Quadratures of Gauss-Stancu Type: Construction and Error Analysis

G. V. Milovanović[a] and M. M. Spalević[b]
[a] University of Niš, Faculty of Electronic Engineering, P. O. Box 73
18000 Niš, Serbia, Yugoslavia
[b] University of Kragujevac, Faculty of Science, P. O. Box 60
34000 Kragujevac, Serbia, Yugoslavia

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Abstract

Quadrature formulas with multiple fixed and free (Gaussian) nodes are studied. Numerical construction of Gaussian nodes and weight coefficients is presented. Also, in the class of analytic functions, an error analysis of Gauss-Turán quadratures is given.

1 Introduction

The idea of numerical integration involving multiple nodes was appeared more than one century after famous method of approximate integration developed by Carl Friedrich Gauss in 1814. Namely, Chakalov (Tschakaloff in German transliteration) [2] in 1948 gave a method for computing *Cotes numbers of higher order* based on the Hermite interpolation. In such way, he obtained an interpolatory quadrature formula with n nodes $\tau_1, \ldots, \tau_n$, and multiplicities $n_1, \ldots, n_n$, respectively, i.e.,

$$\int_{-1}^{1} f(t)dt = \sum_{\nu=1}^{n} \left[A_{0,\nu} f(\tau_\nu) + A_{1,\nu} f'(\tau_\nu) + \cdots + A_{n_\nu-1,\nu} f^{(n_\nu-1)}(\tau_\nu) \right]. \quad (1.1)$$

which is exact for all polynomials of degree at most $n_1 + \cdots + n_n - 1$. Following this idea and taking $n_1 = \cdots = n_n = k$ in (1.1), in 1950 Turán [46] considered numerical quadratures of the form

$$\int_{-1}^{1} f(t)\,dt = \sum_{i=0}^{k-1} \sum_{\nu=1}^{n} A_{i,\nu} f^{(i)}(\tau_\nu) + R(f), \tag{1.2}$$

The quadrature formula (1.2) can be made exact for $f \in \mathcal{P}_{kn-1}$, for any given points $-1 \le \tau_1 \le \cdots \le \tau_n \le 1$. Here $\mathcal{P}_m$ is a set of all algebraic polynomials of degree at most m.

For $k = 1$, this quadrature formula can be exact for $f \in \mathcal{P}_{2n-1}$ if the nodes τ_ν are the zeros of the Legendre polynomial P_n (the well-known Gauss-Legendre quadrature formula). Turán showed that an increase in the degree of exactness can be only for $k = 2s + 1$, $s \ge 0$.

In a general case, such *Gauss-Turán type* quadrature formulae have the form

$$\int_{\mathbb{R}} f(t) d\lambda(t) = \sum_{i=0}^{2s} \sum_{\nu=1}^{n} A_{i,\nu} f^{(i)}(\tau_\nu) + R_{n,s}(f), \tag{1.3}$$

where $d\lambda(t)$ is a given nonnegative measure on the real line $\mathbb{R}$, with compact or unbounded support, for which all moments $\mu_k = \int_{\mathbb{R}} t^k d\lambda(t)$ $(k \ge 0)$ exist and are finite, and $\mu_0 > 0$. The degree of exactness of such quadratures is $2(s+1)n - 1$, i.e., $R_{n,2s}(f) = 0$ for $f \in \mathcal{P}_{2(s+1)n-1}$. The nodes $\tau_1, \ldots, \tau_n$ in (1.3) are the zeros of the monic polynomial $\pi_{n,s}(t)$, which minimizes the integral

$$F(a_0, a_1, \ldots, a_{n-1}) = \int_{\mathbb{R}} [\pi_n(t)]^{2s+2} d\lambda(t),$$

where $\pi_n(t) = t^n + a_{n-1}t^{n-1} + \cdots + a_1 t + a_0$. This minimization leads to the "orthogonality conditions"

$$\frac{1}{2s+2} \cdot \frac{\partial F}{\partial a_k} = \int_{\mathbb{R}} [\pi_n(t)]^{2s+1} t^k d\lambda(t) = 0 \qquad (k = 0, 1, \ldots, n-1). \tag{1.4}$$

The polynomials $\pi_n = \pi_{n,s}$ are known as *s-orthogonal* (or *s-self associated*) *polynomials* on $\mathbb{R}$ with respect to the measure $d\lambda(t)$. For more details on this kind of orthogonality and quadratures with multiple nodes, as well as a list of references see the survey paper [26]. For $s = 0$ polynomials $\pi_{n,s}$ reduce to the standard orthogonal polynomials and (1.3) becomes the well-known Gauss-Christoffel formula.

A generalization of the Turán quadrature formula to rules having nodes with arbitrary multiplicities was derived independently by L. Chakalov [3, 4] and T. Popoviciu [34].

Important theoretical progress on this subject was made by D.D. Stancu [39, 41] (see also [45]). Here, it is important to assume that the nodes τ_ν are ordered, say $\tau_1 < \tau_2 < \cdots < \tau_n$, with multiplicities $n_1, n_2, \ldots, n_n$, respectively. A permutation of the multiplicities $n_1, n_2, \ldots, n_n$, with the nodes held fixed, in general yields a new quadrature rule. Also, only odd multiplicities $n_\nu = 2s_\nu + 1$ $(\nu = 1, 2, \ldots, n)$ contribute toward an increase in the degree of exactness.

For a given sequence of nonnegative integers $\sigma = (s_1, s_2, \ldots, s_n)$ the corresponding quadrature formula

$$\int_{\mathbb{R}} f(t)d\lambda(t) = \sum_{\nu=1}^{n} \sum_{i=0}^{2s_\nu} A_{i,\nu} f^{(i)}(\tau_\nu) + R(f) \tag{1.5}$$

has maximum degree of exactness $d_{\max} = 2\sum_{\nu=1}^{n} s_\nu + 2n - 1$ *if and only if* for $k = 0, 1, \ldots, n-1$

$$\int_{\mathbb{R}} \prod_{\nu=1}^{n} (t - \tau_\nu)^{2s_\nu+1} t^k d\lambda(t) = 0.$$

This *orthogonality conditions* correspond to (1.4) and they could be obtained by the minimization of the integral

$$\int_{\mathbb{R}} \prod_{\nu=1}^{n} (t - \tau_\nu)^{2s_\nu+2} d\lambda(t).$$

Such generalization of s-orthogonal polynomials is known as the σ-*orthogonality*.

The existence of quadrature rules (1.5) was proved by Chakalov [3], Popoviciu [34], Morelli and Verna [32], and existence and uniqueness (subject to $\tau_1 < \tau_2 < \cdots < \tau_n$) by Ghizzetti and Ossicini [17].

The paper is organized as follows. In Section 2 we consider Gauss-Stancu quadrature formulas with multiple fixed and free (Gaussian) nodes. Methods for determination of Gaussian nodes and all weights are analyzed in Sections 3 and 4, respectively. Finally, error bounds for analytic functions for some special Jacobi weight functions are presented in Section 5.

2 Gauss-Stancu Quadratures

Let $\eta_1, \ldots, \eta_m$ ($\eta_1 < \cdots < \eta_m$) be given *fixed* (or *prescribed*) nodes, with multiplicities $m_1, \ldots, m_m$, respectively, and $\tau_1, \ldots, \tau_n$ ($\tau_1 < \cdots < \tau_n$) be *free* nodes, with given multiplicities $n_1, \ldots, n_n$, respectively.

The general quadrature formulae for $I(f) = \int_{\mathbb{R}} f(t)\, d\lambda(t)$ of the form

$$Q(f)=\sum_{\nu=1}^{n}\sum_{i=0}^{n_\nu-1} A_{i,\nu} f^{(i)}(\tau_\nu) + \sum_{\nu=1}^{m}\sum_{i=0}^{m_\nu-1} B_{i,\nu} f^{(i)}(\eta_\nu) \tag{2.1}$$

were investigated by D. D. Stancu [39, 41, 45].

$$\begin{aligned} q_M(t) : &= \prod_{\nu=1}^{m}(t-\eta_\nu)^{m_\nu}, \quad M = \sum_{\nu=1}^{m} m_\nu \\ Q_N(t) : &= \prod_{\nu=1}^{n}(t-\tau_\nu)^{n_\nu}, \quad N = \sum_{\nu=1}^{n} n_\nu \end{aligned}$$

The quadrature formula (2.1) is called *interpolatory* with an algebraic degree of exactness at least $M + N - 1$ if

$$I(f) = Q(f), \qquad f \in \mathcal{P}_{M+N-1}.$$

Choosing the free nodes to increase the degree of exactness leads to so-called Gaussian type of quadratures. If the free (or *Gaussian*) nodes $\tau_1, \ldots, \tau_n$ are such that $I(f) = Q(f)$ for each $f \in \mathcal{P}_{M+N+n-1}$, the corresponding quadrature Q we call the *Gauss-Stancu formula*. The following characterization is well known (see Stancu [42]):

Theorem 2.1 *The nodes $\tau_1, \ldots, \tau_n$ are the Gaussian nodes if and only if*

$$\int_{\mathbb{R}} t^k Q_N(t) q_M(t)\, d\lambda(t) = 0 \tag{2.2}$$

for $k = 0, 1, \ldots, n-1$.

The sufficient conditions for the existence of Gaussian nodes can be done by the following statement:

Theorem 2.2 *If the multiplicities of the Gaussian nodes are odd, e.g., $n_\nu = 2s_\nu + 1$ $(\nu = 1, \ldots, n)$, and if the multiplicities of the fixed knots are even, i.e., $m_\nu = 2r_\nu$ $(\nu = 1, \ldots, m)$, then there exist real distinct knots τ_1, $\ldots$, τ_n.*

The "orthogonality conditions" (2.2) reduce to

$$\int_{\mathbb{R}} t^k \pi_n(t)\, d\mu(t) = 0, \quad k = 0, 1, \ldots, n-1,$$

where $\pi_n(t) = \prod_{\nu=1}^{n} (t - \tau_\nu)$ and

$$d\mu(t) = \left(\prod_{\nu=1}^{n} (t - \tau_\nu)^{2s_\nu} \right) \left(\prod_{\nu=1}^{m} (t - \eta_\nu)^{2r_\nu} \right) d\lambda(t).$$

This means that $\pi_n(t)$ is a polynomial orthogonal with respect to the new nonnegative measure $d\mu(t)$ and, therefore, all zeros $\tau_1, \ldots, \tau_n$ are simple, real, and belong to $\operatorname{supp}(d\mu) = \operatorname{supp}(d\lambda)$. The measure $d\mu(t)$ involves the nodes $\tau_1, \ldots, \tau_n$, i.e., the unknown polynomial $\pi_n(t)$, which is implicitly defined (see Engels [6, pp. 214–226]).

The problem with fixed nodes can be reduced to the new measure (by repeated QR algorithm):

$$d\hat{\lambda}(t) = \left(\prod_{\nu=1}^{m} (t - \eta_\nu)^{2r_\nu} \right) d\lambda(t)$$

In the numerical construction of Gauss-Stancu formulas two tasks are appeared:

1° A nonlinear algebraic problem of finding Gaussian nodes $\tau_1, \ldots, \tau_n$ with respect to the measure $d\hat{\lambda}(t)$ (see Milovanović [24, 25, 26], Milovanović and Spalević [29], and Milovanović, Spalević, Cvetković [31]);

2° Calculations of weights $A_{i,\nu}$ $(i = 0, 1, \ldots, 2s_\nu;\ \nu = 1, \ldots, n)$ and $B_{i,\nu}$ $(i = 0, 1, \ldots, 2r_\nu - 1;\ \nu = 1, \ldots, m)$ (cf. Golub and Kautsky [19], Gautschi and Milovanović [11], Milovanović and Spalević [27, 28], and Milovanović, Spalević, Cvetković [31]). This is a linear problem.

3 Determination of Gaussian Nodes

Let $\{p_j\}_{j\in\mathbb{N}_0}$ be a sequence of orthonormal polynomials with respect to the measure $d\lambda(t)$ on $\mathbb{R}$. These polynomials satisfy the three-term recurrence relation

$$\sqrt{\beta_{j+1}}\, p_{j+1}(t) + \alpha_j p_j(t) + \sqrt{\beta_j}\, p_{j-1}(t) = t p_j(t), \quad j = 0, 1, \ldots ,$$

where $p_{-1}(t) = 0$ and $p_0(t) = 1/\sqrt{\beta_0}$. Usually, we put $\beta_0 = \mu_0 = \int_{\mathbb{R}} d\lambda(t)$.

For a given sequence $\sigma = \sigma_n = (s_1, s_2, \ldots, s_n)$ we rewrite the orthogonality conditions as the following system of nonlinear equations:

$$F_j(\mathbf{t}) \equiv \int_{\mathbb{R}} p_{j-1}(t) \left(\prod_{\nu=1}^{n} (t - \tau_\nu)^{2s_\nu+1} \right) d\lambda(t) = 0, \quad j = 1, \ldots, n, \tag{3.1}$$

where $\mathbf{t} = (\tau_1, \tau_2, \ldots, \tau_n)$. Using the matrix notation

$$\mathbf{t} = [\tau_1\ \tau_2\ \ldots\ \tau_n]^\top, \quad \mathbf{F}(\mathbf{t}) = [F_1(\mathbf{t})\ F_2(\mathbf{t})\ \ldots\ F_n(\mathbf{t})]^\top,$$

for solving the system of nonlinear equations (3.1), we can construct the Newton–Kantorovič method

$$\mathbf{t}^{(k+1)} = \mathbf{t}^{(k)} - W^{-1}(\mathbf{t}^{(k)})\mathbf{F}\big(\mathbf{t}^{(k)}\big), \quad k = 0, 1, 2, \ldots , \tag{3.2}$$

where $\mathbf{t}^{(k)} = [\tau_1^{(k)}\ \tau_2^{(k)}\ \ldots\ \tau_n^{(k)}]^\top$ and

$$W = W(\mathbf{t}) = [w_{j,k}]_{n\times n} = \left[\frac{\partial F_j}{\partial \tau_k}\right]_{n\times n}$$

is the corresponding Jacobian of $\mathbf{F}(\mathbf{t})$, which elements can be calculated by

$$w_{j,k} = -(2s_k+1)\int_{\mathbb{R}} \frac{p_{j-1}(t)}{t-\tau_k}\left(\prod_{\nu=1}^{n}(t-\tau_\nu)^{2s_\nu+1}\right)d\lambda(t), \quad j,k=1,\ldots,n.$$

If $w_{0,k} = 0$ and

$$w_{1,k} = -\frac{2s_k+1}{\sqrt{\beta_0}}\int\limits_{\mathbb{R}}(t-\tau_k)^{2s_k}\left(\prod_{\substack{\nu=1\\ \nu\neq k}}(t-\tau_\nu)^{2s_\nu+1}\right)d\lambda(t), \tag{3.3}$$

in [31] we proved that

$$\sqrt{\beta_{j+1}}\,w_{j+2,k} = (\tau_k-\alpha_j)w_{j+1,k} - \sqrt{\beta_j}\,w_{j,k} - (2s_k+1)F_{j+1}, \tag{3.4}$$

where $j = 0, 1, \ldots, n-2$.

Thus, knowing only F_j and $w_{1,j}$ ($j = 1, \ldots, n$) we calculate the elements of the Jacobian matrix by the nonhomogeneous recurrence relation (3.4). All of the integrals in (3.1) and (3.3) can be calculated exactly, except for rounding errors, by using a Gauss-Christoffel quadrature formula with respect to the measure $d\lambda(t)$ (see [18], [7]),

$$\int_{\mathbb{R}} g(t)d\lambda(t) = \sum_{\nu=1}^{L} A_\nu^{(L)} g\big(\tau_\nu^{(L)}\big) + R_L(g), \tag{3.5}$$

taking $L = n + \sum_{\nu=1}^{n} s_\nu$ nodes. This formula is exact for all polynomials g of degree at most $2L-1 = 2n-1+2\sum_{\nu=1}^{n} s_\nu$.

For a sufficiently good approximation $\mathbf{t}^{(0)}$, the convergence of the method (3.2) is quadratic. This idea has been implemented for finding the corresponding s- and σ-orthogonal polynomials (see [29]). The method was made in two parts. The first part constructs the s-orthogonal polynomial with the maximal value of s_k, i.e., for $\bar{s} = \max\{s_\nu \mid \nu = 1, \ldots, n\}$, and the second one constructs the desired σ-orthogonal polynomial through several steps by reducing only one s_ν to $s_\nu - 1$ in each of steps. Such approach was mainly based on the behavior of the zeros of s-orthogonal polynomials for the Legendre, Laguerre, and Hermite measure, recently presented in [26, Fig. 1–3]. The method is successful for measures on the bounded support (e.g., for the Jacobi measure), but for the measures on the unbounded support (e.g., for the Laguerre and Hermite measures) sometimes the computation can break down, so that the algorithm cannot be applied in such cases. Also, a choice of the initial values of zeros, as well as a lot of computation via several steps in the algorithm, can cause the problems in the application of this method.

Recently, we developed a new iterative algorithm for calculating zeros of s-orthogonal polynomials over the path when the degree of a polynomial increases, and s is a fixed number (see [31]). It needs much less steps (and numerical operations) for constructing the polynomial $\pi_{n,s}(t)$. Precisely, only $n-3$ steps instead of ns steps as in the previous algorithm [29]. Also, the algorithm can be used in constructions for measures with the bounded and unbounded supports.

In this new algorithm, using the zeros of $\pi_{k-2,s}(t)$ and $\pi_{k-1,s}(t)$, i.e.,

$$\mathbf{t}_i = [\tau_1^{(i,s)}\ \tau_2^{(i,s)}\ \ldots\ \tau_i^{(i,s)}]^\top, \quad i = k-2, k-1,$$

we determine at first the starting vector

$$\mathbf{t}_k^{(0)} = [\hat{\tau}_1^{(k,s)}\ \hat{\tau}_2^{(k,s)}\ \ldots\ \hat{\tau}_k^{(k,s)}]^\top, \tag{3.6}$$

and then apply the method (3.2) for solving the corresponding system of k nonlinear equations in order to get the zeros of the polynomial $\pi_{k,s}(t)$. Repeating this procedure $n-3$ times, for $k = 4, \ldots, n$, we obtain the zeros of the polynomial $\pi_{n,s}(t)$. At the beginning of this procedure (for $k = 4$), the zeros of s-orthogonal polynomials of degree two and three, we determine usually by the algorithm proposed in [29].

According to the numerical investigation of zero distribution of s-orthogonal polynomials, we stated in [31] a few appropriate empirical extrapolation formulas for starting vectors (3.6), with components $\hat{\tau}_\nu^{(k,s)} = S_\nu(\mathbf{t}_{k-1}, \mathbf{t}_{k-2})$, $\nu = 1, \ldots, k$. For example, the typical formulas for starting values for the Jacobi measure $d\lambda(t) = (1-t)^\alpha(1+t)^\beta\,dt$ on $(-1,1)$ $(\alpha, \beta > -1)$ and for the Hermite measure $d\lambda(t) = e^{-t^2}\,dt$ on $(-\infty, +\infty)$ are

$$\hat{\tau}_\nu^{(k,s)} = \begin{cases} 2\tau_\nu^{(k-1,s)} - \tau_\nu^{(k-2,s)}, & \nu = 1, 2, \\ \tau_\nu^{(k-1,s)} + \tau_{\nu-1}^{(k-1,s)} - \dfrac{1}{2}\Bigl(\tau_\nu^{(k-2,s)} + \tau_{\nu-2}^{(k-2,s)}\Bigr), & \nu = 3, \ldots, k-2, \\ 2\tau_{\nu-1}^{(k-1,s)} - \tau_{\nu-2}^{(k-2,s)}, & \nu = k-1, k, \end{cases}$$

where $k \geq 5$. In the case of the generalized Laguerre measure $d\lambda(t) = t^\alpha e^{-t}\,dt$ on $(0, +\infty)$ $(\alpha > -1)$, we make the transformation $\tau_\nu^{(k,s)} \to \sqrt{\tau_\nu^{(k,s)}}$.

Beside the classical measures, several other measures (see Chihara [5]) including

1° the generalized Gegenbauer measure on $[-1, 1]$,

$$d\lambda(t) = |t|^{1+2\beta}(1-t^2)^\alpha\,dt;$$

2° the generalized Hermite measure $d\lambda(t) = |t|^{2\mu}e^{-t^2}\,dt$ on $\mathbb{R}$;

3° Abel, Lindelöf, and logistic measure on $\mathbb{R}$, given by

$$d\lambda(t) = \frac{t}{e^{\pi t} - e^{-\pi t}}\,dt, \quad d\lambda(x) = \frac{1}{2\cosh(\pi t)}\,dt, \quad d\lambda(t) = \frac{e^{-t}}{(1+e^{-t})^2}\,dt,$$

respectively, were investigated in [31].

4 Calculation of the Weights

Determination the weight coefficients $A_{i,\nu}$ and $B_{i,\nu}$ in the Gauss-Stancu quadrature formula (2.1) is a linear task, assuming that we previously calculated the Gaussian nodes $\tau_1, \ldots, \tau_n$ (zeros of a certain s- or σ-orthogonal polynomial).

Let the sets of fixed and Gaussian nodes

$$F_m = \{\eta_1, \ldots, \eta_m\} \quad \text{and} \quad G_n = \{\tau_1, \ldots, \tau_n\}$$

be known and let $F_m \cap G_n = \emptyset$. Otherwise, we should make an adjustment as we mentioned in [31, Sect. 1]. Putting

$$X_p = \{\xi_1, \ldots, \xi_p\} := F_m \cup G_n \quad (p = m + n)$$

and denoting the corresponding multiplicity of the node ξ_ν by r_ν ($\nu = 1, \ldots, p$) our task is to determine the coefficients $C_{i,\nu}$ (i.e., $A_{i,\nu}$ and $B_{i,\nu}$) in an interpolatory quadrature formula of the form

$$\int_{\mathbb{R}} f(t)\, d\lambda(t) = \sum_{\nu=1}^{p} \sum_{i=0}^{r_\nu - 1} C_{i,\nu} f^{(i)}(\xi_\nu) + R_p(f). \tag{4.1}$$

Notice that the multiplicity of a Gaussian node must be an odd number.

Defining

$$f_{k,\nu}(t) = (t - \xi_\nu)^k \prod_{i \neq \nu} (t - \xi_i)^{r_i}, \quad \hat{\mu}_{k,\nu} = \int_{\mathbb{R}} (t - \xi_\nu)^k \prod_{i \neq \nu} \left(\frac{t - \xi_i}{\xi_\nu - \xi_i} \right)^{r_i} d\lambda(t),$$

where $0 \leq k \leq r_\nu - 1$, $1 \leq \nu \leq p$, and putting $a_{k,k+j} = f_{k-1,\nu}^{(k-1+j)}(\xi_\nu)$ and

$$\hat{a}_{k,j} = \frac{a_{k,j}}{(j-1)!\, a_{1,1}}, \quad b_k = (k-1)!\, A_{k-1,\nu}, \quad 1 \leq k, j \leq r_\nu,$$

we can state the following result ([31]):

Theorem 4.1 *For fixed ν, $1 \leq \nu \leq p$, the coefficients $C_{i,\nu}$ in the quadrature formula* (4.1) *are given by*

$$\begin{aligned} b_{r_\nu} &= (r_\nu - 1)!\, C_{r_\nu - 1,\nu} = \hat{\mu}_{r_\nu - 1,\nu}, \\ b_k &= (k-1)!\, C_{k-1,\nu} = \hat{\mu}_{k-1,\nu} - \sum_{j=k+1}^{r_\nu} \hat{a}_{k,j} b_j, \quad k = r_\nu - 1, \ldots, 1, \end{aligned}$$

where

$$\hat{a}_{k,k} = 1, \quad \hat{a}_{k,k+j} = -\frac{1}{j}\sum_{\ell=1}^{j} u_\ell \hat{a}_{\ell,j}$$

and

$$u_\ell = \sum_{i\neq\nu} r_i(\xi_i - \xi_\nu)^{-\ell}, \quad \ell = 1, \ldots, r_\nu - 1.$$

Thus, for fixed ν, the coefficients b_k, $1 \le k \le r_\nu$, i.e., the weight coefficients $C_{i,\nu}$ in (4.1), are obtained from the corresponding upper triangular system of equations $\hat{A}\mathbf{b} = \mathbf{c}$, where

$$\hat{A} = [\hat{a}_{ij}], \quad \mathbf{b} = [b_1 \ \ldots \ b_{r_\nu}]^\top, \quad \mathbf{c} = [\hat{\mu}_{0,\nu} \ \ldots \ \hat{\mu}_{r_\nu-1,\nu}]^\top.$$

The normalized moments $\hat{\mu}_{k,\nu}$ can be computed exactly, except for rounding errors, by using the Gauss-Christoffel formula (3.5), taking $L = p + \sum_{\nu=1}^{p} r_\nu$ knots.

5 Error Bounds for Analytic Functions

We consider quadrature formula (4.1) on $(-1, 1)$ with respect to the measure $d\lambda(t) = w(t)\, dt$, where $t \mapsto w(t)$ is a given weight function. In order to study its remainder term $R_p(f)$ for analytic functions we need the following assumptions.

Let Γ be a simple closed curve in the complex plane surrounding the interval $[-1, 1]$ and $\mathcal{D}$ be its interior. Let f be an analytic function in $\mathcal{D}$ and continuous on $\overline{\mathcal{D}}$. Taking any system of p distinct points $\{\xi_1, \ldots, \xi_p\}$ in $\mathcal{D}$ and p nonnegative integers $r_1, \ldots, r_p$, the error in the Hermite interpolating polynomial of f at the point t $(\in \mathcal{D})$ can be expressed in the form (cf. Gončarov [20, Chapter 5])

$$r_p(f;t) = f(t) - \sum_{\nu=1}^{p}\sum_{i=0}^{r_\nu-1} \ell_{i,\nu}(t) f^{(i)}(\xi_\nu) = \frac{1}{2\pi \mathrm{i}} \oint_\Gamma \frac{f(z)\Omega_m(t)}{(z-t)\Omega_m(z)}\, dt,$$

where $\ell_{i,\nu}(t)$ are the fundamental functions of Hermite interpolation and

$$\Omega_p(z) = \prod_{\nu=1}^{p} (z - \xi_\nu)^{r_\nu}.$$

By multiplying this formula with the weight function $w(t)$ and integrating in t over $(-1, 1)$ we get a contour integral representation of the remainder term $R_p(f)$ in the quadrature formula (4.1) with multiple nodes

$$R_p(f) = I(f) - \sum_{\nu=1}^{p} \sum_{i=0}^{r_\nu - 1} C_{i,\nu} f^{(i)}(\xi_\nu) = \frac{1}{2\pi \mathrm{i}} \oint_\Gamma K_p(z, w) f(z) dz, \qquad (5.1)$$

where $C_{i,\nu} = \int_{-1}^{1} \ell_{i,\nu}(t) w(t) dt$ and the kernel $K_p(z, w)$ is given by

$$K_p(z, w) = \frac{\rho_p(z; w)}{\Omega_p(z)}, \quad \rho_p(z; w) = \int_{-1}^{1} \frac{\Omega_p(z)}{z - t} w(t) dt, \quad z \in \mathbb{C} \setminus [-1, 1].$$

The integral representation (5.1) leads to the error estimate

$$|R_p(f)| \le \frac{\ell(\Gamma)}{2\pi} \left(\max_{z \in \Gamma} |K_p(z, w)| \right) \left(\max_{z \in \Gamma} |f(z)| \right), \qquad (5.2)$$

where $\ell(\Gamma)$ is the length of the contour Γ. Therefore, in order to get an estimate of the remainder term, it is important to study the magnitude of $|K_p(z, w)|$ on the contour Γ. The kernels of the remainder term for Gauss-Turán quadratures for classes of analytic functions on elliptical contours with foci at ± 1 and some special Jacobi weights have been recently studied in [30]. This approach for Gaussian type formulas ($s = 0$) was used by Gautschi and Varga [14] (see also [8, 9, 10, 13, 35, 36, 22]).

A general estimate of the remainder term $R_p(f)$ can be obtained by applying the Hölder inequality to (5.1). Namely, for $1 \le r \le +\infty$ and $1/r + 1/r' = 1$, we have

$$|R_p(f)| \le \frac{1}{2\pi} \left(\oint_\Gamma |K_p(z, w)|^r |dz| \right)^{1/r} \left(\oint_\Gamma |f(z)|^{r'} |dz| \right)^{1/r'}.$$

Taking $r = +\infty$, the above estimate reduces to (5.2). On the other side, for $r = 1$ we have

$$|R_p(f)| \leq \frac{1}{2\pi}\left(\oint_\Gamma |K_p(z,w)|\,|dz|\right)\left(\max_{z\in\Gamma}|f(z)|\right).$$

This L^1-type of estimates for Gaussian quadratures on elliptical contours for Chebyshev weights was investigated by Hunter [21]. Also, the L^2-estimate can be of some interest. Such kinds of estimates will be given elsewhere.

In this section we take as the contour Γ an ellipse with foci at the points ± 1 and sum of semiaxes $\varrho > 1$,

$$\mathcal{E}_\varrho = \left\{z \in \mathbb{C} : z = \frac{1}{2}\left(\varrho\, e^{\mathrm{i}\theta} + \varrho^{-1}e^{-\mathrm{i}\theta}\right),\ 0 \leq \theta < 2\pi\right\}.$$

When $\varrho \to 1$, then the ellipse shrinks to the interval $[-1,1]$, while with increasing ϱ it becomes more and more circle-like. There is also another choice of the contour Γ as a circle $\mathcal{C}_\varrho$ with center at origin and radius ϱ (> 1). An advantage of the elliptical contours is that such choice needs the analyticity of f in a smaller region of the complex plane, especially when ϱ is near to 1.

Since the ellipse $\mathcal{E}_\varrho$ has length $\ell(\mathcal{E}_\varrho) = 4\varepsilon^{-1}E(\varepsilon)$, where ε is the eccentricity of $\mathcal{E}_\varrho$, i.e., $\varepsilon = 2/(\varrho + \varrho^{-1})$, and

$$E(\varepsilon) = \int_0^{\pi/2} \sqrt{1 - \varepsilon^2 \sin^2\theta}\, d\theta$$

is the complete elliptic integral of the second kind, the estimate (5.2) reduces to

$$|R_p(f)| \leq \frac{2E(\varepsilon)}{\pi\varepsilon}\left(\max_{z\in\mathcal{E}_\varrho}|K_p(z,w)|\right)\|f\|_\infty, \quad \varepsilon = \frac{2}{\varrho + \varrho^{-1}}\,, \tag{5.3}$$

where $\|f\|_\infty = \max_{z\in\mathcal{E}_\varrho}|f(z)|$. Notice that the bound on the right in (5.3) is a function of ϱ, so that it can be optimized with respect to $\varrho > 1$.

It is well-known the (monic) Chebyshev polynomials of the first kind T_n, orthogonal with respect to $w_1(t) = (1-t^2)^{-1/2}$ on $(-1,1)$, are also

s-orthogonal with the same weight on $(-1,1)$ for each $s \geq 0$ (Bernstein [1]). In 1975 Ossicini and Rosati [33] showed that for three other Jacobi weights (but depending on s),

$$w_2(t) = (1-t^2)^{1/2+s}, \quad w_3(t) = \frac{(1+t)^{1/2+s}}{(1-t)^{1/2}}, \quad w_4(t) = \frac{(1-t)^{1/2+s}}{(1+t)^{1/2}},$$

Chebyshev polynomials of the second kind U_n, the third kind V_n, and the fourth kind W_n are appeared as s-orthogonal, respectively. These polynomials are defined by

$$U_n(t) = \frac{\sin(n+1)\theta}{\sin\theta}, \quad V_n(t) = \frac{\cos(2n+1)\frac{\theta}{2}}{\cos\frac{\theta}{2}}, \quad W_n(t) = \frac{\sin(2n+1)\frac{\theta}{2}}{\sin\frac{\theta}{2}}$$

(cf. Gautschi and Notaris [12]), where $t = \cos\theta$. It is easy to see that $W_n(-t) = (-1)^n V_n(t)$, so that the last weight w_4 could be omitted from any investigation.

Here, we consider the kernel of the remainder term $R_{n,s}(f)$ of Gauss-Turán quadrature formula (1.3) on $(-1,1)$ for classes of analytic functions on elliptical contours $\mathcal{E}_\varrho$, when the weight w is one of the special Jacobi weights $w(t) = w_\nu(t)$, $\nu = 1,2,3$. The corresponding kernel will be denoted by $K_{n,s}(z,w)$.

Some properties of the kernel are given by the following lemma ([30]):

Lemma 5.1 *For each $z \in \mathbb{C} \setminus [-1,1]$,*

$$|K_{n,s}(\overline{z})| = |K_{n,s}(z)|.$$

Moreover, if the weight function is even, i.e., $w(-t) = w(t)$, then

$$|K_{n,s}(-\overline{z})| = |K_{n,s}(z)|.$$

According to (5.3) we are interested in the location on the contour where the modulus of the kernel attains its maximum value.

1° *The measure* $d\lambda_1(t) = (1-t^2)^{-1/2}dt$. Here

$$|K_{n,s}(z,w_1)| = \frac{2^{1-s}\pi}{\varrho^n} \cdot \frac{|Z_{n,s}^{(1)}(\varrho e^{\mathrm{i}\theta})|}{(a_2 - \cos 2\theta)^{1/2}(a_{2n} + \cos 2n\theta)^{s+1/2}} \qquad (z \in \mathcal{E}_\varrho),$$

where $Z_{n,s}^{(1)}(u)$ is given by

$$Z_{n,s}^{(1)}(u) = \sum_{k=0}^{s} \binom{2s+1}{s+k+1} u^{-2nk}$$

and

$$a_j = a_j(\varrho) = \frac{1}{2}(\varrho^j + \varrho^{-j}), \qquad j \in \mathbb{N},\ \varrho > 1.$$

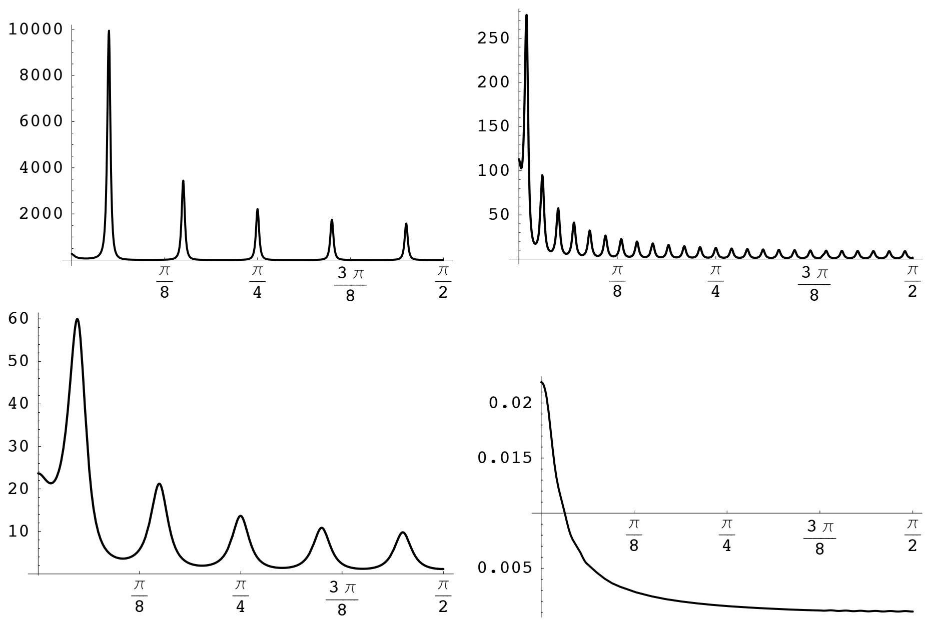

Figure 5.1: Graphics $\theta \mapsto |K_{10,1}(z,w_1)|$ and $\theta \mapsto |K_{50,1}(z,w_1)|$, $z = \frac{1}{2}(\varrho e^{\mathrm{i}\theta} + \varrho^{-1}e^{-\mathrm{i}\theta})$, for $\varrho = 1.01$ (top) and $\varrho = 1.05$ (bottom)

An analysis of $|K_{n,s}(z,w_1)|$ $(z \in \mathcal{E}_\varrho)$ shows that the point of the maximum for a given ϱ depends on n. The graphics $\theta \mapsto |K_{n,1}(z,w_1)|$, $z = \frac{1}{2}(\varrho e^{i\theta} + \varrho^{-1}e^{-i\theta})$, for $n = 10$ and $n = 50$ are displayed in Fig. 5.1, when $\varrho = 1.01$ and $\varrho = 1.05$. The cases for $s = 1, 2, 3$, when $n = 10$ and $\varrho = 1.05$ and 1.10 are presented in Fig. 5.2.

Based on numerical experiments we can state the following conjecture:

Conjecture 5.2 *For each fixed $\varrho > 1$ and $s \in \mathbb{N}_0$ there exists $n_0 = n_0(\varrho, s) \in \mathbb{N}$ such that*

$$\max_{z\in\mathcal{E}_\varrho} |K_{n,s}(z,w_1)| = K_{n,s}\Big(\frac{1}{2}(\varrho+\varrho^{-1}), w_1\Big)$$

for each $n \geq n_0$.

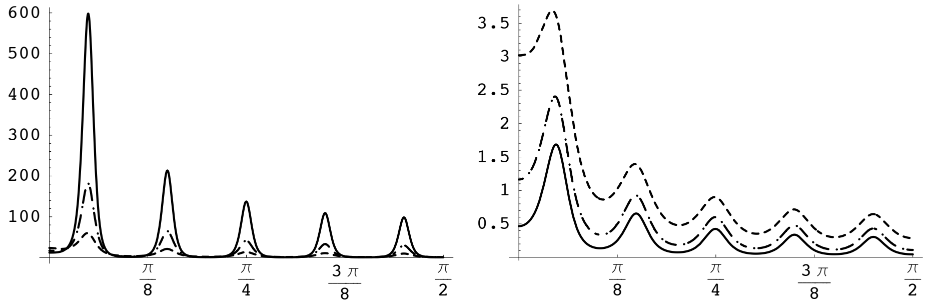

Figure 5.2: The function $\theta \mapsto |K_{10,s}(z,w_1)|$, $z = \frac{1}{2}(\varrho e^{i\theta}+\varrho^{-1}e^{-i\theta})$, for $s = 1$ (dashed line), $s = 2$ (dot-dashed line), $s = 3$ (solid line), when $\varrho = 1.05$ (left) and $\varrho = 1.10$ (right)

2° *The measure $d\lambda_2(t) = (1-t^2)^{s+1/2}dt$, $s \in \mathbb{N}_0$.* In this case

$$|K_{n,s}(z,w_2)| = \frac{\pi}{4^s\varrho^{n+1}}\left(\frac{a_2-\cos 2\theta}{a_{2n+2}-\cos(2n+2)\theta}\right)^{s+1/2}|Z_{n,s}^{(2)}(\varrho e^{i\theta})|,$$

where

$$Z_{n,s}^{(2)}(u) = \sum_{k=0}^{s}(-1)^k\binom{2s+1}{s+k+1}u^{-2(n+1)k}.$$

Theorem 5.3 *If $s \in \mathbb{N}_0$ and n is odd, then*

$$\max_{z\in\mathcal{E}_\varrho} |K_{n,s}(z,w_2)| = \Big| \, K_{n,s}\Big(\frac{\mathrm{i}}{2}(\varrho - \varrho^{-1}), w_2\Big) \Big|,$$

i.e., the maximum of $|K_{n,s}(z,w_2)|$ (n odd) on $\mathcal{E}_\varrho$ is attained on the imaginary axis.

When n is even in the previous theorem, computation shows that the maximum of $|K_{n,s}(z,w_2)|$ on the ellipse $\mathcal{E}_\varrho$ is attained slightly off the imaginary axis. For details see [30].

3° *The measure $d\lambda_3(t) = (1-t)^{-1/2}(1+t)^{s+1/2}dt$, $s \in \mathbb{N}_0$.* This case is very similar to the first one. For $z \in \mathcal{E}_\varrho$ we have (see [30])

$$|K_{n,s}(z,w_3)| = \frac{2^{1-s}\pi}{\varrho^{n+1/2}} \cdot \frac{(a_1+\cos\theta)^{s+1}|Z_{n,s}^{(3)}(\varrho e^{\mathrm{i}\theta})|}{(a_2-\cos 2\theta)^{1/2}(a_{2n+1}+\cos(2n+1)\theta)^{s+1/2}}\,,$$

where

$$Z_{n,s}^{(3)}(u) = \sum_{k=0}^{s} \binom{2s+1}{s+k+1} u^{-(2n+1)k}.$$

On the basis of numerical experiments a similar conjecture for $|K_{n,s}(z,w_3)|$ on the ellipse $\mathcal{E}_\varrho$ as Conjecture 5.2 can be stated.

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