, Ch. 9, §3], who considers $d\lambda(t) = \omega(t)dt$ in (2.1), where ω is a function that is positive at $t = b$, and changes sign exactly at the nodes u_1, u_2, \dots, u_l , which are now assumed interior points of $[a, b]$. Thus, $I(f)$ is an integral with an oscillatory weight function. Since $I(up) = \int_a^b p(t)u(t)\omega(t)dt$, and $u(t)\omega(t) \geq 0$ on $[a, b]$, the nodes τ_ν of the quadrature rule Q_n^* are just the zeros of $\pi_n(\cdot; u\omega dt)$, and $u(\tau_\nu)\lambda_\nu$ the corresponding Christoffel numbers. $Q_n(f)$ in (2.5) then approximates $I(f)$ in (2.1) with degree of exactness $2n - 1 + l$. The required function $(E - P)f$ can be represented in terms of the divided difference of f as $(E - P)f = u(\cdot)[u_1, u_2, \dots, u_l, \cdot]f$.

The special Christoffel formula for $d\lambda(t) = dt$ on $[-1, 1]$, with $l = 2$, $u_1 = -u_2 = 1$, has already been obtained by Lobatto [1852, §§207–210]. It is customary, therefore, to call (2.2), (2.3), when $l = 2$, $u_1 = a$, $u_2 = b$ (hence $[a, b]$ is finite), a *Gauss-Lobatto formula*. The same formula, together with the simpler one with $l = 1$, $u_1 = a$ or $u_1 = b$, was also discussed (for $d\lambda(t) = dt$) by Radau [1880]; the latter is commonly referred to as the *Gauss-Radau formula*. All weights of a Gauss-Radau and a Gauss-Lobatto formula are necessarily positive. Shohat [1929] has a systematic study of the Gauss-Legendre-Lobatto formula. The two Gauss-Radau formulae for the Chebyshev measure $d\lambda(t) = (1 - t^2)^{-1/2}dt$ on $[-1, 1]$, as well as the respective Gauss-Lobatto formula, can be expressed explicitly in terms of trigonometric functions (Markov [1885]). All three formulas have equal coefficients associated with all interior nodes. For the last one, this equicoefficient property is proved by Gatteschi, Monegato & Vinardi [1976] to be characteristic among Gauss-Lobatto formulae with Jacobi weight function, even if multiple fixed nodes are admitted. Gauss-Radau and Gauss-Lobatto formulae for some classical measures $d\lambda$ are reviewed extensively in Bouzitat [1952], where in particular one finds explicit constructions of these formulae for all measures with square root singularities at one or both endpoints. For other examples see Ljaščenko & Olešnik [1974], [1975].

There are various generalizations of Christoffel's theorem. It is a simple matter, e.g., to observe that the theorem remains valid for *multiple nodes* u_λ , if the appropriate rows in the determinant of (2.4) are replaced by rows of derivatives (Szegö [1921]). A more substantial generalization is due to Uvarov [1959], [1969], who considers $d\sigma(t) = [u(t)/v(t)]d\lambda(t)$, where

$$u(t) = \pm \prod_{\lambda=1}^l (t - u_\lambda), \quad v(t) = \prod_{\mu=1}^m (t - v_\mu)$$

are such that the measure $d\sigma$ they generate is a positive Stieltjes measure on $[a, b]$. Assuming the roots u_λ pairwise distinct, and the same for the v_μ , Uvarov establishes the *generalized Christoffel's theorem*

$$(2.7) \quad u(t)\pi_n\left(t; \frac{u}{v} d\lambda\right) = \text{const} \cdot \begin{vmatrix} p_{n-m}(t) & p_{n-m+1}(t) & \cdots & p_{n+1}(t) \\ p_{n-m}(u_1) & p_{n-m+1}(u_1) & \cdots & p_{n+1}(u_1) \\ \cdot & \cdot & \cdot & \cdot \\ p_{n-m}(u_l) & p_{n-m+1}(u_l) & \cdots & p_{n+1}(u_l) \\ r_{n-m}(v_1) & r_{n-m+1}(v_1) & \cdots & r_{n+1}(v_1) \\ \cdot & \cdot & \cdot & \cdot \\ r_{n-m}(v_m) & r_{n-m+1}(v_m) & \cdots & r_{n+1}(v_m) \end{vmatrix}, \quad m \leq n,$$

and another similar theorem in the case $m > n$. Here, $p_k = p_k(\cdot; d\lambda)$ are the orthogonal polynomials with respect to the measure $d\lambda$, and

$$r_k(z) = \int_a^b \frac{p_k(t)}{z - t} d\lambda(t), \quad k = 0, 1, 2, \dots$$

The case of confluent zeros u_λ or v_μ is handled similarly as in the classical Christoffel theorem. Interestingly, Christoffel [1877] already has an example of (2.7), namely the case $d\lambda(t) = dt$ on $[-1, 1]$ and $u(t) = 1, v(t) = t^2 + a^2$, but he refrains from giving any explanation. Kumar [1974a, b] and Price [1979], apparently unaware of Uvarov's result, discuss further examples. See also Szegö [1922, Kap. II], Grinšpun [1966].

2.1.2. *Kronrod's extension of quadrature rules.* Motivated by a desire to provide a practical means of estimating the error in numerical integration, Kronrod [1964a, b] initiates a study of *pairs* (Q_1, Q_2) of *quadrature rules*,

$$Q_i(f) = \sum_{\nu=1}^{n_i} \lambda_{\nu,i} f(\tau_{\nu,i}), \quad i = 1, 2.$$

The intent here is to use the more accurate of the two, say Q_2 , to estimate the error of the other, Q_1 , the integral to be approximated being the weighted integral in (2.1). One defines the degree of exactness of the pair (Q_1, Q_2) by

$$d(Q_1, Q_2) = \min(d(Q_1), d(Q_2))$$

(cf. Section 1.1). The number of distinct points that are either nodes of Q_1 or nodes of Q_2 is denoted by $n(Q_1, Q_2)$. Assuming Q_1 not identical with Q_2 , one has

$$n(Q_1, Q_2) \geq d(Q_1, Q_2) + 2, \quad Q_1 \neq Q_2,$$

since otherwise $d(Q_1, Q_2) > n(Q_1, Q_2) - 2$, hence $d(Q_1) \geq n(Q_1, Q_2) - 1$ and $d(Q_2) \geq n(Q_1, Q_2) - 1$, which would imply $Q_1 = Q_2$, both Q_1 and Q_2 being interpolatory on the set of (distinct) nodes of Q_1 and Q_2 .

Following Kronrod, we pose the following problem: Given an interpolatory quadrature rule Q_1 for the integral I in (2.1), find a quadrature rule $Q_2 \neq Q_1$ such that $d(Q_2)$ is as large as possible, subject to

$$(2.8) \quad d(Q_2) \geq d(Q_1), \quad n(Q_1, Q_2) = d(Q_1, Q_2) + 2 = d(Q_1) + 2.$$

In other words, we wish to maximize the degree of exactness of Q_2 under the condition that the pair (Q_1, Q_2) have maximum degree of exactness [the first condition in (2.8)] and the minimum number of nodes [the second condition in (2.8)]. We consider this optimum Q_2 , if it exists, to have $n(Q_1, Q_2)$ nodes, those in Q_1 or Q_2 , although some of the weights, conceivably, could be zero. We call Q_2 the *minimum node Kronrod extension* of Q_1 . The same problem can be posed with $n(Q_1, Q_2)$ prescribed arbitrarily, $n(Q_1, Q_2) \geq d(Q_1) + 2$. We then call Q_2 simply a *Kronrod extension* of Q_1 . Since the quadrature rule Q_2 contains among its nodes all those of Q_1 , we may think of the Kronrod extension as a quadrature formula with *preassigned nodes* (those of Q_1). What differs from Christoffel's theory (cf. Section 2.1.1) is the fact that the preassigned nodes are now located *within* the interval $[a, b]$, and the corresponding node polynomial is no longer of constant sign.

Since Q_1 has n_1 nodes, and is interpolatory, $d(Q_1) \geq n_1 - 1$, and therefore $n(Q_1, Q_2) \geq n_1 + 1$. Let ω_{Q_1} denote the node polynomial (of degree n_1) of Q_1 . Then the following can be shown (which generalizes slightly a result of Kronrod [1964b, Thms. 5 and 6]): *If there exists a monic polynomial ω of degree $n(Q_1, Q_2) - n_1$, orthogonal with respect to $\omega_{Q_1} d\lambda$ to all polynomials of lower degree,*

$$\int_a^b \omega(t) t^k \omega_{Q_1}(t) d\lambda(t) = 0, \quad k = 0, 1, 2, \dots, n(Q_1, Q_2) - n_1 - 1,$$

then there exists a unique Kronrod extension Q_2 of Q_1 , having degree of exactness $d(Q_2) \geq 2n(Q_1, Q_2) - n_1 - 1$. The extension is the unique interpolatory quadrature rule that has as nodes the n_1 nodes of Q_1 and the $n(Q_1, Q_2) - n_1$ zeros of ω . [If one of the latter happens to coincide with a node of Q_1 , the quadrature rule $Q_2(f)$ also involves the derivative of f at that node.] In general, there is no assurance that the nodes of Q_2 are real and contained in $[a, b]$.

Perhaps the most interesting case is the one originally considered by Kronrod: Q_1 is the n -point Gauss-Christoffel quadrature rule. In this case the minimum node Kronrod extension Q_2 has degree of exactness $d(Q_2) \geq 2(2n+1) - n - 1 = 3n + 1$, and the new nodes to be inserted in Q_1 are the zeros of the (monic) polynomial ω_{n+1} of degree $n+1$ satisfying

$$\int_a^b \omega_{n+1}(t) t^k \pi_n(t) d\lambda(t) = 0, \quad k = 0, 1, 2, \dots, n.$$

Here π_n is the node polynomial of Q_1 , i.e. $\pi_n = \pi_n(\cdot; d\lambda)$. If $d\lambda(t) = (1-t^2)^{\mu-1/2} dt$ on $[-1, 1]$, $0 \leq \mu \leq 2$, the polynomial ω_{n+1} exists uniquely and has $n+1$ distinct zeros in $[-1, 1]$ which are separated by the zeros of π_n (cf. Section 3.1.2). Rabinowitz [1980] in this case (and similarly for the Kronrod extension of Gauss-Lobatto formulae) proves that $d(Q_2)$ equals, but does not exceed, $2[(3n+3)/2] - 1$, except when $\mu = 0$ or $\mu = 1$, in which cases $d(Q_2)$ is larger (if $n \geq 4$). Monegato [1978a] shows that all weights of Q_2 are positive if $0 \leq \mu \leq 1$. In the case $\mu = 1/2$ (i.e., $d\lambda(t) = dt$), tables of Q_2 , accurate to 16 decimal digits, have been computed by Kronrod [1964b] for $n = 1(1)40$. Baratella [1979] has tables for Kronrod extensions of Gauss-Radau formulae.

Nothing, in principle, prevents us from repeating the process of extension and generating a sequence Q_1, Q_2, Q_3, \dots of successively extended quadrature rules. Whether indeed this is possible, and yields rules Q_i with all nodes real, has not been proved, not even in the case $d\lambda(t) = dt$.

Kronrod extensions of Gauss-Lobatto formulae, as well as repeated extensions of a low-order Gauss-Legendre rule, have been computed by Patterson [1968]. The latter are used in an automatic integration routine of Cranley & Patterson [1971] and Patterson [1973]. Piessens [1973a] uses a Kronrod pair (Q_1, Q_2) for $d\lambda(t) = dt$, $n = 10$, for similar purposes.

Particularly simple are the (minimum node) Kronrod extensions of the Gauss-Chebyshev rules, with $d\lambda(t) = (1-t^2)^{-1/2} dt$ and $d\lambda(t) = [(1-t)/(1+t)]^{1/2} dt$ on $[-1, 1]$, which can be written down explicitly and extended infinitely often (Mysovskih [1964], Monegato [1976]). Weight distributions $d\lambda(t)$ with infinite support, on the other hand, seem to resist satisfactory Kronrod extension. Kahaner & Monegato [1978], e.g., prove that minimum node extensions of the n -point (generalized) Gauss-Laguerre rule, with $d\lambda(t) = t^\alpha e^{-t} dt$ on $[0, \infty)$, $-1 < \alpha \leq 1$, do not exist for $n \geq 23$ if one requires that all nodes be real and all coefficients positive. Moreover, the ordinary Gauss-Laguerre formula ($\alpha = 0$) cannot be so extended if $n > 1$, nor can the Gauss-Hermite formula, unless $n = 1, 2$, or 4 , confirming earlier empirical results of Ramskiĭ [1974]. Further remarks on the difficulties of Kronrod extension can be found in Monegato [1979].

Computational methods for generating Kronrod extensions of Gauss and Lobatto rules are discussed by Patterson [1968], Piessens & Branders [1974], and Monegato [1978b].

2.2. Gaussian quadrature with multiple nodes

Gauss' principle applied to quadrature sums involving derivative values in addition to function values not only uncovers new theoretical foundations, but also yields formulae of considerable practical value in situations where derivatives are readily accessible. The breakthrough came in 1950, through the work of Turán, and has led to intensive further developments, particularly in Romanian and Italian schools of numerical analysis.

2.2.1. *The quadrature rule of Turán.* The quadrature rule for the integral I in (2.1), considered by Turán [1950], has multiple nodes τ_ν , each having the same multiplicity $r \geq 1$,

$$(2.9) \quad \begin{aligned} I(f) &= Q_n(f) + R_n(f), \\ Q_n(f) &= \sum_{\nu=1}^n [\lambda_\nu f(\tau_\nu) + \lambda'_\nu f'(\tau_\nu) + \dots + \lambda^{(r-1)}_\nu f^{(r-1)}(\tau_\nu)]. \end{aligned}$$

We continue to use ω_n to denote the node polynomial $\omega_n(t) = \prod_{\nu=1}^n (t - \tau_\nu)$. The appropriate interpolation process for the Newton-Cotes approach is now *Hermite interpolation*, which, given any set of (distinct) nodes τ_ν , will yield a degree of exactness $m - 1$ for (2.9). We therefore call (2.9) *interpolatory* if $d(Q_n) = m - 1$. Jacobi's theory is easily adapted (replace ω_n by ω'_n in Section 1.3) to show that (2.9) has degree of exactness $d(Q_n) = m - 1 + k, 0 \leq k \leq n$, if and only if (2.9) is interpolatory and $I(\omega'_n p) = 0$ for all $p \in \mathbf{P}_{k-1}$. Thus, it is now the r -th power of ω_n , not ω_n , which must be orthogonal to all polynomials of degree $\leq k - 1$. We call this new type of orthogonality *power orthogonality* or, specifically, *r-th power orthogonality*. Unless $k = 0$, the power r must be *odd*, since otherwise $I(\omega'_n) > 0$, and ω'_n could not be orthogonal to constants, let alone to \mathbf{P}_{k-1} . We assume, therefore, that

$$r = 2s + 1, \quad s \geq 0.$$

We then have $k \leq n$, since otherwise $p = \omega_n$ would yield $I(\omega'_n p) = 0$, which is obviously impossible. We see, therefore, that (2.9) has maximum degree of exactness $d(Q_n) = (r + 1)n - 1$ precisely if

$$(2.10) \quad \int_a^b [\omega_n(t)]^{2s+1} t^k d\lambda(t) = 0, \quad k = 0, 1, \dots, n - 1.$$

In the special case $s = 0$ one recovers the Gauss-Christoffel formula.

Turán [1950] proves that there exists a unique polynomial $\omega_n = \pi_{n,s}(\cdot; d\lambda)$ for which (2.10) is satisfied. Moreover, $\pi_{n,s}$ has n distinct real zeros which are all contained in the open interval (a, b) . The same is proved independently, and by entirely different methods, by Ossicini [1966]. Turán furthermore identifies $\pi_{n,s}$ as the solution of the extremal problem

$$(2.11) \quad \int_a^b [\omega(t)]^{2s+2} d\lambda(t) = \min,$$

where the minimum is sought among all monic polynomials ω of degree n . (The system (2.10) is formally obtained from (2.11) by differentiating the objective function in (2.11) with respect to all coefficients of ω .) The special case $s = 0$ in (2.11) expresses a well-known extremal property of the orthogonal polynomial $\omega = \pi_n(\cdot; d\lambda)$. Many essential features of the Gauss-Christoffel theory are thus seen to generalize naturally to quadrature rules (2.9) with multiple nodes. One important feature, however, the positivity of the weights, does not completely carry over. For the case $r = 3$, Turán observes that $\lambda_\nu^{(2)} > 0$, while for general r , Ossicini & Rosati [1978] prove $\lambda_\nu^{(\rho)} > 0$ whenever $\rho \geq 0$ is even. The weights $\lambda_\nu^{(\rho)}$, for ρ odd, may have either sign, in general. This is always true for symmetric integrals, but happens also in other cases, e.g., when $d\lambda(t) = e^{-t} dt$ on $[0, \infty]$ and $n \geq 3$ (cf. the tables in Stroud & Stancu [1965]).

The Chebyshev measure $d\lambda(t) = (1-t^2)^{-1/2} dt$, as always, provides for interesting examples. Bernstein [1930] indeed proves that for each $s \geq 0$ the extremal polynomial in (2.11) is precisely the Chebyshev polynomial $\omega = 2^{1-n} T_n$. Therefore, the Chebyshev points $\tau_\nu = \cos((2\nu - 1)\pi/2n)$, $\nu = 1, 2, \dots, n$, serve as nodes for all Turán formulas (2.9) with $r = 1, 3, 5, \dots$, i.e. there are weights $\lambda_\nu^{(\rho)}$ such that

$$(2.12) \quad \int_{-1}^1 \frac{f(t)}{(1-t^2)^{1/2}} dt = \sum_{\nu=1}^n \sum_{\rho=0}^{2s} \lambda_\nu^{(\rho)} f^{(\rho)}\left(\cos\left(\frac{2\nu-1}{2n}\pi\right)\right) + R_n(f),$$

with $R_n(f) = 0$ for all $f \in \mathbf{P}_{2(s+1)n-1}$ (Turán [1950]). Equivalently, there exist weights $\mu_\nu^{(\rho)}$ such that

$$(2.12') \quad \int_{-\pi}^{\pi} g(t) dt = \sum_{\nu=1}^n \sum_{\rho=0}^{2s} \mu_\nu^{(\rho)} g^{(\rho)}\left(\frac{2\nu-1}{2n}\pi\right) + R_n(g),$$

where $R_n(g) = 0$ for all even trigonometric polynomials g of degree $\leq 2(s+1)n - 1$. The coefficients $\mu_\nu^{(\rho)}$ in (2.12') admit simple explicit expressions, already obtained by Kis [1957], and rediscovered repeatedly (Rosati [1968], Riess [1976]). Micchelli & Rivlin [1972] generalize (2.12) to

$$(2.13) \quad \int_{-1}^1 \frac{f(t)}{(1-t^2)^{1/2}} dt = \frac{\pi}{n} \left\{ \sum_{\nu=1}^n f(\tau_\nu) + \sum_{\sigma=1}^{\infty} \alpha_\sigma [\tau_1^{2\sigma}, \tau_2^{2\sigma}, \dots, \tau_n^{2\sigma}] f' \right\},$$

$$\alpha_\sigma = (-1)^\sigma \binom{-1/2}{\sigma} / (2\sigma \cdot 4^{(n-1)\sigma}),$$

where $[\tau_1^{2\sigma}, \dots, \tau_n^{2\sigma}] f'$ denotes the divided difference of f' formed with the nodes τ_ν , each taken with multiplicity 2σ , and f is holomorphic. If $f \in \mathbf{P}_{2(s+1)n-1}$ then (2.13) reduces to (2.12). The case $s = 1$ is easily worked out; for $s = 2$ the

formulas are given in Riess [1975]. Micchelli & Rivlin also obtain the ‘‘Lobatto analogue’’ of (2.13).

The remainder R_n in Turán’s formula (2.9) is studied by Ionescu [1967] and Ossicini [1968], the remainder in (2.12) by Pavel [1967]. It is shown, in particular, that the Peano kernel $K_{(r+1)n}$ (cf. Section 4.2) is positive, a fact that follows also from earlier work of Chakalov [1954] concerning more general quadrature rules (those of Section 2.2.2). For finite intervals $[a, b]$, and holomorphic functions f , Ossicini & Rosati [1975] find the contour integral representation

$$R_n(f) = \frac{1}{2\pi i} \oint_r \frac{\rho_{n,s}(z)}{[\pi_{n,s}(z)]^{2s+1}} f(z) dz, \quad \rho_{n,s}(z) = \int_a^b \frac{[\pi_{n,s}(t)]^{2s+1}}{z-t} d\lambda(t),$$

where $\pi_{n,s} = \pi_{n,s}(\cdot; d\lambda)$ is the s -orthogonal polynomial for the measure $d\lambda$ (cf. Section 2.2.3). This reduces to a classical formula, when $s = 0$ (cf. Section 4.1.1, Eq. (4.1)).

Convergence of Turán’s quadrature formula, in the case of a finite interval $[a, b]$ and $f \in C^{2s}[a, b]$, is established by Ossicini & Rosati [1978]. Roghi [1978] estimates the rate of convergence.

2.2.2. *Arbitrary multiplicities and preassigned nodes.* Chakalov [1954], [1957] and Popoviciu [1955], independently, generalize Turán’s work to quadrature rules having nodes with arbitrary multiplicities, hence quadrature sums of the form

$$(2.14) \quad Q_n(f) = \sum_{\nu=1}^n \sum_{\rho=0}^{r_\nu-1} \lambda_\nu^{(\rho)} f^{(\rho)}(\tau_\nu), \quad r_\nu \geq 1.$$

It is important, now, to assume the nodes ordered, say

$$(2.15) \quad a \leq \tau_1 < \tau_2 < \dots < \tau_n \leq b,$$

so that r_1 refers to the multiplicity of the first node, r_2 to that of the second, etc. (A permutation of the multiplicities r_1, r_2, \dots, r_n with the nodes held fixed, in general yields a new quadrature rule, a point emphasized only recently by Ghizzetti & Ossicini [1975].)

The maximum possible degree of exactness can again be determined by a simple adaptation of Jacobi’s theory (cf. Section 1.3). One finds

$$(2.16) \quad \max d(Q_n) = 2 \sum_{\nu=1}^n \left[\frac{r_\nu + 1}{2} \right] - 1,$$

so that multiplicities r_ν that are even do not contribute toward an increase in the degree of exactness. For this reason one normally assumes all r_ν to be *odd* integers,

$$r_\nu = 2s_\nu + 1.$$

The maximum degree of exactness (2.16) is then attained if and only if

$$(2.17) \quad \int_a^b \prod_{\nu=1}^n (t - \tau_\nu)^{2s_\nu+1} t^k d\lambda(t) = 0, \quad k = 0, 1, \dots, n-1.$$

Interestingly enough, there again exists a unique set of ordered nodes τ_ν for which (2.17) is satisfied; all nodes, moreover, are contained in the open interval (a, b) . The existence is proved by

Chakalov [1954], Popoviciu [1955], and Morelli & Verna [1969], existence and uniqueness (subject to (2.15)) by Ghizzetti & Ossicini [1975]. Karlin & Pinkus [1976a] prove the latter also for Stancu's generalization of (2.14) [see (2.19) below]. An extremal property analogous to (2.11) holds also for (2.14),

$$(2.18) \quad \int_a^b \prod_{\nu=1}^n (t - \tau_\nu)^{2s_\nu+2} d\lambda(t) = \min.$$

Once the nodes τ_ν are obtained, either from (2.17) or from (2.18), the quadrature rule (2.14) can be constructed in the usual way by Hermite interpolation. The weights $\lambda^{(\rho)}$, for which Chakalov [1954] and others have explicit expressions, normally vary in sign. Examples (with only one multiple node) in which all weights are positive, however, have been constructed; see Richert [1979].

The positivity of the Peano kernel $K_{d(C_n), r+1}$ for the error functional R_n is again secured, as is shown by Chakalov [1954]. See also Pavel [1968a].

In a series of papers, Stancu [1957a, b], [1959] generalizes the formula of Chakalov and Popoviciu in the same way as Christoffel generalized Gauss' formula. Thus, the quadrature sum is now

$$(2.19) \quad Q_n(f) = \sum_{\nu=1}^n \sum_{\rho=0}^{r_\nu-1} \lambda^{(\rho)} f^{(\rho)}(\tau_\nu) + \sum_{\lambda=1}^l \sum_{\kappa=0}^{k_\lambda-1} \mu_\lambda^{(\kappa)} f^{(\kappa)}(u_\lambda),$$

where u_λ are preassigned nodes such that

$$u(t) = \pm \prod_{\lambda=1}^l (t - u_\lambda)^{k_\lambda} \geq 0 \quad \text{on } [a, b].$$

The theory of Chakalov and Popoviciu, including their discussion of the remainder term, extends readily to this more general situation, the results pertaining to (2.17) and (2.18) remaining in full force if $d\lambda(t)$ is replaced by $u(t)d\lambda(t)$ throughout. (The remainder is also discussed by Pavel [1968b].) Special cases of (2.19), in part supplemented by numerical tables, are further considered by Stancu & Stroud [1963], Stroud & Secrest [1966, Tables 13, 14], Ossicini [1968], Morelli [1967/68], and Rebolia [1973]. The case $r_1 = r_2 = \dots = r_n = 1$, which (for $l \leq 2$) includes generalized Radau and Lobatto formulae, is of particular interest and is studied by Ionescu [1951], Gatteschi [1963/64], Ramskii [1968], Esser [1972], Maskell & Sack [1974], and Porath & Wenzlaff [1976].

Further generality can be introduced by imposing constraints on the weights, e.g., that some selected weights, either λ 's or μ 's, be equal to zero. Maximizing the degree of exactness under such constraints is more difficult, the underlying interpolation process now being of the Birkhoff-Hermite type. The special case $r_1 = r_2 = \dots = r_n = r$, $\lambda^{(\rho)} = 0$ for $0 \leq \rho < r - 1$, and $l = 1$, $u_1 = 0$, $k_1 = 2[(r - 1)/2] + 1$, with $d\lambda(t) = dt$ on $[-1, 1]$, is considered by Hammer & Wicke [1960] and leads to interesting nonclassical orthogonal polynomials, for which Struble [1960] has numerical tables. See also Patterson [1969] for a similar example. The case of simple nodes τ_ν , and zero constraints on some of the μ -weights, is treated by Michelli & Rivlin [1973b, Thm. 4]. Lorentz & Riemenschneider [1978] and Dyn [1979] discuss the general Birkhoff-Hermite case. For generalizations to nonpolynomial quadrature rules, see Section 2.3.3.

2.2.3. *Power-orthogonal polynomials.* The condition (2.10) gives rise to a sequence of (monic) polynomials $\pi_{n,s}(\cdot; d\lambda)$ of degree n , $n = 0, 1, 2, \dots$, each having the property that its $(2s + 1)$ -st power is orthogonal to all polynomials of lower degree. Thus, in particular,

$$\int_a^b [\pi_{n,s}(t)]^{2s+1} \pi_{k,s}(t) d\lambda(t) = 0, \quad \text{all } k < n.$$

The polynomials $\pi_{n,s}$ are called *s-orthogonal polynomials* (Ghizzetti & Ossicini [1967], [1970, p. 74f]); they reduce to ordinary orthogonal polynomials when $s = 0$.

More generally, given a sequence of arbitrary nonnegative integers, $\sigma = \{s_1, s_2, s_3, \dots\}$, $s_i \geq 0$, the condition (2.17) defines a sequence of polynomials

$$\pi_{n,\sigma}(t) = \prod_{\nu=1}^n (t - \tau_\nu^{(\sigma)}), \quad a < \tau_1^{(\sigma)} < \tau_2^{(\sigma)} < \dots < \tau_n^{(\sigma)} < b, \quad n = 0, 1, 2, \dots,$$

such that

$$\int_a^b \prod_{\nu=1}^n (t - \tau_\nu^{(\sigma)})^{2s_\nu + 1} \cdot \pi_{k,\sigma}(t) d\lambda(t) = 0, \quad \text{all } k < n.$$

These are called σ -orthogonal polynomials (Ghizzetti & Ossicini [1974/75]). The s -orthogonal polynomials correspond to the special sequence $\sigma = \{s, s, s, \dots\}$.

Very little is known about such power-orthogonal polynomials. From Bernstein's observation, leading to (2.12), one knows that the Chebyshev polynomials T_n are s -orthogonal on $[-1, 1]$ for each $s = 0, 1, 2, \dots$, with respect to the Chebyshev measure $d\lambda(t) = (1 - t^2)^{-1/2} dt$. Three other measures $d\lambda$ are presently known (they all depend on s) for which the s -orthogonal polynomials can be identified (Ossicini & Rosati [1975]). Except for Rodrigues' formula, which has an analogue for σ -orthogonal polynomials (Ghizzetti & Ossicini [1974, 1974/75]), no general theory is currently available.

2.2.4. Constructive aspects and applications. Quadrature rules such as (2.14) are usually computed in two steps: First, one generates the nodes τ_ν , either by solving directly the associated extremal problem (2.18), or by solving a system of nonlinear equations which derives from the orthogonality condition (2.17). Then, one determines the weights $\lambda_\nu^{(p)}$ of the quadrature rule, usually by solving a linear system of equations expressing the interpolatory character of the rule.

The first step is clearly the more critical one, computationally. In view of the many powerful optimization techniques currently available, however, it is reasonable to expect that the minimum problem (2.18) can be solved more or less routinely, provided the objective function and its gradient can be computed accurately and efficiently. In this connection, observe that an N -point Gauss-Christoffel quadrature rule, relative to the measure $d\lambda$ (or $ud\lambda$ in the case of quadrature rules (2.19)), where $N = n + 1 + \sum_{\nu=1}^n s_\nu$, will evaluate the objective function and its gradient exactly, except for rounding errors. The required quadrature rules, on the other hand, may be obtained by the methods discussed in Section 5.

When setting up the linear system for the weights $\lambda_\nu^{(p)}$, some care must be exercised in the selection of the polynomial basis functions. One wants the system to be reasonably well-conditioned and sparse. A choice that offers some of these advantages is that of the Newton polynomials $1, t - \tau_1, \dots, (t - \tau_1)^1, (t - \tau_1)^1(t - \tau_2), \dots, (t - \tau_1)^1(t - \tau_2)^2 \dots (t - \tau_n)^{s_n - 1}$, which leads to a triangular system. Note that the right-hand vector of the linear system can again be computed by Gauss-Christoffel integration.

Quadrature rules of the Turán type have been applied by Micchelli & Rivlin [1972] to the calculation of Fourier coefficients, and by Kastlunger & Wanner [1972] to the construction of implicit Runge-Kutta formulas for integrating ordinary differential equations. These turn out to be "A-stable", if $r = 1$ and $r = 3$, hence are useful for stiff differential equations, but are only A(α)-stable, for some $\alpha < \pi/2$, when $r \geq 5$.

2.3. Further miscellaneous extensions

2.3.1. Product-type quadrature rules. When integrating a product of two functions it may be desirable to sample the two functions independently on two different sets of points, "at their own speed" as it were. This leads naturally to product-type quadrature rules of the form

$$(2.20) \quad \int_a^b f(t)g(t)d\lambda(t) = \sum_{\mu=1}^m \sum_{\nu=1}^n f(\tau_\mu)\lambda_{\mu,\sigma}(\sigma_\nu) + R_{m,n}(f, g),$$

first introduced and studied by Boland & Duris [1971]. We assume that $d\lambda(t)$ is a positive measure, and $\{\tau_\mu\}, \{\sigma_\nu\}$ two sets of pairwise distinct real nodes. We denote the node polynomials by

$$\omega_m(t) = \prod_{\mu=1}^m (t - \tau_\mu), \quad \chi_n(t) = \prod_{\nu=1}^n (t - \sigma_\nu).$$

One says that the quadrature rule $Q(f, g)$ in (2.20) has *joint degree of exactness* $d(Q) = (k, l)$ if $R_{m,n}(f, g) = 0$ whenever $f \in P_k$ and $g \in P_l$. The formula (2.20) is called *interpolatory* if it has joint degree of exactness $d(Q) = (m - 1, n - 1)$. Equivalently, (2.20) is interpolatory if the quadrature sum in (2.20) is the result of integrating the product of two interpolation polynomials, one of degree $m - 1$ interpolating f at the nodes τ_μ , the other of degree $n - 1$ interpolating g at the nodes σ_ν . The quadrature weights are then given by

$$\lambda_{\mu\nu} = \int_a^b \frac{\omega_m(t)}{\omega'_m(\tau_\mu)(t - \tau_\mu)} \frac{\chi_n(t)}{\chi'_n(\sigma_\nu)(t - \sigma_\nu)} d\lambda(t), \quad 1 \leq \mu \leq m, \quad 1 \leq \nu \leq n.$$

Interpolatory product-type quadrature rules are the analogues of Newton-Cotes formulas for ordinary integrals. They are uniquely determined by the nodes τ_μ and σ_ν .

Given m and n , where for definiteness we assume $m \geq n$, it is of interest to determine the domain of all possible joint degrees of exactness. The most complete answer is due to Gribble [1977]. Let C, G_1 and G_2 be disjoint subsets of the Gaussian integers defined by $C = \{(k, l) : 0 \leq k \leq m - 1, 0 \leq l \leq n - 1\}$, $G_1 = \{(k, l) : k \geq 0, l \geq n, k + l \leq 2n - 1\}$, $G_2 = \{(k, l) : 0 \leq l \leq n - 1, k \geq m, k + l \leq 2m - 1\}$ (see Figure 2.1). Then a product-type quadrature rule Q can have joint degree of exactness $d(Q) = (k, l)$ if and only if $(k, l) \in C \cup G_1 \cup G_2$. Those rules Q with

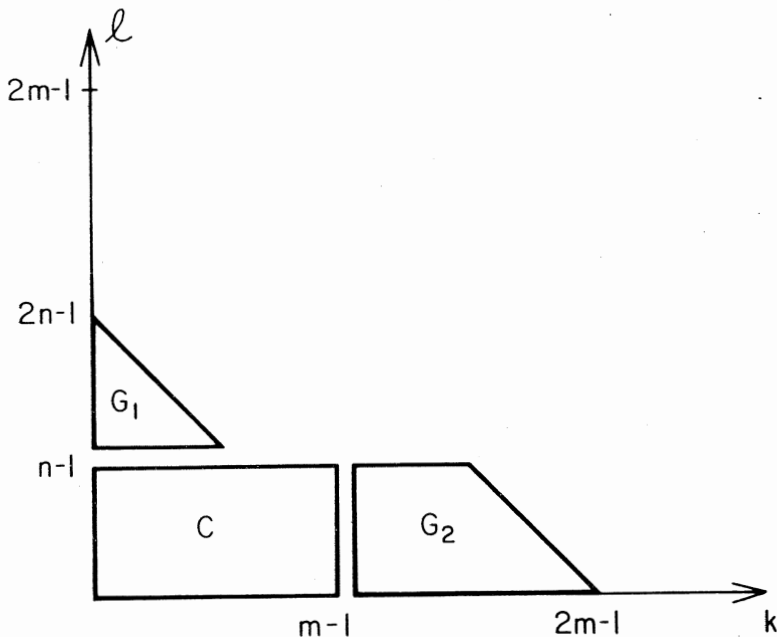


Fig. 2.1. Degrees of exactness for product-type quadrature rules

$d(Q) = (m - 1, n - 1)$, hence also $d(Q) \in C$, are precisely the interpolatory quadrature rules, which, as already observed, can be constructed for arbitrary nodes τ_μ, σ_ν . It is natural to consider the quadrature rules Q with $d(Q) \in G_1 \cup G_2$, as being "of Gaussian type". They exist only if some of their nodes are suitably restricted. Indeed, for a quadrature rule Q to have $d(Q) \in G_1$, it is necessary and sufficient that the nodes σ_ν be such that

$$(2.21) \quad \int_a^b \chi_s(t) t^s d\lambda(t) = 0 \quad \text{for } s = 0, 1, \dots, k + l - n.$$

The nodes τ_μ can then be selected arbitrarily. Since $k + l - n \leq n - 1$ for $(k, l) \in G_1$, the condition (2.21) can always be satisfied with pairwise distinct real nodes σ_ν , and uniquely so, if $k + l = 2n - 1$. Similarly, a quadrature rule Q with $d(Q) \in G_2$ exists if and only if

$$\int_a^b \omega_r(t) t^r d\lambda(t) = 0 \quad \text{for } r = 0, 1, \dots, k + l - m,$$

in which case the nodes σ_ν can be chosen arbitrarily. In particular, if $m = n$, it follows (Boland [1973]) that the only quadrature rule Q for which simultaneously $d(Q) = (n - 1, n)$ and $d(Q) = (n, n - 1)$ is the ordinary Gauss-Christoffel quadrature rule, in which $\tau_\nu = \sigma_\nu, \nu = 1, 2, \dots, n$, are the Gaussian nodes, λ_ν the Christoffel numbers, and $\lambda_\mu = 0$ for $\mu \neq \nu$.

The error term $R_{m,n}(f, g)$, and convergence results, are discussed in Boland & Duris [1971] and Boland [1972].

2.3.2. *Gaussian quadrature involving interval functionals.* All quadrature sums considered so far involve point evaluation functionals, i.e. the values of a function (and perhaps some of its derivatives) at certain well-determined points. In physical applications it is not uncommon that no such function values are accessible, but only certain averages

$$I(u_k, v_k; f) = \frac{1}{\text{meas}[u_k, v_k]} \int_{u_k}^{v_k} f(t) d\mu_k(t), \quad \text{meas}[u_k, v_k] = \int_{u_k}^{v_k} d\mu_k(t), \quad k = 1, 2, \dots, n,$$

taken over small intervals $[u_k, v_k], u_k < v_k$. In such cases, it is meaningful to employ quadrature rules of the type

$$(2.22) \quad \int_a^b f(t) d\lambda(t) = \sum_{k=1}^n \lambda_k I(u_k, v_k; f) + R_n(f).$$

Ordinary quadrature rules are contained in (2.22) as the limit case $u_k \rightarrow \tau_k, v_k \rightarrow \tau_k, k = 1, 2, \dots, n$.

The study of quadrature rules (2.22) involving interval functionals was initiated independently by Omladič, Pahor & Suhadolc [1975/76] and Pittnauer & Reimer [1976]. They showed, first of all, that the theory of interpolatory quadrature rules (Newton-Cotes formulae) carries over completely: Given any n nonoverlapping intervals $[u_k, v_k]$ (some possibly degenerate), one can construct a unique quadrature rule (2.22) which is exact for all polynomials of degree $\leq n - 1$. In the special case $d\lambda(t) = d\mu_k(t) = dt$ on $[-1, 1]$, Pittnauer & Reimer [1976], [1979a] also extend the theory of Gaussian quadrature. In particular, they establish the following interesting extremal characterization of Gauss-Legendre formulae. For given numbers $\sigma_k > 1, k = 1, 2, \dots, n$, consider the function

$$G_n(u, v) = \int_{-1}^1 \Omega_n(t; u, v) dt - \sum_{k=1}^n \sigma_k \int_{u_k}^{v_k} \Omega_n(t; u, v) dt,$$

where $u \in \mathbb{R}^n, v \in \mathbb{R}^n$ are points in the closed polyhedron $P: -1 \leq u_1 \leq v_1 \leq \dots \leq u_n \leq v_n \leq 1$, and

$$\Omega_n(t; u, v) = \prod_{k=1}^n (t - u_k)(t - v_k).$$

Then the minimum of $G_n(u, v)$ on P is necessarily attained at an interior point of P . If (u, v) is such an interior minimum point, and $\lambda_k = (v_k - u_k)\sigma_k$, then (2.22) is a Gauss-Legendre quadrature formula, i.e. exact for all $f \in P_{2n-1}$. Higher degree of exactness, when (u, v) is an interior point of P , is unattainable.

Every choice of numbers $\sigma_k > 1$ will produce a Gauss-Legendre formula of the type (2.22). Uniqueness, therefore, no longer holds, but the positivity of the weights λ_k is still guaranteed.

We remark that the property just described, when subject to the constraint $u = v$, yields the classical characterization of the Legendre polynomial $\pi_n(t; dt)$ as the monic n -th degree polynomial of minimum L_2 -norm.

Peano estimates of the remainder (cf. Section 4.2), as well as a convergence theory for quadrature rules (2.22), are developed in Pittnauer & Reimer [1979b].

2.3.3. *Nonpolynomial Gaussian quadrature.* Gauss' principle can be extended in a natural way to nonpolynomial functions. Thus, given a system of linearly independent functions

$$(2.23) \quad u_1(t), u_2(t), u_3(t), \dots, \quad a \leq t \leq b,$$

usually chosen to be complete in some suitable function space, the quadrature rule

$$(2.24) \quad \int_a^b f(t) d\lambda(t) = \sum_{\nu=1}^n \lambda_\nu f(\tau_\nu) + R_n(f)$$

is to be constructed in such a way as to integrate exactly as many successive functions in (2.23) as possible. If the first $2n$ functions are integrated exactly, one calls the rule (2.24) *Gaussian with respect to the system* (2.23).

Gaussian formulae, indeed also Gauss-Radau formulae, for the system $u_\alpha(t) = t^{\alpha_1}$, $0 \leq \alpha_1 < \alpha_2 < \dots$, on $[0, 1]$ are already established by Stieltjes [1884c]. Trigonometric functions $u_1(t) = 1$, $u_2(t) = \cos t$, $u_3(t) = \sin t$, $u_4(t) = \cos 2t$, ... yield quadrature rules exact for trigonometric polynomials up to a certain degree. Assuming $d\lambda(t) = dt$ on $[0, 2\pi]$, and $0 \leq \tau_1 < \tau_2 < \dots < \tau_n < 2\pi$, Schmidt [1947] shows that the maximum possible degree is $n-1$, and is attained precisely if $\tau_\nu = \nu(2\pi/n) - \gamma$, $0 \leq \gamma < 2\pi/n$, and $\lambda_\nu = 2\pi/n$. This elevates the trapezoidal rule to a Gaussian formula for trigonometric functions. The case of an arbitrary finite interval $[a, b]$, in the context of trigonometric (and also exponential) systems, is discussed by Crout [1929/30, §16], Newbery [1969] and Knight & Newbery [1970]; integrals with arbitrary positive measures $d\lambda(t)$ on $[0, 2\pi]$ by Turečik [1959], [1960] and Keda [1961a]. Keda [1961b] and Rosati [1968] obtain trigonometric Gauss formulae with multiple nodes. For Gauss formulae with respect to spline functions, see Schoenberg [1958] and Micchelli & Pinkus [1977]. Harris & Evans [1977/78] have Gauss formulae for systems (2.23) that include algebraic powers together with functions exhibiting endpoint singularities.

Nonpolynomial Gaussian formulae can sometimes be obtained via ordinary Gaussian formulae through suitable transformations. Thus, for example, the n -point formula for $d\lambda(t) = t^r e^{-t} dt$ on $[0, \infty]$, Gaussian with respect to the system $u_r(t) = (t+1)^{-r}$, $r = 0, 1, 2, \dots$ (Krylov, Korolev & Skoblja [1959], Pal'cev & Skoblja [1965]), is simply related to the n -point Gauss-Christoffel formula with measure $(t+1)^{-2n} d\lambda(t)$ on $[0, \infty]$. A similar example, involving Fourier transforms, is discussed in Kruglikova & Krylov [1961]. See also Stroud & Secrest [1966, §3.2].

Ghizzetti [1954/55], inspired by work of Radon on the remainder term (cf. Section 4.2), constructs a very general class of Gauss formulae (2.24) which are exact for all solutions of a linear homogeneous differential equation $Lf = 0$ of order $2n$. The existence of such formulae depends on the homogeneous n -point boundary value problem

$$(2.25) \quad Ly = 0, \quad y(\tau_\nu) = 0, \quad \nu = 1, 2, \dots, n.$$

If (2.25) has exactly q linearly independent eigensolutions $y_r(t)$, $n \leq q \leq 2n - 1$, Gauss formulae exist if and only if

$$(2.26) \quad \int_a^b y_r(t) d\lambda(t) = 0, \quad r = 1, 2, \dots, q,$$

and then, in fact, ∞^q many. The classical case corresponds to $L = D^{2n}$, $D = d/dt$, where (2.25) has exactly n linearly independent solutions $y_r(t) = t^{r-1} \prod_{v=1}^{n-r} (t - \tau_v)$, $r = 1, 2, \dots, n$, and (2.26) expresses the usual orthogonality criterion for $\omega_n(t) = \prod_{v=1}^n (t - \tau_v)$. Since $q = n$ in this case, the formula is unique.

Gauss formulae for harmonic functions have been proposed in connection with the Dirichlet problem for Laplace's equation (Stroud [1974]). If D is a bounded, simply connected two-dimensional open domain, with rectifiable boundary ∂D , the solution of $\Delta^2 u = 0$ in D , with u prescribed on ∂D , has the known representation $u(P) = - \int_{\partial D} (\partial G / \partial n)(P, Q) u(Q) ds$, where G is the Green's function of D and $\partial G / \partial n$ its normal derivative (known to be nonpositive). Treating $-\partial G / \partial n$ as a weight function it is natural to seek an approximation of the form $u(P) \approx \sum_{v=1}^n g_v u(Q_v)$, where $g_v \in \mathbf{R}$ and $Q_v \in \partial D$ depend on P , and try to make the formula exact for harmonic polynomials of as high a degree as possible. Since there are $2n$ free parameters and $2n - 1$ linearly independent harmonic polynomials of degree $\leq n - 1$, one expects that one parameter, say Q_n , can be selected arbitrarily on ∂D and all others determined such that the formula has harmonic degree of exactness $n - 1$. Barrow & Stroud [1976] indeed show that this is possible by proving the existence of at least one Gaussian formula of harmonic degree $n - 1$. Their proof is based on degree theory for mappings and homotopy arguments. Numerical procedures for computing such formulae are discussed in Stroud [1974]. Johnson & Riess [1979] construct formulas for circular regions. Similar ideas are pursued in Barrow [1976], [1977] in connection with the heat equation and other parabolic equations.

A generalization in another direction is due to Engels [1972], [1973], who extends Markov's derivation of Gaussian quadrature rules (cf. Section 1.4) in the sense that the underlying Hermite interpolation operator, though still linear, need no longer be polynomial. It turns out that a number of known quadrature rules, e.g. the optimal quadrature rule of Wilf [1964] and more general optimal quadrature rules (Engels [1977]), become Gaussian in this generalized sense. A further extension of this theory to quadrature rules with prescribed (simple or double) nodes is given in Engels [1974].

The existence of a Gaussian quadrature rule (2.24) with respect to the system (2.23) is always guaranteed if the first $2n$ functions of this system form a Chebyshev system on $[a, b]$. In the language of moment spaces, the Gauss formula corresponds to the unique *lower principal representation* of the measure $d\lambda(t)$ (see, e.g., Karlin & Studden [1966, §3]). Gaussian quadrature rules with multiple nodes, based on extended Chebyshev systems, are established in Karlin & Pinkus [1976a, b] and Barrow [1978] (cf. also Section 2.2.2).

3. Extension of Integrals Accessible to Gauss-Christoffel Quadrature

3.1. Nonpositive integrals

The positivity $d\lambda(t) \geq 0$ of the measure of integration is a sufficient, but by no means a necessary, condition for the existence and uniqueness of the orthogonal polynomial $\pi_n(\cdot; d\lambda)$, and hence for the unique existence of the n -point Gauss-Christoffel quadrature formula (cf. Section 1.4). Viewing the orthogonality conditions $\int_a^b \pi_n(t) t^k d\lambda(t) = 0$, $k = 0, 1, \dots, n - 1$, as a system of linear algebraic equations for the coefficients of π_n , one finds, indeed, that a necessary and sufficient condition is merely

$$(3.1) \quad \Delta_n = \det \begin{bmatrix} \mu_0 & \mu_1 & \dots & \mu_{n-1} \\ \mu_1 & \mu_2 & \dots & \mu_n \\ \dots & \dots & \dots & \dots \\ \mu_{n-1} & \mu_n & \dots & \mu_{2n-2} \end{bmatrix} \neq 0,$$

$$\mu_r = \int_a^b t^r d\lambda(t), \quad r = 0, 1, 2, \dots$$

If also $\Delta_{n+1} \neq 0$, then $\int_a^b \pi_n^2(t) d\lambda(t) \neq 0$, and the degree of exactness of the Gauss-Christoffel formula cannot exceed $2n - 1$.

If $d\lambda(t) \geq 0$ then (3.1) is certainly true, even in the strengthened form $\Delta_n > 0$, all $n \geq 1$, as is known from the theory of the moment problem (Wall [1948, p. 325]). If $d\lambda$ is an arbitrary measure, the condition (3.1) may still be valid, but some of the familiar properties of orthogonal polynomials may cease to hold. Thus, the zeros of π_n need no longer be real, let alone contained in (a, b) , and the Christoffel numbers need no longer be positive. Concerning the latter, all one can say is that (for real-valued $d\lambda$ and real nodes) the number of positive [negative] Christoffel numbers equals the number of positive [negative] eigenvalues of the Hankel matrix in (3.1) (Stroud [1963]).

While there is some general theory concerning orthogonal polynomials with sign-variable weight functions (Struble [1963], Monegato [1980]), we will consider here only a few examples of nonpositive (including complex-valued) measures $d\lambda$ that are of interest in applications.

3.1.1. *Odd and even weight functions on symmetric intervals.* Let $\omega(t)$ be an odd function on a symmetric interval $[-a, a]$, $a > 0$, and $d\lambda(t) = \omega(t)dt$. Assume further that $n = 2m$ is even. Then the determinant in (3.1) has a checkerboard pattern of zero and nonzero elements, from which it follows, by Laplace expansion, that

$$(3.2) \quad \Delta_n = (-1)^n \det \begin{bmatrix} \mu_1 & \mu_3 & \dots & \mu_{n-1} \\ \mu_3 & \mu_5 & \dots & \mu_{n+1} \\ \dots & \dots & \dots & \dots \\ \mu_{n-1} & \mu_{n+1} & \dots & \mu_{2n-3} \end{bmatrix}^2$$

There is, therefore, a unique n -point Gauss-Christoffel quadrature formula if n is even and the determinant in (3.2) is different from zero. The latter is certainly true if ω is nonnegative on $[0, a]$, since then

$$\mu_{2r-1} = \int_{-a}^a t^{2r-1} \omega(t) dt = \int_0^{a^2} t^{r-1} \omega(\sqrt{t}) dt, \quad r = 1, 2, 3, \dots,$$

are moments of the nonnegative measure $d\sigma(t) = \omega(\sqrt{t})dt$ on $[0, a^2]$. The desired Gauss-Christoffel formula indeed can be constructed in terms of the m -point Gauss-Christoffel formula for $d\sigma$ (Radau [1880, p. 317f], Piessens

[1970a]). For a similar construction in the case of multiple nodes see also Levin [1974]. If n is odd, the Gauss–Christoffel formula does not exist, as is already observed by Christoffel [1877] in the special case $d\lambda(t) = tdt$ on $[-1, 1]$.

Among examples of odd weight functions that have received attention are $d\lambda(t) = t^{2s+1}dt$ on $[-1, 1]$ (Rothmann [1961]) and $d\lambda(t) = \sin t dt$ on $[-\pi, \pi]$ (Piessens [1970a]). Another interesting example, $d\lambda(t) = \ln((1+t)/(1-t))dt$ on $[-1, 1]$, arises in the evaluation of a certain two-dimensional Cauchy principal value integral describing the aerodynamical load on a lifting body (Song [1969]). For this example, Piessens, Chawla & Jayarajan [1976] have numerical tables.

If $\omega(t)$ is even, but not necessarily of constant sign, and $n = 2m + 1$ is odd, then a unique n -point Gauss–Christoffel formula exists if

$$\det \begin{bmatrix} \mu_0 & \mu_2 & \dots & \mu_{n-1} \\ \mu_2 & \mu_4 & \dots & \mu_{n+1} \\ \dots & \dots & \dots & \dots \\ \mu_{n-1} & \mu_{n+1} & \dots & \mu_{2n-2} \end{bmatrix} \cdot \det \begin{bmatrix} \mu_2 & \mu_4 & \dots & \mu_{n-1} \\ \mu_4 & \mu_6 & \dots & \mu_{n+1} \\ \dots & \dots & \dots & \dots \\ \mu_{n-1} & \mu_{n+1} & \dots & \mu_{2n-4} \end{bmatrix} \neq 0.$$

It can be constructed in terms of the m -point Gauss–Radau formula for the weight function $\omega(\sqrt{t})/\sqrt{t}$ on $[0, a^2]$ or, equivalently, the m -point Gauss–Christoffel formula for $d\sigma(t) = \sqrt{t}\omega(\sqrt{t})dt$ on $[0, a^2]$ (Piessens [1972a]). As always, in such cases, there is no assurance that all nodes are real. An example of interest in Fourier analysis is $d\lambda(t) = \cos t dt$ on $[-\pi, \pi]$ (Piessens [1972a]).

3.1.2. *Oscillatory weight functions.* An interesting example of an oscillating weight function is $d\lambda(t) = \pi_m(t; d\sigma)d\sigma(t)$ for some positive measure $d\sigma$ on $[a, b]$. Here, $\mu_r = \int_a^b t^r \pi_m(t) d\sigma(t) = 0$ if $r < m$, and $\mu_m > 0$, so that (3.1) cannot hold unless $n \geq m + 1$. The case $n = m + 1$, already considered by Stieltjes in his last letter to Hermite (Baillaud & Bourget [1905, Vol. II, p. 439]), is of particular interest in connection with Kronrod’s extension of Gauss–Christoffel quadrature rules (cf. Section 2.1.2). In this case,

$$\Delta_n = \det \begin{bmatrix} 0 & 0 & \dots & 0 & \mu_m \\ 0 & 0 & \dots & \mu_m & \mu_{m+1} \\ \dots & \dots & \dots & \dots & \dots \\ \mu_m & \mu_{m+1} & \dots & \mu_{2m-1} & \mu_{2m} \end{bmatrix} = \mu_m^n > 0 \quad (n = m + 1),$$

showing that $\pi_n(\cdot; d\lambda)$ exists uniquely. Stieltjes conjectures that the zeros of $\pi_n(\cdot; d\lambda)$ are all real, simple, contained in (a, b) , and separated by the zeros of $\pi_m(\cdot; d\sigma)$. Unfortunately, the conjecture is not true in this generality, but has been proved by Szegő [1935] for ultraspherical polynomials, $d\sigma(t) = (1-t^2)^{\mu-1/2} dt$, with $0 < \mu \leq 2$. The special case $\mu = 0$ (of the Chebyshev polynomial $\pi_m(\cdot; d\sigma) = 2^{1-m}T_m$) yields $\pi_n(t; d\lambda) = 2^{1-m}(t^2 - 1)U_{m-1}(t)$, where

U_{m-1} is the Chebyshev polynomial of the second kind. The corresponding Gauss-Christoffel quadrature formula, interestingly enough, has degree of exactness $3m - 1$ if $m > 1$, not $2m + 1$, as one might expect (Micchelli & Rivlin [1972], Riess & Johnson [1974]).

3.1.3. *Complex-valued weight functions.* Gauss-Christoffel quadrature rules with a complex weight function were first introduced by Salzer [1955], [1961] in connection with the inversion of the Laplace transform. The integral of interest here is the Bromwich integral

$$I(f) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{\zeta} \zeta^{-s} f(\zeta) d\zeta, \quad s > 0,$$

where f is assumed holomorphic in a half-plane containing the contour $\text{Re } \zeta = c$, and bounded as $\zeta \rightarrow \infty$ in $|\arg \zeta| < \pi/2$. Salzer [1955], in the case $s = 1$, and Skoblja [1961], Krylov & Skoblja [1961], Wellekens [1970], Piessens [1971a, c], in the case of general $s > 0$, approximate $I(f)$ by a (complex) quadrature sum

$$(3.3) \quad Q_n(f) = \sum_{\nu=1}^n c_\nu f(\zeta_\nu)$$

which is Gaussian in the sense that $Q_n(f) = I(f)$ whenever f is a polynomial of degree $\leq 2n - 1$ in $1/\zeta$. This calls for polynomials π_r in the variable $1/\zeta$ satisfying the orthogonality condition

$$\frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{\zeta} \zeta^{-s} \pi_k(1/\zeta) \pi_l(1/\zeta) d\zeta = 0, \quad k \neq l.$$

Such polynomials $\pi_r = \pi_{r,s}(z)$ exist uniquely. Indeed, $\Delta_n \neq 0$ for all $n \geq 1$ (Krylov & Skoblja [1974, p. 94ff]), where Δ_n is the determinant in (3.1) formed with the moments

$$\mu_r = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{\zeta} \zeta^{-s-r} d\zeta = \frac{1}{\Gamma(s+r)}, \quad r = 0, 1, 2, \dots$$

It turns out that $\pi_{n,s}(z) = y_n(z; s, -1)$, where $y_n(z; a, b)$ is the generalized Bessel polynomial of Krall & Frink [1949]. (Bessel polynomials have a long history, and many interesting applications; see Grosswald [1978] for a recent exposition.) The nodes ζ_ν in (3.3) — the reciprocals of the zeros of $\pi_{n,s}(z)$ — are all contained in the right half-plane, when $s \geq 1$ (Wimp [1965]). Extensive numerical tables (Krylov & Skoblja [1968], Piessens [1969a]) in fact suggest that $\text{Re } \zeta_\nu > 0$ even for $s > 0$. This has been proved by Martinez [1977]. More precise results concerning the zeros of $\pi_{n,s}$ can be found in de Bruin, Saff & Varga [to appear].

The convergence $Q_n(f) \rightarrow I(f)$ as $n \rightarrow \infty$ is discussed in Luke [1969, p. 254].

The quadrature rule (3.3) may be constructed by the method of Golub & Welsch (cf. Section 5.1), since the three-term recurrence relation for Bessel polynomials is known explicitly. For a discussion of this, see Luvison [1974] and Piessens [1975]. Piessens [1973b] has a Fortran program for generating Q_n , which uses the Newton-Raphson method.

Instead of applying (3.3) directly to f , Salzer [1976] proposes to apply Q_n to a Lagrange or Hermite interpolation polynomial of degree $2n - 1$ based on interpolation points on the real line. This obviates the need of evaluating f in the complex plane and still often produces satisfactory results (Pexton [1976]).

Kronrod extensions of Q_n in (3.3) (cf. Section 2.1.2) are discussed by Piessens [1969b], [1971b], who also constructs Radau type formulas with the prescribed point at infinity.

Gauss-Christoffel quadrature rules with other complex weight functions, in particular Jacobi weight functions $(1-t)^\alpha(1+t)^\beta$ with complex parameters α, β , satisfying $\operatorname{Re} \alpha > -1$, $\operatorname{Re} \beta > -1$, are used in atomic scattering theory by Nuttall & Wherry [1978], and in elasticity theory by Theocaris & Ioakimidis [1977]. Jacobi measures in which α, β are no longer subject to the restriction $\operatorname{Re} \alpha > -1$, $\operatorname{Re} \beta > -1$, and correspondingly the integral is to be interpreted as an appropriate loop integral, are discussed by Maskell & Sack [1974].

3.2. Cauchy principal value integrals

Quadrature rules can be adapted to deal with Cauchy-type singular integrals extended over segments of the real line, or over the circle, or over more general curves in the complex plane. We consider here only Cauchy principal value integrals of the form

$$(3.4) \quad I(f)(x) = \int_a^b \frac{f(t)}{x-t} d\lambda(t), \quad x \in (a, b),$$

where $[a, b]$ is a finite or infinite interval and $d\lambda(t) = \omega(t)dt$ a measure of integration that admits Gauss-Christoffel quadrature formulae and is such that the integral in (3.4) is meaningful. (Hölder continuity of f on $[a, b]$ usually suffices.) Singular integrals over the circle, which give rise to principal value integrals $\int_0^{2\pi} f(t) \cot((x-t)/2) dt$ with Hilbert kernel (and 2π -periodic functions f) are best treated by trigonometric interpolation at equally spaced points. For this, see Gaier [1964, Ch. 2, §2], Korneičuk [1964], Gabdulhaev [1976]. Rabinowitz [1978] has a survey of numerical methods for evaluating Cauchy principal value integrals.

We distinguish between two types of quadrature rules for (3.4). In the first type, the parameter x enters as a node,

$$(3.5) \quad Q_n(f)(x) = c_0(x)f(x) + \sum_{\nu=1}^n c_\nu(x)f(\tau_\nu);$$

in the other, it does not,

$$(3.5^*) \quad Q_n^*(f)(x) = \sum_{\nu=1}^n c_\nu^*(x) f(\tau_\nu).$$

All nodes τ_ν are assumed independent of x . We will call (3.5^{*}) a *quadrature rule in the strict sense*, and (3.5) a *modified quadrature rule*. The two quadrature rules have essentially different character: (3.5) can be made "Gaussian", i.e. of degree of exactness $2n$, whereas (3.5^{*}) cannot. The degree of exactness of (3.5^{*}), indeed, cannot exceed $n-1$ (Sanikidze [1970a]), since otherwise $I(f)(x) \equiv 0$ when $f(t) = \sum_{\nu=1}^n (t - \tau_\nu)$, which contradicts well-known inversion formulas for Cauchy singular integrals (Gahov [1958, §42.3], Mushelišvili [1946, §86]).

3.2.1. *Modified Gauss-Christoffel quadrature formulae.* Let $\{\pi_k\}$ denote the (monic) orthogonal polynomials belonging to $d\lambda$, and let

$$(3.6) \quad G_n(f) = \sum_{\nu=1}^n \lambda_\nu f(\tau_\nu)$$

denote the n -point Gauss-Christoffel quadrature rule for the measure $d\lambda$. In analogy to the Gauss-Christoffel theory (cf. Section 1.4) we define

$$L(x) = \int_a^b \frac{d\lambda(t)}{x-t}, \quad \rho_n(x) = \int_a^b \frac{\pi_n(t)}{x-t} d\lambda(t),$$

$$\sigma_n(x) = \int_a^b \frac{\pi_n(x) - \pi_n(t)}{x-t} d\lambda(t).$$

Clearly,

$$\pi_n(x)L(x) = \sigma_n(x) + \rho_n(x),$$

and, the integrand of σ_n being a polynomial of degree $\leq n-1$ in the variable t ,

$$\sigma_n(x) = G_n \left[\frac{\pi_n(x) - \pi_n(\cdot)}{x - \cdot} \right] = \pi_n(x) G_n \left[\frac{1}{x - \cdot} \right].$$

Consequently,

$$(3.7) \quad L(x) - G_n \left[\frac{1}{x - \cdot} \right] = \frac{\rho_n(x)}{\pi_n(x)}.$$

Now in order to approximate the integral $I(f)(x)$ in (3.4), we write

$$(3.8) \quad I(f)(x) = f(x) \int_a^b \frac{d\lambda(t)}{x-t} - \int_a^b \frac{f(x) - f(t)}{x-t} d\lambda(t),$$

and observe that the second integral is integrated exactly by the rule G_n whenever $f \in \mathbf{P}_{2n}$. Therefore,

$$I(f)(x) = f(x) \left\{ L(x) - G_n \left[\frac{1}{x - \cdot} \right] \right\} + G_n \left[\frac{f(\cdot)}{x - \cdot} \right] + R_n(f),$$

or, by virtue of (3.7),

$$(3.9) \quad I(f)(x) = \frac{\rho_n(x)}{\pi_n(x)} f(x) + \sum_{\nu=1}^n \lambda_\nu \frac{f(\tau_\nu)}{x - \tau_\nu} + R_n(f).$$

Here $R_n(f) = 0$ for all $f \in \mathbf{P}_{2n}$. We call (3.9) — a quadrature rule of the type (3.5) — the *modified Gauss–Christoffel quadrature formula* for $I(f)(x)$.

We remark that (3.9) is valid for any interpolatory quadrature rule G_n , if π_n is understood to be the node polynomial of G_n . The degree of accuracy, of course, will be correspondingly smaller. In particular, we may construct modified versions of the Gauss–Radau, Gauss–Lobatto, etc., formulae for $I(f)(x)$. A simple limit argument will show that, for any quadrature rule G_n ,

$$(3.10) \quad \lambda_\nu = - \frac{\rho_n(\tau_\nu)}{\pi_n'(\tau_\nu)}, \quad \nu = 1, 2, \dots, n.$$

If f is holomorphic in a neighborhood of the interval $[a, b]$, the formula (3.9) can also be obtained by applying the residue theorem to the function $f(\zeta) \hat{\pi}_n(t) / [(x - \zeta)(\zeta - t)\pi_n(\zeta)]$ and subsequent integration over the variable t . This yields the useful contour integral representation of the remainder,

$$(3.11) \quad R_n(f)(x) = \frac{1}{2\pi i} \oint_{\Gamma} \frac{\rho_n(z)}{(x - z)\pi_n(z)} f(z) dz,$$

where Γ is a contour encircling the interval $[a, b]$.

Particularly noteworthy is the special case in which x is a root of $\rho_n(x) = 0$. Then (3.9) becomes

$$(3.9^\circ) \quad I(f)(x) = \sum_{\nu=1}^n \lambda_\nu \frac{f(\tau_\nu)}{x - \tau_\nu} + R_n(f) \quad (\rho_n(x) = 0),$$

and we get a formula that looks like what would have been obtained had we simply applied G_n to the integral in (3.4), treating the principal value integral as if it were an ordinary integral. If G_n is a Gauss–Christoffel formula, then again $R_n(f) = 0$ for $f \in \mathbf{P}_{2n}$. Korneičuk [1964] appears to be the first who noted the simple and elegant formula (3.9°). He also observes that between any two zeros of π_n there is at least one zero of ρ_n , if all $\lambda_\nu > 0$. (This was already noted by Stieltjes [1883] through an examination of the behavior of $\rho_n(x)/\pi_n(x)$ on (a, b) and taking note of (3.10).) Inevitably, the formula (3.9°) has been rediscovered many times (see, e.g., Lebedev & Baburin [1965], Delves [1967/68], Piessens [1970c], Stark [1971], Erdogan & Gupta [1971/72], Krenk [1975/76]).

As x approaches a node τ_ν , the quadrature sum in (3.9) tends to a finite value, even though one term tends to $+\infty$ and another to $-\infty$. The limit, in fact, is

$$(3.12) \quad I(f)(\tau_\nu) = \left[\frac{\rho'_n(\tau_\nu)}{\pi'_n(\tau_\nu)} + \frac{1}{2} \lambda_\nu \frac{\pi''_n(\tau_\nu)}{\pi'_n(\tau_\nu)} \right] f(\tau_\nu) + G_n^\nu \left[\frac{f(\cdot)}{\tau_\nu - \cdot} \right] - \lambda_\nu f'(\tau_\nu) + R_n(f),$$

where

$$G_n^\nu(f) = \sum_{\substack{\mu=1 \\ \mu \neq \nu}}^n \lambda_\mu f(\tau_\mu),$$

or, equivalently,

$$(3.12') \quad I(f)(\tau_\nu) = \left\{ \rho_0(\tau_\nu) - G_n^\nu \left[\frac{1}{\tau_\nu - \cdot} \right] \right\} f(\tau_\nu) + G_n^\nu \left[\frac{f(\cdot)}{\tau_\nu - \cdot} \right] - \lambda_\nu f'(\tau_\nu) + R_n(f).$$

Although the limits (3.12), (3.12') are well-determined, the evaluation of $I(f)(x)$ in (3.9), when x is close to one of the nodes τ_ν , is subject to severe cancellation errors. To avoid them, one must reorganize the computation in a different way, as will be discussed in Section 3.2.3.

When $[a, b]$ is a finite interval, say $[-1, 1]$, and $d\lambda(t) = dt$, the integral (3.4) can always be transformed into the form

$$\int_{-1}^1 \frac{f(t)}{t} dt,$$

with a new f , for example by a linear fractional transformation. Using as base rule (3.6) the Gauss-Legendre formula, for which $\rho_n(x) = (1/2)Q_n(x)$ is the Legendre function of the second kind, one finds $\rho_n(0) = 0$ if n is even, so that (3.9') becomes applicable with $x = 0$. This gives (Price [1960], Lebedev & Baburin [1965], Piessens [1970c])

$$\int_{-1}^1 \frac{f(t)}{t} dt = \sum_{\nu=1}^n \frac{\lambda_\nu}{\tau_\nu} f(\tau_\nu) + R_n(f), \quad n \text{ even},$$

which is exact for $f \in P_{2n}$. An analogous formula holds if $d\lambda(t) = \omega(t)dt$ is an even measure on a symmetric interval.

If n is odd, no such Gaussian formula exists (cf. Section 3.1.1). However, in this case π_n vanishes for $\tau_\nu = 0$, so that (3.12) becomes applicable (Hunter [1972]),

$$\int_{-1}^1 \frac{f(t)}{t} dt = \lambda_\nu f'(0) + \sum_{\substack{\mu=1 \\ \mu \neq \nu}}^n \frac{\lambda_\mu}{\tau_\mu} f(\tau_\mu) + R_n(f), \quad n \text{ odd}, \quad \tau_\nu = 0.$$

This formula, too, is exact for $f \in P_{2n}$.

The quadrature rule (3.9) can be generalized to incorporate poles, either on or outside of $[a, b]$, in addition to, or in place of the pole at x , with an appropriate extension of the remainder formula in (3.11); see Hunter [1972], Chawla & Ramakrishnan [1974], Chawla & Jayarajan [1975], Ioakimidis &

Theocaris [1977b], Lether [1977]. Remainder expressions of the Markov type (see Section 1.4) have been obtained in the special case (3.9°) by Železnova, Korneičuk & Markov [1965], and in the general case (3.9) [and (3.13) below] by Elliott & Paget [1979].

For the Jacobi measure $d\lambda(t) = (1-t)^\alpha(1+t)^\beta dt$, $\alpha > -1$, $\beta > -1$, Tsamasphyros & Theocaris [1977] claim convergence of (3.9) for functions f which are Hölder continuous with exponent μ , $0 < \mu \leq 1$. Convergence in the case of an arbitrary weight function on a compact interval $[a, b]$ is proved for functions $f \in C^1[a, b]$ by Elliott & Paget [1979] and discussed for Hölder continuous functions by Elliott [1979].

3.2.2. *Gauss-Christoffel quadrature formulae in the strict sense.* An alternative use of the quadrature formula (3.6) in (3.8) can be made as follows: Use (3.6) to approximate the second integral on the right of (3.8) and, at the same time, approximate the factor $f(x)$ multiplying the first integral by the interpolation polynomial of degree $n-1$ based on the nodes τ_ν of the quadrature rule (3.6). The result is a quadrature formula for $I(f)(x)$ of the type (3.5*), namely

$$(3.13) \quad I(f)(x) = \sum_{\nu=1}^n \left(\frac{\rho_n(x)}{\pi'_n(\tau_\nu)(x - \tau_\nu)} + \frac{\lambda_\nu}{x - \tau_\nu} \right) f(\tau_\nu) + R_n(f),$$

or, equivalently, by virtue of (3.10),

$$(3.13') \quad I(f)(x) = \sum_{\nu=1}^n \frac{\rho_n(x) - \rho_n(\tau_\nu)}{\pi'_n(\tau_\nu)(x - \tau_\nu)} f(\tau_\nu) + R_n(f).$$

As pointed out earlier, this formula has degree of exactness at most equal to $n-1$, unless x is a zero of $\rho_n(x)$, in which case (3.13) reduces to (3.9°) and has degree of exactness $d(G_n) + 1$. The formula (3.13) can also be obtained more directly by replacing f in (3.4) by the polynomial of degree $\leq n-1$ interpolating f at the nodes τ_ν of (3.6). Korneičuk [1964], taking for G_n the Gauss-Christoffel formula, appears to be the first to obtain (3.13). The special case of Jacobi weight functions is considered by Sanikidze [1970a] and Šeško [1976], and interpolatory quadrature rules based on Chebyshev points of the first and second kind, with $d\lambda(t) = dt$, are used by Sanikidze [1968], [1970c], [1970d], Chawla & Jayarajan [1975], Šeško [1976] and Chawla & Kumar [1978]. Sanikidze [1970b] also discusses interpolatory formulae based on the zeros of two consecutive orthogonal polynomials. Many convergence criteria and error estimates can be found in the work of Sanikidze. Paget & Elliott [1972] also have error estimates based on contour integration. Perhaps the most remarkable convergence results are due to Elliott & Paget [1975], [1976a] and Šeško [1976], who, independently, in the case of the Gauss-Jacobi formula for $d\lambda(t) = (1-t)^\alpha(1+t)^\beta dt$, $\alpha > -1$, $\beta > -1$, prove convergence of (3.13) for all functions f that are Hölder continuous on $[-1, 1]$ with exponent μ , $0 < \mu \leq 1$.

Šeško [1976] indeed proves uniform convergence if $\alpha > 0, \beta > 0$, not only for the Gauss-Jacobi formula, but also for the interpolatory formula based on Chebyshev points. Analogous results for $d\lambda(t) = (1-t)^\alpha(1+t)^\beta \ln((1-t)/(1+t))dt$ can be found in Šeško & Jakimenko [1980]. Sanikidze [1972] has similar convergence results for the Kronrod extension (cf. Section 2.1.2) of (3.13) in the case of the Gauss-Chebyshev formula. See also Chawla & Kumar [1978], [1979].

Formulas of the type (3.13) for infinite intervals and Hermite measure $d\lambda(t) = e^{-t^2}dt$, including their convergence, are discussed by Kas'janov [1977]. Velev, Semanov & Soliev [1977] use Hermite interpolation processes to derive quadrature rules with multiple nodes for the approximation of singular integrals (3.4) with $d\lambda(t) = (1-t^2)^{-1/2}dt$.

For the use of Gauss-type quadrature rules to approximate Cauchy principal value integrals in higher dimensions, see Gabdulhaev [1975], Gabdulhaev & Onegov [1976], Velev, Semenov & Soliev [1977], Šeško [1979], Tsamasphyros & Theocaris [1979] and Theocaris, Ioakimidis & Kazantzakis [1980].

3.2.3. *Computational considerations.* Although the quadrature rules (3.9) and (3.13) are numerically unstable when x is near one of the nodes τ_v , a device already used by Korneičuk [1964] allows us to evaluate the quadrature sums in a stable manner for arbitrary $x \in (a, b)$. We describe the procedure for the formula (3.13), assuming that the underlying quadrature formula is a Gauss-Christoffel formula.

We represent the polynomial $p_{n-1}(f; \cdot)$ of degree $\leq n-1$ interpolating f at the zeros τ_v of $\pi_n(\cdot; d\lambda)$ in the form

$$(3.14) \quad p_{n-1}(f; t) = \sum_{k=0}^{n-1} a_k \pi_k(t),$$

where, by virtue of the discrete orthogonality property of orthogonal polynomials,

$$(3.15) \quad a_k = h_k^{-1} \sum_{v=1}^n \lambda_v \pi_k(\tau_v) f(\tau_v), \quad k = 0, 1, \dots, n-1,$$

with $h_k = \int_a^b \pi_k^2(t) d\lambda(t)$. Integrating (3.14) yields (3.13) in the form

$$(3.16) \quad I(f)(x) = \sum_{k=0}^{n-1} a_k \rho_k(x) + R_n(f).$$

The polynomials $\{\pi_k(x)\}$ and functions $\{\rho_k(x)\}$ required in (3.15) and (3.16) both satisfy the recurrence relation (cf. Section 1.4)

$$(3.17) \quad y_{k+1} = (x - \alpha_k)y_k - \beta_k y_{k-1}, \quad k = 0, 1, 2, \dots,$$

the initial values being $\pi_{-1}(x) = 0, \pi_0(x) = 1$ for $\{\pi_k(x)\}$, and

$$(3.18) \quad \rho_{-1}(x) = 1, \quad \rho_0(x) = \int_a^b \frac{d\lambda(t)}{x-t},$$

for $\{\rho_k(x)\}$. (We assume that $\beta_0 = \int_a^b d\lambda(t)$ in (3.17).) The computation of $\rho_n(x)$ by means of (3.17), (3.18) is quite stable if x is in the interior of $[a, b]$. The only nontrivial computation, therefore, is that of $\rho_0(x)$ in (3.18). For many of the standard measures $d\lambda$, however, $\rho_0(x)$ can be expressed, and thus evaluated, in terms of known special functions. The sum in (3.16) is most effectively evaluated by Clenshaw's algorithm (Paget & Elliott [1972]).

A similar procedure applies to the quadrature rule (3.9) (Elliott & Paget [1979]). The approach, indeed, is capable of dealing with a much wider class of integrals, for example

$$I(f)(x) = \int_a^b K(x, t)f(t)d\lambda(t),$$

where $K(x, t)$ is a singular (or weakly singular) kernel, or a kernel that otherwise exhibits unpleasant behavior. For work along these lines see Bahvalov & Vasil'eva [1968], Piessens & Poleunis [1971], Branders & Piessens [1975], Patterson [1976/77], Elliott & Paget [1976b], [1978], Sloan [1978], and Smith & Sloan [1980].

An adaptive automatic integration routine for singular integrals (3.4) (with $d\lambda(t) = dt$) is developed in Piessens, VanRoy-Branders & Mertens [1976].

3.2.4. *Applications to singular integral equations.* The quadrature rules developed in Sections 3.2.1 and 3.2.2 are widely used for the approximate solution of singular integral equations in problems of elasticity theory, fluid flow, aerodynamics and electromagnetic scattering. In one of its simpler forms, the problem consists in finding a solution $y(t)$ of an integral equation of the first kind,

$$(3.19) \quad \int_{-1}^1 \frac{y(t)}{x-t} dt + \int_{-1}^1 k(x, t)y(t)dt = f(x), \quad -1 < x < 1,$$

where k and f are given, usually smooth, functions. Depending on whether or not one seeks a solution that is bounded at one or both of the endpoints, there may be no solution (unless a compatibility condition is fulfilled), a unique solution, or infinitely many solutions. When solutions exist, they will be of the form

$$(3.20) \quad y(t) = u(t)\omega(t)$$

where ω exhibits square root singularities at the endpoints, and u is smooth, if k and f are. The exact type of singularity of ω is well-determined, once the boundedness characteristics of y have been defined.

For the numerical solution of (3.19) one now substitutes (3.20) into (3.19), applies the quadrature rule (3.9) with the appropriate $d\lambda(t) = \omega(t)dt$ to the first integral in (3.19) and the parent quadrature rule G_n in (3.6) to the second. If one further chooses for x the roots x_i of $\rho_n(x) = 0$, there results a system of linear equations

$$(3.21) \quad \sum_{\nu=1}^n \lambda_{\nu} \left[\frac{1}{x_i - \tau_{\nu}} + k(x_i, \tau_{\nu}) \right] u_{\nu} = f(x_i)$$

for the unknowns u_{ν} which approximate $u(\tau_{\nu})$. If there are fewer than n zeros of $\rho_n(x)$, additional equations — usually physically meaningful ones — can be adjoined.

Similarly one deals with integral equations of the second kind,

$$a(x)y(x) + b(x) \int_{-1}^1 \frac{y(t)}{x-t} dt + \int_{-1}^1 k(x, t)y(t)dt = f(x), \quad -1 < x < 1,$$

the solution of which again admits representations of the form (3.20), but with ω now a more general Jacobi type weight function. To again arrive at a linear system of the type (3.21), the "collocation points" x_i must now be chosen as roots of the equation (Theocaris [1976], Ioakimidis & Theocaris [1978a])

$$a(x)\omega(x) + b(x) \frac{\rho_n(x)}{\pi_n(x)} = 0.$$

Best results (when u in (3.20) is smooth) can be expected from the employment of the appropriate Gauss-Jacobi quadrature rule (3.6). This indeed has been the choice in the work of Stark [1971], Erdogan & Gupta [1971/72], Krenk [1975/76], Theocaris & Ioakimidis [1978a] and others. In many applications the value of u at one or both endpoints is physically meaningful, and

indeed may be the only quantity of interest. In such cases the Gauss-Radau and Gauss-Lobatto rules are appropriate and are the preferred choice in the work of Ioakimidis & Theocaris [1977a], [1978a, b], Theocaris & Ioakimidis [1977/78], [1978b], Krenk [1978], and Theocaris & Tsamaphyros [1979]. Occasionally, other types of singularity arise in singular integral equations and must be dealt with accordingly. Theocaris & Ioakimidis [1977], [1979a], for example, consider a problem with complex Jacobi-type singularities, Theocaris, Chrysakis & Ioakimidis [1979] one with a logarithmic singularity, while Cohen [1978] considers problems on an infinite interval. Interpolation schemes that allow $u(t)$ to be obtained for arbitrary $t \neq \tau_v$, with an accuracy comparable to the one of the approximations u_v , are discussed in Theocaris & Ioakimidis [1979b]. For convergence results, see Ioakimidis & Theocaris [1980].

Similar methods can also be applied to singular integro-differential equations; see Ioakimidis & Theocaris [1979].

4. The Remainder Term and Convergence

The analysis of the remainder of a quadrature rule has a long and extensive history and continues to be an active topic of research. There are three major areas of concern: The representation of the remainder in some form or another, the estimation of its magnitude, and conclusions concerning the convergence behavior of the quadrature rule. We only review work that relates specifically to Gauss-Christoffel quadrature rules.

One of the early representations of the remainder, Markov's formula for $R_n(f)$ in terms of the $2n$ -th derivative of f (cf. Section 1.4), while widely quoted, is of limited practical value, as it stands. For one, high-order derivatives are usually difficult to estimate. Then the formula cannot be applied to functions of low-order continuity. And finally, it does not lend itself easily for a comparison with other quadrature rules which may have different degrees of exactness. For these reasons, other representations are being used, notably representations valid for functions that can be extended holomorphically into the complex plane, and others valid for real functions of a given continuity class.

4.1. The remainder term for holomorphic functions

There are several approaches for estimating the remainder $R_n(f)$ when f is holomorphic. Among the oldest is the method of contour integration. More recent approaches use tools of functional analysis and approximation theory. Whatever the approach, the results are often quite comparable.

4.1.1. *Estimates based on contour integration.* For simplicity we assume that $[a, b]$ is a finite interval, which we standardize to $[-1, 1]$. The use of contour integration to represent the remainder $R_n(f)$ can be traced back at least to Heine [1881] whose work immediately yields (cf. Section 1.4)

$$(4.1) \quad R_n(f) = \frac{1}{2\pi i} \oint_{\Gamma} \frac{\rho_n(z)}{\pi_n(z)} f(z) dz.$$

It is assumed in (4.1) that f is single-valued holomorphic in a domain D which includes the interval $[-1, 1]$ in its interior, Γ is a contour in D surrounding $[-1, 1]$, π_n the appropriate orthogonal polynomial, and

$$\rho_n(z) = \int_{-1}^1 \frac{\pi_n(t)}{z-t} d\lambda(t).$$

Two choices of Γ are most frequently made: $\Gamma = C_r$, the circle $|z| = r$, $r > 1$, and $\Gamma = \mathcal{E}_\rho$, the ellipse with foci at ± 1 and sum of its semiaxes equal to ρ , $\rho > 1$. The parameters r and ρ can be varied in certain intervals $1 < r \leq r^*$, $1 < \rho \leq \rho^*$ determined by the domain of holomorphy of f . Circles, of course, can only be used if D is sufficiently large so as to contain a circle C_r for some $r > 1$. In this respect, ellipses \mathcal{E}_ρ have the advantage of shrinking to the interval $[-1, 1]$ when $\rho \rightarrow 1$, which makes them suitable to deal with functions which are analytic on the segment $[-1, 1]$. Having families of contours Γ at disposal provides for flexibility and gives an opportunity for optimization in the estimates of $|R_n(f)|$ to be made. These estimates follow directly from (4.1), and have the form

$$(4.2) \quad |R_n(f)| \leq \frac{1}{2\pi} \gamma_n l(\Gamma) \max_{z \in \Gamma} |f(z)|,$$

where $l(\Gamma)$ is the length of Γ and γ_n either a strict upper bound for $|\rho_n(z)/\pi_n(z)|$ on Γ , or an asymptotic estimate valid for $n \rightarrow \infty$. In the latter case, (4.2) is only an approximate relation. Strict error bounds are obtained in this manner, for some of the classical Gauss-Christoffel formulae, by McNamee [1964], Chawla [1967], [1968], Kambo [1970], [1970/71], Donaldson [1973], Kumar [1974a, b], Porath & Wenzlaff [1976], asymptotic estimates by Fock [1932], Barrett [1960/61], Chawla & Jain [1968a, b], Donaldson & Elliott [1972], Ramakrishnan [1973] and Smith [1977]. As pointed out in some of these references, the method can be extended to infinite intervals, and is easily adapted to incorporate poles and other singularities of f .

An equivalent form of (4.1) is (cf. Section 1.4)

$$(4.1') \quad R_n(f) = \frac{1}{2\pi i} \oint_{\Gamma} R_n\left(\frac{1}{z-\cdot}\right) f(z) dz.$$

In this form the remainder is studied extensively by Takahasi & Mori [1970], [1971], who display many revealing contour maps of $|R_n(1/(z-\cdot))|$ for Gauss-Legendre and other quadrature rules. Lether [1980] expands $(z-\cdot)^{-1}$ in (4.1') in a series of Chebyshev polynomials of the second kind and obtains an estimate of $R_n(f)$ for arbitrary measure $d\lambda(t)$ on a finite interval.

Freud [1973], [1975a, b] establishes the new representation

$$(4.3) \quad R_n(f) = \sum_{\nu=0}^{\infty} \frac{h_\nu}{2\pi i} \oint_{\Gamma_\nu} \frac{f(z) dz}{\pi_\nu(z) \pi_{\nu+1}(z)},$$

valid for arbitrary measures $d\lambda(t)$, where π_k are the (monic) orthogonal polynomials, $h_\nu = \int_a^b \pi_\nu^2(t) d\lambda(t)$, and Γ_ν are contours enclosing all zeros of π_ν and $\pi_{\nu+1}$. In the first paper, Freud combines (4.3) with asymptotic results for orthogonal polynomials to derive asymptotic estimates for $|R_n(f)|$ under the assumption that $d\lambda(t)$ has support in $[-1, 1]$ and is such that $\ln \lambda'(\cos \theta)$ is Lebesgue integrable on $[-\pi, \pi]$. In the subsequent papers these estimates are further developed into strict upper bounds. (Cf. also Section 4.1.3, in particular v. Sydow [1977/78].)

Assuming $d\lambda(t) = \omega(t)dt$ on $[-1, 1]$, where ω is even, positive, and Lebesgue integrable, and assuming f holomorphic in $|z| < 1$ and continuous on $|z| = 1$, Stenger [1966] uses (4.1) to derive the expansion

$$(4.4) \quad R_n(f) = \sum_{\nu=0}^{\infty} a_{2n+2\nu} r_{n,\nu},$$

where a_{2k} are the coefficients in the Maclaurin series of f . The quantities $r_{n,\nu} = R_n(t^{2n+2\nu})$ are shown to be positive, and to satisfy $r_{n,\nu+1} - r_{n+1,\nu} > 0$, for all $n \geq 1$, $\nu \geq 0$. This has the interesting consequence that $R_n(f) \geq R_{n+1}(f) \geq 0$ for all $n \geq n_0$, whenever $a_{2k} \geq 0$ for all $k \geq n_0$. (See also Section 4.3, in particular Brass [1978].) Upper bounds for $|R_n(f)|$ can be obtained from (4.4) by applying Schwarz's or Hölder's inequality (if $\{r_{n,\nu}\}_{\nu=0}^{\infty} \in l_p$, $1 \leq p \leq \infty$), and by using Cauchy's inequality to estimate $|a_{2k}|$.

Representations of $R_n(f)$, similar to the one in (4.4), in terms of other expansions are obtained for various special Gauss-Christoffel formulae by Chawla [1970a], [1971a], Kambo [1971] and Jayarajan [1974], who use expansions in Chebyshev or Legendre polynomials. This again yields error bounds if one suitably estimates the expansion coefficients. Luke [1975], for arbitrary measure $d\lambda(t)$, expands f in orthogonal polynomials $\pi_k(t; d\lambda)$ and works out the corresponding expansion for $R_n(f)$. This is extended in Luke, Ting & Kemp [1975] to the case of Christoffel quadratures (with preassigned nodes).

4.1.2. *Hilbert space norm estimates.* The idea of using Hilbert space methods to estimate linear functionals that are important in approximation (such as the error functional $R_n(f)$ in a quadrature rule) was first introduced by Davis [1953]. Here the scenario calls for a Hilbert space $\mathcal{H} = \mathcal{H}(D)$ of functions which are single-valued holomorphic in a domain D that contains the interval $[-1, 1]$. If, then, R_n is a bounded linear functional in \mathcal{H} , one gets immediately

$$(4.5) \quad |R_n(f)| \leq \sigma_n \|f\|,$$

where $\sigma_n = \|R_n\|$ is the norm of the error functional R_n and $\|f\|$ the norm of f in the Hilbert space \mathcal{H} . The former depends only on the quadrature rule in question, the latter only on the function to which the rule is applied. Indeed, if $\{p_k\}$ is a complete orthonormal system in \mathcal{H} , then

$$(4.6) \quad \sigma_n^2 = \sum_{k=0}^{\infty} |R_n(p_k)|^2.$$

Davis [1953] originally, and Stetter [1968], Riess [1971], Haber [1971], [1971/72], Kofron [1972], Hämmerlin [1972] subsequently, use circular domains bounded by C_r , $r > 1$, and equip \mathcal{H} with the inner product $(f, g) = \int_{C_r} f(z) \overline{g(z)} ds$. The orthonormal system then consists of powers, $p_k(z) = (2\pi r)^{-1/2} (z/r)^k$. The norm of f in (4.5) can be further estimated to yield

$$|R_n(f)| \leq \tau_n \sup_{z \in C_r} |f(z)|, \quad \tau_n = \sigma_n \sqrt{2\pi r}.$$

For reasons already indicated in the previous section, domains bounded by an ellipse \mathcal{E}_ρ , $\rho > 1$ (with semimajor axis a and semiminor axis b , $a + b = \rho$) are the preferred choice of many authors. They are used, e.g., by Davis & Rabinowitz [1954], Davis [1962], Barnhill [1968], Chawla [1969], Riess & Johnson [1969], Haber [1971/72], in conjunction with the double integral inner product $(f, g) = \iint_{\text{int}(\mathcal{E}_\rho)} f(z) \overline{g(\bar{z})} dx dy$. This yields estimates of the form

$$(4.7) \quad |R_n(f)| \leq \tau_n \sup_{z \in \mathcal{E}_\rho} |f(z)|, \quad \tau_n = \sigma_n \sqrt{\pi ab},$$

where σ_n can be computed (or estimated) from (4.6), the p_k being essentially Chebyshev polynomials of the second kind. For a number of quadrature rules, including Gaussian rules, the quantities σ_n are tabulated for selected values of a (or ρ) in Lo, Lee & Sun [1965] and Stroud & Secrest [1966]. (Earlier tables in Davis & Rabinowitz [1954] and Davis [1962] contain a systematic error.) Somewhat sharper bounds result through the use of the line integral inner product $(f, g) = \int_{\mathcal{E}_\rho} f(z) \overline{g(\bar{z})} |1 - z^2|^{-1/2} ds$, as is shown in Chawla [1968/69], [1969] and Rabinowitz & Richter [1970], or through the use of $(f, g) = \int_{\mathcal{E}_\rho} f(z) \overline{g(\bar{z})} |\omega(z)| ds$, where $d\lambda(t) = \omega(t) dt$ (Chawla [1970b]). The orthonormal functions in the former case are Chebyshev polynomials of the first kind. Nearly identical results are derived by other means in Chawla [1971b]. Knauff [1976/77] uses Banach space methods to obtain estimates of the type (4.7) for Gauss-Chebyshev quadratures. Indeed, there are many other ways such estimates can be derived; Rabinowitz [1969] compares five of them in the case of Gauss-Legendre formulae.

Nicholson, Rabinowitz, Richter & Zeilberger [1971], and Curtis & Rabinowitz [1972] study the error of Gauss-Legendre, Radau and Lobatto formulae when applied to Chebyshev polynomials. In view of (4.6), this yields information on the error norms σ_n in the respective Hilbert spaces $\mathcal{H}(\mathcal{E}_\rho)$.

4.1.3. *Estimates via approximation theory.* If $[a, b]$ is a finite interval, f continuous on $[a, b]$, and if p_{2n-1}^* achieves the best uniform approximation $E_{2n-1}(f)$ of f by polynomials of degree $\leq 2n - 1$,

$$E_{2n-1}(f) = \inf_{p \in \mathbf{P}_{2n-1}} \max_{a \leq t \leq b} |f(t) - p(t)| = \|f - p_{2n-1}^*\|_\infty,$$

then it is a simple matter to observe that for any Gauss-Christoffel formula, $|R_n(f)| = |R_n(f - p_{2n-1}^*)| \leq 2\mu_0 \|f - p_{2n-1}^*\|_\infty$, hence

$$(4.8) \quad |R_n(f)| \leq 2\mu_0 E_{2n-1}(f), \quad \mu_0 = \int_a^b d\lambda(t).$$

This was already noted by Bernstein [1918], who combines (4.8) with his own estimates of $E_{2n-1}(f)$ for holomorphic functions. The same observation, similarly applied to holomorphic functions, is made by Stenger [1966] and Locher & Zeller [1968]. The strongest result is due to v. Sydow [1977/78], who proves

$$(4.9) \quad |R_n(f)| \leq 4\mu_0(1 - \rho^{-2})^{-1} \rho^{-2n} \cdot \max_{z \in \mathcal{G}_\rho} |f(z)|$$

for arbitrary measure $d\lambda(t)$ and functions f that are holomorphic in the interior of \mathcal{G}_ρ and continuous on the boundary. The formula (4.9) is typical for many results obtained previously in special cases by the methods of Sections 4.1.1 and 4.1.2. Locher [1974] makes a somewhat different use of (4.8).

4.2. The Peano representation of the remainder

Kronecker's stern dictum "... ohne Restglied ist es keine Formel!" (Kronecker [1894]) has lost much of its punch since Peano [1913], [1914] showed that essentially every linear functional that annihilates polynomials up to a certain degree automatically generates its own remainder term. Thus, for a quadrature rule over a finite interval $[a, b]$, if the error functional R_n satisfies $R_n(p) = 0$ for all $p \in \mathbf{P}_{s-1}$ 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

$$(4.10) \quad R_n(f) = \int_{-\infty}^{\infty} K_s(t) f^{(s)}(t) dt,$$

where

$$(4.11) \quad K_s(t) = R_n \left[\frac{(\cdot - t)_+^{s-1}}{(s-1)!} \right].$$

Here the plus sign on the right is the "cutoff" symbol, indicating that the function on which it acts is to be set equal to zero if the argument is negative. K_s in (4.11) is called the s -th Peano kernel of R_n ; it is a spline function of degree $s - 1$, with knots at the quadrature nodes and compact support $[a, b]$. (The integral in (4.10) could therefore be extended over $[a, b]$.) The formula (4.10) simplifies if K_s has constant sign on $[a, b]$, in which case

$$(4.10') \quad R_n(f) = c_s f^{(s)}(\bar{t}), \quad c_s = \int_{-\infty}^{\infty} K_s(t) dt = R_n \left(\frac{t^s}{s!} \right),$$

where \bar{t} is some (unknown) intermediate value in $[a, b]$.

A quadrature rule which has degree of exactness d (but not $d + 1$) thus generates exactly $d + 1$ Peano kernels K_1, K_2, \dots, K_{d+1} . We have $d = 2n - 1$ for the n -point Gauss–Christoffel formula, $d = 2n - 2$ for the Radau formula, etc.

Peano's representation (4.10) can be used in different ways to estimate the remainder. For example,

$$(4.12) \quad |R_n(f)| \cong e_s \max_{a \leq t \leq b} |f^{(s)}(t)|,$$

where

$$(4.13) \quad e_s = \int_{-\infty}^{\infty} |K_s(t)| dt, \quad s = 1, 2, \dots, d + 1.$$

The numbers e_s are often referred to as the *Peano constants* of R_n . (Their dependence on n is suppressed in the notation). Equality in (4.12) can be attained for special f . Note also that for Gauss–Christoffel formulae, according to Markov (cf. Section 1.4), $e_{2n} = [(2n)!]^{-1} \int_a^b \pi_n^2(t) d\lambda(t)$. Alternatively, if $f^{(s)}$ is of bounded variation, $|R_n(f)| \leq \text{Var}(f^{(s)}) \max_t |K_{s+1}(t)|$. Still another use of the Peano representation is made by Cosma Cagnazzi [1970] who for quadrature rules with positive coefficients derives estimates of the form $|R_n(f)| \leq e_s^* o_s$, where $o_s = \max_{a \leq t \leq b} f^{(s)}(t) - \min_{a \leq t \leq b} f^{(s)}(t)$ is the oscillation of $f^{(s)}$ on $[a, b]$, and $e_s^* = (s!)^{-1} \int_a^b (t - a)^s d\lambda(t)$ are certain constants depending only on s , but not on the specific quadrature rule under consideration.

Once the first few Peano constants are known, (4.12) is especially useful for estimating the quadrature error in cases where only low-order derivatives of f exist, or are accessible. The importance of this point was already stressed by v. Mises [1933], who in fact, apparently unaware of Peano's work, constructs the Peano kernels by repeated integration (v. Mises [1936]). v. Mises also observes that the Peano kernel K_s of the n -point Gauss–Legendre formula has exactly $2n - s$ sign changes in $[-1, 1]$ (hence none if $s = 2n$), a fact noted later again by Roghi [1967]. Similar statements hold for Gauss–Radau and Gauss–Lobatto formulae (cf., e.g., Brass [1977, Satz 82]).

Stroud [1966] makes the point that the Peano estimate (4.12), for functions of low-order continuity, often compares favorably with other estimates of the same form obtained by approximation-theoretic means. See Rabinowitz [1968], Riess & Johnson [1969], Chui [1972], for estimates of the latter kind.

The Peano constants provide a convenient means of measuring the quadrature error for functions of a given continuity class. This allows comparisons of different quadrature rules on a common basis. It is remarkable, in this respect, that the Gauss–Legendre formula, even for functions of low continuity, compares favorably with other common integration rules, such as Romberg integration, which use the same number of points (Stroud [1965]). According to Stroud & Secrest [1966], the first two Peano constants indeed are only marginally larger than the corresponding constants for the best quadrature

rules (which minimize the integral in (4.13)). It appears therefore, contrary to widespread belief, that Gauss-Christoffel formulae are not only effective for highly regular functions, but also handle functions of low-order continuity at least as well as other common quadrature rules.

Selected Peano constants e_s , $s = 1, 2, 4, 8, \dots$, including e_{2n} , are tabulated in Stroud & Secrest [1966] for many Gauss-Christoffel and related quadrature rules. Their computation, particularly for large s , is quite difficult because of severe cancellation problems.

Peano-type error estimates in the case of infinite intervals $[a, b]$, particularly for Gauss-Laguerre formulae, are obtained by Stroud & Chen [1972].

Radon [1935], Rémès [1940] and Milne [1949] generalize Peano's theory to functionals R that do not annihilate polynomials, but instead annihilate all solutions of a linear homogeneous differential equation of order s . If L is the associated linear differential operator, and $g(\tau, t)$ the Green's function of the initial value problem, then

$$Rf = \int_{-\infty}^{\infty} K(t)(Lf)(t)dt,$$

where the Peano kernel is now given by

$$K(t) = R[g_+(\cdot, t)].$$

Here, $g_+(\tau, t) = g(\tau, t)$ if $\tau < t$, and $g_+(\tau, t) = 0$ otherwise. For Peano kernels of constant sign,

$$Rf = (Lf)(\bar{t}) \cdot R w, \quad a < \bar{t} < b,$$

where w is any solution of $Lw = 1$. Still further generalizations are due to Sard [1948], who also makes precise the class of functionals R to which Peano's theory applies.

4.3. Convergence

The convergence theory for quadrature rules of the form

$$(4.14) \quad \int_a^b f(t)d\lambda(t) = \sum_{\nu=1}^n \lambda_{\nu}^{(n)} f(\tau_{\nu}^{(n)}) + R_n(f), \quad n = 1, 2, 3, \dots,$$

$$a \leq \tau_n^{(n)} < \tau_{n-1}^{(n)} < \dots < \tau_1^{(n)} \leq b,$$

is particularly simple if $[a, b]$ is a *finite* interval. By a theorem of Steklov [1916] and Pólya [1933] the quadrature rule in (4.14) converges for every continuous function,

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

precisely if

$$(4.15) \quad \left\{ \begin{array}{l} \lim_{n \rightarrow \infty} R_n(p) = 0 \quad \text{for every polynomial } p \\ \text{and } \sum_{\nu=1}^n |\lambda_{\nu}^{(n)}| \leq K \quad \text{for all } n = 1, 2, 3, \dots, \end{array} \right.$$

where $K > 0$ is a constant not depending on n . If (4.14) are Gauss–Christoffel quadrature formulae then the first condition in (4.15) is trivially true, $R_n(p)$ being zero if $2n$ exceeds the degree of p , and the second follows from the positivity of the Christoffel numbers,

$$\sum_{\nu=1}^n |\lambda_{\nu}^{(n)}| = \sum_{\nu=1}^n \lambda_{\nu}^{(n)} = \int_a^b d\lambda(t).$$

Thus, Gauss–Christoffel quadrature rules on a finite interval always converge for every continuous function. We can see this also directly from (4.8) and Weierstrass’s approximation theorem. Stieltjes [1884a], in a beautiful memoir, indeed proves convergence for every function that is Riemann–Stieltjes integrable.

Mindful, however, of the fact (Lipow & Stenger [1972]) that for every quadrature rule which converges on $C[a, b]$ there is an $f \in C[a, b]$ for which convergence is arbitrarily slow, one ought to be less concerned with convergence as such, and more with the quality of convergence. In this regard the estimates discussed in Sections 4.1.1–4.1.3 provide useful insights. Bernstein’s estimate (4.8), e.g., when used in conjunction with results of Jackson and Bernstein, yields $R_n(f) = o(n^{-s})$ if $f \in C^s[a, b]$, $\limsup |R_n(f)|^{1/n} < 1$ if f is analytic on $[a, b]$, and $|R_n(f)|^{1/n} = o(1)$ if f is entire. Similarly, the bound in (4.9) assures us of geometric convergence in the case of holomorphic functions and tells us how the convergence rate increases with the size of the domain of holomorphy. For results on convergence rates in terms of the r -th modulus of continuity see Butzer, Scherer & Westphal [1973] and Butzer [1979/80].

The convergence of Gauss–Christoffel formulae on *infinite* intervals is a more subtle question. It is intimately related to the determinacy of the moment problem for $d\lambda(t)$. That such a connection exists, in the case of a half-infinite interval $[0, \infty]$, is suggested by a result of Stieltjes according to which the moment problem is determined if and only if the continued fraction corresponding to the integral $\int_0^{\infty} d\lambda(t)/(z - t)$ converges. The determinacy of the moment problem therefore implies convergence of the Gauss–Christoffel rule for $f(t) = (z - t)^{-1}$, $z \notin [0, \infty]$ (cf. Section 5, Eq. (5.7)). For more general functions f the theory gradually evolved through the work of Uspensky [1916], [1928], Shohat [1927], Jouravsky [1928] and Shohat & Tamarkin [1943]. Assuming that $\int_{-\infty}^{\infty} f(t)d\lambda(t)$ exists as an (improper) Riemann–Stieltjes integral and that the moment problem on $[-\infty, \infty]$ is determined for $d\lambda(t)$, the Gauss–Christoffel quadrature rule converges if $|f(t)| \leq A + Bt^{2s}$ for all real t , where A, B are positive constants and $s \geq 1$ an integer (Freud [1971, Ch. 3,

Thm. 1.1]). In fact, this is true for every sequence of positive quadrature rules (i.e., $\lambda_n^{(v)} \geq 0$ in (4.14)) which converge on polynomials. For the determinacy of the moment problem one has well-known criteria due to Carleman, M. Riesz and others (see, e.g., Shohat & Tamarkin [1943, p. 19f]). More general theorems of this type, for arbitrary intervals $[a, b]$, are known in which the condition on f is replaced by the condition that for suitable functions G_a, G_b the limits $\lim_{t \downarrow a} f(t)/G_a(t)$, $\lim_{t \uparrow b} f(t)/G_b(t)$ be zero (Ivanova [1955], Freud [1971, Ch. 3, Thms. 1.6, 1.6a, 1.6b]), or at least finite (Esser [1971b]). If $[a, b]$ is compact, these conditions allow f to become singular at one or both endpoints. Concrete theorems of this kind for classical Gauss-Christoffel formulae are summarized in Freud [1971, p. 96].

The Steklov-Pólya criterion (4.15) can be extended to quadrature rules that have multiple nodes with arbitrary multiplicities, so long as the multiplicities do not exceed a fixed integer s for all n . If the criterion is fulfilled one gets convergence for all $f \in C^s[a, b]$ (Bandemer [1966], [1967]). In particular, all Christoffel-Stancu quadrature rules on finite intervals converge in this sense (Filippi & Esser [1970], Esser [1971a], [1972]). Convergence theorems for Gauss-Radau formulae on infinite intervals are included in Freud [1971, Ch. 3, Thm. 1.4]; for the Gauss-Laguerre measure, see also Krylov & Fedenko [1962].

Another aspect of convergence is monotonicity. While monotone convergence cannot hold for all $f \in C[a, b]$ (Filippi & Esser [1970, Satz 9]), Brass [1978], for the quadrature rule $Q_n(f)$ in (4.14), shows $Q_n(f) \leq Q_m(f)$ for all $m > n$, if $f^{(2n)}$ is continuous on $[a, b]$ and nonnegative. If this condition holds for each n , convergence is monotone. For an alternative proof, see Locher [1980].

Finally, attempts may be made to speed up the convergence of quadrature rules through appropriate acceleration techniques. The use of the ε -algorithm for this purpose is studied empirically by Chisholm, Genz & Rowlands [1972].

5. Computation of Gauss-Christoffel Quadrature Formulae; Numerical Tables

Generating Gauss-Christoffel quadrature rules is closely related to the problem of generating orthogonal polynomials (see Section 1.4). In principle, this problem was already solved by Chebyshev [1859a] for discrete measures, and by Stieltjes [1884a] for general measures. If the measure in question is $d\lambda(t)$, and $(f, g) = \int_a^b f(t)g(t)d\lambda(t)$ denotes the inner product of f and g , then the (monic) orthogonal polynomials $\{\pi_k\}$ satisfy the three-term recurrence relation

$$(5.1) \quad \begin{aligned} \pi_{k+1}(t) &= (t - \alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t), & k = 0, 1, 2, \dots, \\ \pi_{-1}(t) &= 0, & \pi_0(t) = 1, \end{aligned}$$

where the coefficients α_k, β_k are given by

$$(5.2) \quad \alpha_k = \frac{(t\pi_k, \pi_k)}{(\pi_k, \pi_k)}, \quad k = 0, 1, 2, \dots,$$

$$(5.3) \quad \beta_k = \frac{(\pi_k, \pi_k)}{(\pi_{k-1}, \pi_{k-1})}, \quad k = 1, 2, 3, \dots$$

(Darboux [1878], Stieltjes [1884a]). If $d\lambda(t) \geq 0$, as we shall assume, then (5.3) shows that $\beta_k > 0$ for $k \geq 1$. Since π_0 is known, and β_0 is arbitrary, we obtain α_0 from (5.2), whence π_1 from (5.1). Knowing π_0 and π_1 , we now compute α_1 and β_1 from (5.2) and (5.3), and then again π_2 from (5.1). Continuing in this manner, we can generate as many polynomials, and therefore as many of the coefficients α_k, β_k , as are desired. This is the *procedure of Stieltjes*.

While Stieltjes' procedure is very elegant, it leaves an important point unanswered: How are we to compute the inner products in (5.2), (5.3)? The manner in which the recursion coefficients α_k, β_k are determined, indeed, turns out to be rather critical for the numerical stability of the procedure. We find it convenient, therefore, to first assume that all coefficients α_k, β_k are explicitly known. (This is true for "classical" orthogonal polynomials.) An efficient algorithm for computing Gauss-Christoffel formulae can then be based on the associated Jacobi matrix. This is discussed in Section 5.1. The more difficult situation in which the coefficients α_k, β_k must be generated along with the polynomials π_k is deferred to Sections 5.2 and 5.3. In Section 5.4 we review numerical tables available for Gauss-type formulae.

5.1. Methods based on the Jacobi matrix

Suppose we wish to generate the n -point Gauss-Christoffel quadrature rule

$$(5.4) \quad \int_a^b f(t)d\lambda(t) = \sum_{\nu=1}^n \lambda_\nu f(\tau_\nu) + R_n(f).$$

We associate with the measure $d\lambda(t)$ the symmetric tridiagonal matrix of order n ,

$$(5.5) \quad J_n = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \ddots & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{n-1}} \\ 0 & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{bmatrix},$$

where α_k, β_k are the recursion coefficients in (5.1). We refer to J_n as the n -th *Jacobi matrix* of $d\lambda(t)$. The polynomial π_n , then, is precisely the characteristic polynomial of J_n . The nodes τ_ν , being the zeros of π_n , are therefore the eigenvalues of J_n . Denoting by v_ν the (normalized) eigenvector corresponding to τ_ν ,

$$J_n v_\nu = \tau_\nu v_\nu, \quad v_\nu^T v_\nu = 1, \quad \nu = 1, 2, \dots, n,$$

Wilf [1962, Ch. 2, Exercise 9] (and Goertzel around 1954 before him (Wilf [1980])) observes that the Christoffel numbers λ_ν are expressible in terms of the first components $v_{\nu,1}$ of v_ν by means of

$$\lambda_\nu = \mu_0 v_{\nu,1}^2, \quad \nu = 1, 2, \dots, n, \quad \mu_0 = \int_a^b d\lambda(t).$$

Obtaining the n -point Gauss-Christoffel formula (5.4), therefore, amounts to calculating the eigenvalues and first components of the corresponding eigenvectors of the symmetric tridiagonal matrix J_n (a fact noted also by Gordon [1968]).

This is accomplished most effectively by Francis' QR algorithm (Golub & Welsch [1969], Wilkinson & Reinsch [1971, p. 241ff], Sack & Donovan [1971/72], Gautschi [1979b]), or by Rutishauser's LR algorithm (Sack & Donovan [1971/72], Capovani, Ghelardoni & Lombardi [1976a, b]), both executed with appropriate shift strategies. These methods are indeed extremely fast. According to Capovani et al. [1976b], e.g., it takes only 7.24 seconds of machine time on an IBM 370/168 to generate a 1000-point Gauss-Hermite formula! Alternative procedures based on the Newton-Raphson method, or other rootfinding methods, which compute τ_ν as zeros of π_n , not only require considerable care in the selection of initial approximations (Stroud & Secrest [1966], Laurie [1977], Laurie & Rolfes [1979]), but also tend to be slower (Gautschi [1979b]).

For special measures, such as the Legendre measure $d\lambda(t) = dt$, faster methods can be obtained by combining high-order rootfinding procedures with a judicious choice of initial approximations; see, e.g., Lether [1978], Gatteschi [1979], Gautschi [1979b].

The eigenvalue method described for Gauss-Christoffel formulae can be modified to produce Gauss-Radau and Gauss-Lobatto formulae; for this, see Golub [1973].

In the case of measures supported on the non-negative real axis an ingenious algorithm is due to Rutishauser [1962a, b]. It departs from Stieltjes' integral and its corresponding continued fraction ("S-fraction"),

$$(5.6) \quad \int_a^b \frac{d\lambda(t)}{z-t} \sim \frac{\mu_0}{z} - \frac{q_1}{1-z} - \frac{e_1}{z-1} - \frac{q_2}{1-z} - \frac{e_2}{z} - \dots$$

(This continued fraction is not to be confused with the associated continued fraction, the “*J*-fraction”, already used by Gauss, which is a contraction of the *S*-fraction. Accordingly, (5.6) is valid only for $0 \leq a < b \leq \infty$; see Perron [1957, Satz 4.1].) The coefficients q_k, e_k are all positive, and are readily obtained from the recursion coefficients α_k, β_k in (5.1), by virtue of

$$\left. \begin{aligned} \alpha_0 &= q_1 \\ \alpha_k &= e_k + q_{k+1} \\ \beta_k &= e_k q_k \end{aligned} \right\} \quad k = 1, 2, 3, \dots$$

The connection between the *S*-fraction in (5.6) and Gauss–Christoffel formulae is expressed by the relation

$$(5.7) \quad \sum_{\nu=1}^n \frac{\lambda_\nu}{z - \tau_\nu} = \frac{\mu_0}{z - 1} \frac{q_1}{1 - z} \frac{e_1}{z - 1} \frac{q_2}{1 - z} \dots \frac{e_{n-1}}{z - 1} \frac{q_n}{z - 1},$$

i.e., the Gauss–Christoffel nodes τ_ν are the poles, and the Christoffel numbers λ_ν the corresponding residues, of the $2n$ -th convergent of the continued fraction in (5.6). Rutishauser now computes the poles of this convergent in a Graeffe-like manner, generating a sequence of finite continued fractions, all of the same form as in (5.7), each having as poles the squares of the poles of the preceding continued fraction. The process converges quadratically, and yields the poles τ_ν and residues λ_ν simultaneously.

5.2. Generation of the Jacobi matrix

Given the first $2n$ moments

$$(5.8) \quad \mu_k = \int_a^b t^k d\lambda(t), \quad k = 0, 1, 2, \dots, 2n - 1,$$

it is possible to generate the Jacobi matrix (i.e., the coefficients $\alpha_k, \beta_k, k = 0, 1, \dots, n - 1$) by means of Stieltjes’ procedure. It suffices to represent each polynomial $\pi_k(t)$ explicitly in terms of powers of t and to compute the inner products in (5.2), (5.3) by “multiplying out” term by term. In this manner each α_k, β_k is obtained as a ratio of two quadratic forms in the coefficients of π_k and π_{k-1} , the matrices involved being Hankel matrices in the moments (5.8).

In terms of modern digital computation, however, the procedure is subject to two major criticisms: In the first place, the algorithm is highly unstable, especially for finite intervals $[a, b]$. This is ultimately a manifestation of the fact that the Gauss–Christoffel nodes τ_ν and weights λ_ν , considered as functions of the moments μ_k , become progressively more ill-conditioned (i.e., more sensitive to small perturbations in the moments) as n increases (Gautschi [1968a], [1978]). Secondly, the procedure is unnecessarily expensive, requiring, as it

does, of the order $O(n^3)$ arithmetic operations. Both these deficiencies can be alleviated.

The numerical stability is greatly enhanced (Sack & Donovan [1971/72]) if instead of the moments μ_k one employs the “modified moments”

$$(5.9) \quad \nu_k = \int_a^b p_k(t) d\lambda(t), \quad k = 0, 1, \dots, 2n - 1,$$

where $\{p_k\}$ is a suitable system of polynomials (usually orthogonal on $[a, b]$ with respect to some other, classical, measure $ds(t)$). The resulting improvement in the numerical condition is analyzed in Gautschi [1970a].

To arrive at an efficient algorithm, assume that $\{p_k\}$ satisfies a three-term recurrence relation analogous to the one in (5.1),

$$p_{k+1}(t) = (t - a_k)p_k(t) - b_k p_{k-1}(t), \quad k = 0, 1, \dots, 2n - 1,$$

$$p_{-1}(t) = 0, \quad p_0(t) = 1,$$

with coefficients a_k, b_k that are known explicitly. (If they are all zero, then $p_k(t) = t^k$, and the modified moments reduce to ordinary moments.) The desired recursion coefficients α_k, β_k can then be obtained via the “mixed moments”

$$\sigma_{k,l} = \int_a^b \pi_k(t) p_l(t) d\lambda(t), \quad k, l \geq -1,$$

in the following manner. One initializes

$$(5.10^0) \quad \begin{cases} \sigma_{-1,l} = 0, & l = 1, 2, \dots, 2n - 2, \\ \sigma_{0,l} = \nu_l, & l = 0, 1, \dots, 2n - 1, \\ \alpha_0 = a_0 + \frac{\nu_1}{\nu_0}, & \beta_0 = 0, \end{cases}$$

and then continues, for $k = 1, 2, \dots, n - 1$, with

$$(5.10^k) \quad \begin{cases} \sigma_{k,l} = \sigma_{k-1,l+1} - (\alpha_{k-1} - a_l)\sigma_{k-1,l} - \beta_{k-1}\sigma_{k-2,l} + b_l\sigma_{k-1,l-1} & l = k, k + 1, \dots, 2n - k - 1, \\ \alpha_k = a_k - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}} + \frac{\sigma_{k,k+1}}{\sigma_{k,k}}, & \beta_k = \frac{\sigma_{k,k}}{\sigma_{k-1,k-1}}. \end{cases}$$

The algorithm (5.10) not only furnishes the coefficients $\alpha_k, \beta_k, k \leq n - 1$, hence the orthogonal polynomials $\{\pi_k\}_{k=0}^n$, but also, at the same time, the normalization factors $\sigma_{k,k} = \int_a^b \pi_k^2(t) d\lambda(t), k \leq n - 1$. The number of arithmetic operations is clearly of the order $O(n^2)$, one order less than what is required in Stieltjes’ procedure.

In the special case of ordinary moments ($a_k = b_k = 0$), and discrete

measures $d\lambda(t)$, the algorithm (5.10) reduces to one of Chebyshev [1859a]. The general case is due to Sack & Donovan [1971/72] who obtained an algorithm equivalent to (5.10). In the form (5.10) it was given, independently, by Wheeler [1974]. A derivation can also be found in Gautschi [1978]. Earlier algorithms of Golub & Welsch [1969] and Gautschi [1970a] are not competitive, as they too require $O(n^3)$ operations.

The performance of (5.10) appears to be most satisfactory if the interval $[a, b]$ is finite and $\{p_k\}$ are orthogonal on $[a, b]$ with respect to some (standard) weight function. For infinite intervals, a certain degree of ill-conditioning unfortunately persists (Gautschi [1970a]). The success of the algorithm, moreover, depends critically on the ability to compute the modified moments (5.9) accurately. This is often possible through a judicious use of recurrence relations, as for example in the case of Chebyshev and Gegenbauer moments (Piessens & Branders [1973], Branders [1976], Luke [1977], Lewanowicz [1979]). In other cases, closed form expressions can be obtained (Gautschi [1970a, examples (i), (iii)], Wheeler & Blumstein [1972], Blue [1979], Gautschi [1979a], Gatteschi [1980]).

As an application of the algorithm (5.10) we show how Christoffel's theorem (cf. Section 2.1.1) can be implemented in algorithmic form. Thus, we seek polynomials $\{\pi_k\}$ orthogonal on $[a, b]$ with respect to the measure $d\lambda(t) = u(t)ds(t)$, where u is a polynomial of some fixed degree m . Assuming that $ds(t)$ has a set of known orthogonal polynomials, we use these as the polynomials p_k in the modified moments (5.9). Writing u in the form

$$(5.11) \quad u(t) = \sum_{k=0}^m c_k p_k(t),$$

we find

$$\nu_k = \begin{cases} c_k \int_a^b p_k^2(t) ds(t), & k \leq m \\ 0, & \text{otherwise.} \end{cases}$$

Applying now the algorithm (5.10) immediately yields the recursion coefficients α_k, β_k for the desired polynomials π_k . Note that algorithm (5.10) requires only $O(n)$ operations in this case, since $\nu_k = 0$ for all $k > m$.

In some applications, e.g. to Christoffel quadrature rules with preassigned nodes (cf. Section 2.1.1), one is not given the coefficients c_k in (5.11), but rather the zeros of u . An algorithmic implementation of Christoffel's theorem for this situation is given in Galant [1971].

Branders [1976], Laurie [1977], and Laurie & Rolfes [1979] implement Stieltjes' algorithm by expanding π_k in Chebyshev polynomials and by taking advantage of special properties, notably formulae for the product of two

Chebyshev polynomials, to carry out the computations. This approach relies on the Chebyshev moments of $d\lambda(t)$ and therefore represents but another realization of algorithm (5.10).

5.3. A discretization method

An approximative method for computing Gauss-Christoffel formulae, based on discrete orthogonal polynomials, is proposed by Gautschi [1968a]. It is applicable whenever the weight function $\omega(t)$ in $d\lambda(t) = \omega(t)dt$ can be evaluated for arbitrary t . We now describe a variant of this method which incorporates algorithm (5.10) and the method of Golub & Welsch.

Assuming first $[a, b]$ a finite interval, let $\{d\lambda_N(t)\}_{N=1}^{\infty}$ be a sequence of discrete N -point measures on $[a, b]$, approximating $d\lambda(t)$ in the sense that

$$(5.12) \quad \lim_{N \rightarrow \infty} \int_a^b p(t) d\lambda_N(t) = \int_a^b p(t) d\lambda(t)$$

for every polynomial p . The Jacobi matrix $J_{n,N}$ of order n , belonging to $d\lambda_N(t)$, then converges to J_n , the desired Jacobi matrix in (5.5), as $N \rightarrow \infty$,

$$\lim_{N \rightarrow \infty} J_{n,N} = J_n.$$

The following procedure, therefore, suggests itself: Select a suitable system of classical orthogonal polynomials $\{p_k\}$ and compute the corresponding modified moments

$$(5.13) \quad \nu_{k,N} = \int_a^b p_k(t) d\lambda_N(t), \quad k = 0, 1, \dots, 2n - 1.$$

(These are easily obtained, since the integral in (5.13) is now a finite sum.) Apply algorithm (5.10) to generate the elements $\alpha_{k,N}$, $\beta_{k,N}$ of $J_{n,N}$. Increase N until $J_{n,N}$ sufficiently approximates J_n . Then obtain the desired Gauss-Christoffel formula from $J_{n,N} \approx J_n$, using the method described in Section 5.1.

The quality of this procedure depends crucially on the choice of the discretization $d\lambda_N(t)$ of $d\lambda(t)$. If, as in many applications, $d\lambda(t) = \omega(t)dt$, where ω is continuous and positive in the open interval (a, b) , and integrable at both endpoints (although possibly singular there), then a discrete measure $d\lambda_N(t)$ may be obtained by applying a suitable N -point quadrature rule Q_N to the integral on the right of (5.12),

$$\int_a^b p(t) d\lambda_N(t) = Q_N(p\omega).$$

The condition (5.12) requires that Q_N be convergent when applied to $p\omega$, i.e. convergent even in the possible presence of endpoint singularities. Fortunately, most quadrature rules have this property, at least if the singularity is monotone,

or can be majorized by a monotone singularity (Bezиковић [1939], Rabinowitz [1967], [1970], [1977], [1979], Gautschi [1967], Feldstein & Miller [1971], Miller [1971], el-Tom [1971]; see also Freud [1971, Ch. 3, Thm. 1.6(b)], Mikloško [1970b], Esser [1971b]). A specific quadrature rule recommended by Gautschi [1968a] is the Fejér quadrature formula, i.e. the interpolatory quadrature rule based on the Chebyshev points on $[a, b]$. This often yields satisfactory convergence rates.

If the interval $[a, b]$ is infinite, it can be reduced to a finite interval by means of a suitable transformation of variables, whereupon the procedure described again applies (Gautschi [1968a]). For reasons of numerical stability, however, it is now advisable to compute the approximate Jacobi matrix $J_{n,N}$ by Stieltjes' procedure.

5.4. Numerical tables

A large number of numerical tables of Gauss-type quadrature rules have been prepared to assist the occasional user. They are summarized below in Tables 1–6. Early tables, later superseded by more extensive and more accurate ones, are not included in this summary. For convenience we divide the Gauss–Christoffel formulae into four groups (Tables 1–4), in accordance with the type of weight function involved. Gauss–Radau and Gauss–Lobatto formulae are collected in Table 5, where “R” in column 1 stands for “Radau”, and “L” for “Lobatto”. The letter “ n ” in the heading denotes the number of free nodes. Turán formulae are listed in Table 6. Here “ n ” means the number of distinct nodes, while “ r ” refers to the multiplicity of each. Throughout these tables we use the notation “ $a(h)b$ ” to indicate the sequence of numbers $a, a+h, a+2h, \dots, b$. If the step h is not constant, we write “var” in place of “ h ”. The accuracy of the tables is indicated in terms of the number of significant digits (S) or the number of decimal digits after the decimal point (D), as appropriate.

Gauss–Christoffel formulae for Jacobi measures $d\lambda(t) = (1-t)^\alpha(1+t)^\beta dt$ with $\alpha = \pm 1/2$, $\beta = \pm 1/2$ are explicitly known in terms of trigonometric functions, hence need not be tabulated (cf. Section 1.4). The same is true for Gauss–Radau and Gauss–Lobatto formulae with Chebyshev measure $d\lambda(t) = (1-t^2)^{-1/2} dt$; see, e.g. Bouzitat [1952].

Tables of Gauss–Lobatto formulae having double nodes at the endpoints are given for $d\lambda(t) = dt$ in Gatteschi [1963/64].

Extensive tabulations for weight functions depending on a parameter can sometimes be avoided by expanding the nodes and weights in suitable series in that parameter, or by using other curve fitting procedures. It then suffices to tabulate the coefficients in the respective expansions or approximations. King & Dupuis [1976] adopt this approach for the measure $d\lambda(t) = e^{-xt^2} dt$ on

$[-1, 1]$, which is of interest in quantum mechanics, while Lambin & Vigneron [1979] provide series in Chebyshev polynomials for the Laguerre measure $d\lambda(t) = t^\alpha e^{-t} dt$ on $[0, \infty]$, $-1 < \alpha \leq 1$.

Ultimately, however, it is more productive to have high-quality computer software available for generating arbitrary Gauss-type formulae. Although, at the present time, this is still an elusive goal, computer programs with various degrees of generality and efficacy have been published; see, e.g., Rutishauser [1962b], Stroud & Secrest [1966], Gautschi [1968b], Golub & Welsch [1969], Davis & Rabinowitz [1975] and Laurie & Rolfes [1979]. A computer algorithm for the complex weight function $e^{\zeta} \zeta^{-s}$ on $[c - i\infty, c + i\infty]$ (cf. Section 3.1.3) is given in Piessens [1973b].

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TABLE 1. Gauss-Jacobi formulae.

Weight Function	$[a, b]$	n	Accuracy	Reference
1	$[-1, 1]$	2(1)64(4)96(8)168 256, 384, 512	30S	Stroud & Secrest [1966]
$(1 - t^2)^\alpha$ $\alpha = -1/2(1/2)3/2 (\alpha \neq 0)$	$[-1, 1]$	2(1)20	30S	"
$(1 + t)^\alpha, \beta = 1$ $\beta = 2(1)4$	$[-1, 1]$	2(1)30 2(1)20	30S 30S	" "
$ t ^\alpha, \alpha = 1(1)4$	$[-1, 1]$	2(1)20	30S	"
t^α and $t^\alpha(1 - t)^\alpha$ $\alpha = -.9(.1)3.$ $\alpha = -2/3(1/3)8/3 (\alpha \neq 0, 1, 2)$ $\alpha = -3/4(1/2)11/4$	$[0, 1]$	1(1)15	20S	Krylov & Vorob'eva [1971]
$t^{q-1}(1-t)^{p-q}$ $q = .1(.1)1.$ $p = (2q - 1)(.1)(q + 1)$	$[0, 1]$	2(1)15	15-16S	Glonti [1971]
t^2	$[0, 1]$	1(1)20	15D	Sprung & Hughes [1965]
$t^{\alpha-1}(1-t)^{\beta-1}$ $\alpha, \beta = 1/2(\text{var.})3/2$	$[0, 1]$	2(1)12	12S	Boujot & Maroni [1968]
$t^\alpha, \alpha = 0(1)5$	$[0, 1]$	1(1)8	12D	Fishman [1957]
$t^\beta(1-t)^\alpha$ $\alpha, \beta = -.9(.1)3., \beta \leq \alpha$	$[0, 1]$	1(1)8	8S	Krylov et al. [1963]
$ t ^\alpha, \alpha = -3/4(\text{var.}) - 1/4$	$[-1, 1]$	1(1)8	8S	Bertova et al. [1953]
$t^s, s = 0(2)10$	$[-1, 1]$	2(1)4	7S	Rothmann [1961]
$s = 1(2)11$	$[-1, 1]$	2, 4	7S	"

Table 2. Gauss-Laguerre and Gauss-Hermite formulae.

Weight Function	$[a, b]$	n	Accuracy	Reference
e^{-t}	$[0, \infty]$	2(1)32(4)68	30S	Stroud & Secrest [1966]
e^{-t}	$[0, \infty]$	100, 150, 200, 300	24S	Berger & Danson [1968]
e^{-t}	$[0, \infty]$	400(100)900	23-24S	Berger et al. [1969]
e^{-t^2}	$[-\infty, \infty]$	2(1)64(4)96(8)136	30S	Stroud & Secrest [1966]
e^{-t^2}	$[-\infty, \infty]$	300	15S	Afshar et al. [1973]
$t t ^\alpha e^{-t^2}, \alpha = 1, 2, 3$	$[-\infty, \infty]$	2(1)20	30S	Stroud & Secrest [1966]
$t^\alpha e^{-t}, \alpha = -.5(5)10.$	$[0, \infty]$	4(4)16(8)32(16) 64(32)128	25S	Shao et al. [1964b]
$ t ^{2\lambda} e^{-t^2}, \lambda = 0(1)10$	$[-\infty, \infty]$	8(8)32(16)64(32) 128(64)256	25S	"
$t^\alpha e^{-t}, \alpha = -.5(1)3.5$	$[0, \infty]$	4, 8, 16, 32	25S	Shao et al. [1964a]
$ t ^{2\lambda} e^{-t^2}, \lambda = 0(1)4$	$[-\infty, \infty]$	8, 16, 32, 64	25S	"
$t^s e^{-t}, s = 1(1)5$	$[0, \infty]$	4(4)16	18S	Rabinowitz & Weiss [1959]
$t^\alpha e^{-t}, \alpha = 0(-.01) -.99$	$[0, \infty]$	2(1)16	15S	Dekanosidze [1966]
$\alpha = -.75, -.5, -.25$	$[0, \infty]$	1(1)15	15-17S	Concus et al. [1963]
$\alpha = -1/3, -2/3$	$[0, \infty]$	1(1)15	15-17S	Concus [1964]
$t^s e^{-t}$	$[0, \infty]$	1(1)15	8S	Aizenstat et al. [1962]
$s = -.9(.02)(.05)3.$				
$s = -.75, -.25$				
$s = -2/3(1/3)8/3$				
$(s \neq 0, 1, 2)$				

¹) This table gives the modified Christoffel numbers, i.e. the Christoffel numbers divided by the weight function evaluated at the respective node.

Table 3. Gauss-Christoffel formulae for power and logarithmic singularities.

Weight Function	$[a, b]$	n	Accuracy	Reference
$\ln(1/t)$	$[0, 1]$	2(1)16	30S	Stroud & Secrest [1966]
$t^\alpha [\ln(1/t)]^m, \alpha = 0, -.5, m = 1, 2, 3$	$[0, 1]$	2(1)20	30S	Kutt [1976]
$t^\alpha \ln(1/t)$	$[0, 1]$	3(var.)50	25S	Piessens & Branders [1975]
$\alpha = -1/2, -1/3, -1/4, -1/5, 1/3, 1/2$				
$\alpha = 0, -1/2$	$[0, 1]$	5, 10(10)100	20S	Branders & Piessens [1971]
$(1-t)^\alpha t^\beta \ln(1/t)$	$[0, 1]$	3(var.)50	25S	Piessens & Branders [1975]
$\alpha, \beta = -1/2, -1/3, -1/4, -1/5, 1/3, 1/2$				

$\ln(1/(1-t^2))$	$[-1, 1]$	1(1)30	25S	Laurie & Rolles [1977]
$\ln[(1+t)/(1-t)]$	$[-1, 1]$	2(2)18	20S	Piessens et al. [1976]
$t^\alpha \ln(e/t), \alpha = -.9(01)0(.1)5.$	$[0, 1]$	1(1)10	15S	Krylov & Pal'cev [1967]
$t^\alpha \ln(e/t)\ln(e/(1-t)), \alpha = 0(1)5$	$[0, 1]$	1(1)10	15S	"
$t^\alpha e^{-t} \ln(1+1/t), \alpha = 0(1)5$	$[0, \infty]$	1(1)10	15S	"
$t^{\alpha-1} [\ln(1/t)]^{\beta-1}, \alpha = 1/2(1/2)5/2, \beta = 1/2(\text{var.})2$	$[0, 1]$	2(1)12	12S	Boujot & Maroni [1968]
$t^{-1}(1-t)^{\beta-1}/(\pi^2 + \ln^2(t^{-1}-1)), \beta = 0, 1$	$[0, 1]$	2(1)12	12S	"

TABLE 4. Miscellaneous Gauss-Christoffel formulae.

Weight function	$[a, b]$	n	Accuracy	Reference
$(t-a)^\alpha$ $a = -1.1, -1.01, -1.001,$ $\alpha = -.5, -1, -2$	$[-1, 1]$	3(var.)50	25S	Piessens & Branders [1975]
$(t^2+a^2)^\alpha$ $a = 1, .1, .01, .001,$ $\alpha = -.5, -1, -2$	$[-1, 1]$	3(var.)50	25S	"
$t^\gamma(1-t^\alpha)^\beta$ $\alpha = 3, 4, 6, 8, \beta = \pm 1/2,$ $\gamma = 0, \pm 1/2$ $\alpha = 2, \beta = -3/4, -2/3,$ $\gamma = 0$	$[0, 1]$	2(2)8(4)16, 24	25S	Byrd & Galant [1970]
$(1+t^2)^{-k-1}, k = 3(1)10^2)$ $k = 5(1)10$	$[-\infty, \infty]$ $[-\infty, \infty]$	4 6	10D 10D	Harper [1962] "
$(1+t^2)^{-1}$	$[-1, 1]$	2(1)7	7S	Reiz [1950b]
$(1-t^2)^{-1/2}(1+t^2)^{-1}$	$[-1, 1]$	1(1)4	8D	Kumar [1974a]
$t(1+t)^{-13/3}$	$[0, \infty]$	1(1)5	8S	Kumar & Jain [1974]
$1-\sqrt{t}$	$[0, 1]$	1(1)10	5-15S	Struble [1960]
$(1-\sqrt{t})^2/2\sqrt{t}$	$[0, 1]$	1(1)10	5-15S	"
$\cos t$ $\sin t$	$[-\pi, \pi]$	3(var.)50	25S	Piessens & Branders [1975]
$\sin t$ $\cos t$	$[-\pi, \pi]$ $[-\pi/2, \pi/2]$	2(2)18 1(1)4	16S 12D	Piessens [1970b] Piessens [1970a]
$1 + \frac{\cos}{\sin}(2\pi kt), k = 1, 2, 3, 5$	$[0, 1]$	6, 8, 11, 13	10-15D	Mikloško [1970a]
$\frac{1}{2} \left(1 + \frac{\cos}{\sin} m\pi t \right), m = 1(1)12$	$[-1, 1]$	1(1)8, 16, 32	12D	Gautschi [1970b]
$1 - \frac{\cos}{\sin} kt, k = 1, 1024$	$[0, 2\pi]$	1(1)4	6-7S	Zamfirescu [1963]

TABLE 4. (continued)

Weight Function	$[a, b]$	n	Accuracy	Reference
$\left(1 + \frac{\cos t}{\sin t}\right)(1+t)^{-2n-1+s}$ $s = 1.05(.05)4.$	$[0, \infty]$	1(1)10	10S	Krylov & Kruglikova [1968]
$ t ^\alpha e^{- t }, \alpha = 1, 2, 3$	$[-\infty, \infty]$	2(1)20	30S	Stroud & Secrest [1966]
$t^\alpha e^{-at}, a = 1, 2, 5,$ $\alpha = -.5, 0, .5$	$[0, 1]$	3(var.)50	25S	Piessens & Branders [1975]
$e^{-at^2}, a = 1, 2, 5, 10$	$\{[-1, 1]$	3(var.)50	25S	"
	$\{[0, 1]$	3(var.)50	25S	"
$e^{-kt}, \begin{cases} k = 2, 7 \\ k = 2(1)16 \end{cases}$	$[-1, 1]$	2, 7	15S	Cecchi [1967]
	$[-1, 1]$	2(1)10	15S	Cecchi [no date]
$2\pi^{-1/2}e^{-t^2}$	$[0, \infty]$	1(1)20	20S	Galant [1969]
e^{-t^2}	$\{[0, \infty]$	2(1)15	15S	Steen et al. [1969]
	$\{[0, 1]$	2(1)10	15S	"
$e^{-x^2}, x = 0, .5, 10$	$[-1, 1]$	10	20S	King & Dupuis [1976]
$t^{-m}e^{-t}, m = 0(1)10$	$[1, \infty]$	2(1)10	16S	Olson [1969]
$t^\alpha(t+1)^{-2n}e^{-t}, \alpha = -.5(.5)5$	$[0, \infty]$	1(1)10	10S	Pal'cev & Skobljia [1965]
$E_1(t)$ (exponential integral)	$[0, \infty]$	10, 20	12S	Danloy [1973]
$E_m(t), m = 1(1)5$ $m = 1(1)3$	$[0, \infty]$	2, 3	6-8S	Reiz [1950a]
	$[0, \infty]$	4	7-8S	"
$E_m(t), m = 1, 2$ $\tau = .1(\text{var.})\infty$	$[0, \tau]$	3, 4	4-6S	Kegel [1962]
	$[0, \infty]$	2(1)12	12-16S	Vigneron & Lambin [1980]
$(-1)^s J_m(t)$ (Bessel function) $m = 0(1)2, s = 1(1)20$	$[j_{m,s-1}, j_{m,s}]$	2(2)8	14D	Piessens [1972b]
$\text{const} \cdot t^{-2/3} e^{-t} \text{Ai}((3t/2)^{2/3})$	$[0, \infty]$	1, 2, 4, 6	17S	Schulten et al. [1979]
$N(i, k; t), k = 2, 4, i = 1(1)k$ (normalized B -spline of degree $k-1$)	$[-1, 1]$	1(1)17	14S	Phillips & Hanson [1974]
$(2\pi i)^{-1} p^{-1} e^p$	$[c - i\infty, c + i\infty]$	2(1)24	30S	Stroud & Secrest [1966]
$(2\pi i)^{-1} p^{-s} e^p, s = 1(1)5$ $s = .01(.01)3. (s \neq 1, 2, 3)$	$[c - i\infty, c + i\infty]$	1(1)15	20S	Krylov & Skobljia [1968]
	$[c - i\infty, c + i\infty]$	1(1)10	7-8S	"
$s = .1(\text{var.})4$	$[c - i\infty, c + i\infty]$	6(1)12	16S	Piessens [1969a]

²) The orthogonal polynomial system is finite in this case. The Gauss-Christoffel nodes and weights are expressible in terms of Jacobi nodes and weights; see Haber [1964].

³) The orthogonal polynomial system is finite in this case.

TABLE 5. Gauss-Radau and Gauss-Lobatto formulae.

Weight Function	$[a, b]$	n	Accuracy	Reference
1 (R)	$[-1, 1]$	2(1)19(4)47	30S	Stroud & Secrest [1966]
e^{-t} (R)	$[0, \infty]$	3(1)5	20S	Stancu & Stroud [1963]
$t^s e^{-t}$, $s = 0, -1/3, -1/2, -2/3$ (R)	$[0, \infty]$	1(1)15	16S	Cassity [1965]
$s = -.99(\text{var.})10$ (R)	$[0, \infty]$	1(1)15	16S	Cassity & Hopper [1964]
1 (L)	$[-1, 1]$	2(1)32(4)96	30S	Stroud & Secrest [1966]
1 (L)	$[-1, 1]$	1(1)14(8)46(16)94	20D	Michels [1963]
1 (L)	$[-1, 1]$	3(4)23(8)47, 63	19D	Rabinowitz [1960]
\sqrt{t} (R)	$[0, 1]$	1(1)5	8D	Akkerman [1959]
t and t^2 (L)	$[0, 1]$	1(1)4	8D	"

TABLE 6. Turán formulae.

Weight Function	$[a, b]$	n	r	Accuracy	Reference
1	$[-1, 1]$	2(1)7	3, 5	20S	Stroud & Stancu [1965]
1 ^{*)}	$[-1, 1]$	2(1)9 2(1)7 2(1)5	3 5 7	11S	Lo Cascio [1973]
1 (L)	$[-1, 1]$	4(1)7	3, 5	12-16S	Rebolia [1973]
e^{-t}	$[0, \infty]$	1(1)3	3, 5	20S	Stroud & Stancu [1965]
e^{-t}	$[0, \infty]$	1	3(2)23	12S	Verna [1969]
e^{-t^2}	$[-\infty, \infty]$	2(1)7	3, 5	20S	Stroud & Stancu [1965]
e^{-t^2}	$[-\infty, \infty]$	2(1)3	3(2)7	12S	Verna [1969]

*) Only the nodes are tabulated. Some of the tabular entries are inaccurate.

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