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QUADRATURE PROCESSES – DEVELOPMENT AND NEW DIRECTIONS

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A b s t r a c t. We present a survey on quadrature processes, beginning with Newton's idea of approximate integration and Gauss' discovery of his famous quadrature method, as well as significant contributions of Jacobi and Christoffel. Beside the stable construction of Gauss-Christoffel quadratures for classical and non-classical weights we give some recent applications in the summation of slowly convergent series and moment-preserving spline approximation. Also, we consider quadratures of the maximal degree of precision with multiple nodes, as well as a more general concept of orthogonality with respect to a given linear moment functional and corresponding quadratures of Gaussian type. A short account of non-standard quadratures of Gaussian type is also included. Finally, we mention the Gaussian integration which is exact on the space of Müntz polynomials.

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1. *Introduction*

In this paper we give an account of the classical Newton-Cotes and Gauss-Christoffel quadratures, as well as several their generalizations and extensions. We consider only one dimensional cases.

The paper is organized as follows. In Sections 2 and 3, beside the basic ideas of Isaac Newton (1643–1727) and Carl Friedrich Gauss (1777–1855), including significant contributions of Carl Gustav Jacob Jacobi (1804–1851) and Elwin Bruno Christoffel (1829–1900), we give several recent results on the Gauss-Christoffel quadrature rules for classical and non-classical weight functions, where the theory of orthogonal polynomials is a basic tool. We also mention some recent applications of such quadratures in the summation of slowly convergent series and the moment-preserving spline approximation.

In Section 4 we consider the quadratures with multiple nodes introduced fifty years ago by Chakalov, Popoviciu and Turán, but intensively studied using the s- and σ-orthogonality up to date.

Section 5 is devoted to the concept of orthogonality with respect to a given linear moment functional and to the corresponding quadrature rules of Gaussian type. As illustrations we mention only orthogonality on the semicircle introduced in our joint papers with Gautschi and Landau and recent results on orthogonal polynomials for oscillatory weights obtained with Cvetković. In the first case, the corresponding quadratures of Gaussian type can be applied for calculating the Cauchy principal value integrals and for numerical differentiation of analytic functions. In the second one, they can be applied for numerical calculation of integrals involving highly oscillatory integrands.

In Section 6 we give some considerations on the so-called non-standard quadratures of Gaussian type, which have been introduced and investigated recently. Such quadratures are based on operator values for a general family of linear operators, acting of the space of algebraic polynomials, such that the degrees of polynomials are preserved.

Finally, in Section 7 we consider the Gaussian integration which is exact on the space of Müntz polynomials. The extensions to trigonometric systems and the other non-polynomial systems are not included.

2. *Theory of Newton and Gauss*

The major advance in integration came in the 17th century with the independent discovery of the fundamental theorem of calculus by Newton and

Leibniz. This theorem gives a connection between integration and differentiation. Formalizing integrals (B. F. Riemann) and formulating different definitions of integrals (H. Lebesgue, T. J. Stieltjes, S. Bochner, ...), founded in measure theory, integration becomes an important modern theory.

Numerical integration also begins by Newton's idea from 1676 for finding the weight coefficients A_1, A_2, ..., A_n in the so-called *n-point quadrature formula*

$$I(f) = \int_a^b f(t)\,dt \approx Q_n(f) = A_1 f(\tau_1) + A_2 f(\tau_2) + \cdots + A_n f(\tau_n), \qquad (1)$$

for given (usually equidistantly) n points (nodes) τ_1, τ_2, ..., τ_n, such that (1) is exact for all algebraic polynomials of degree at most $n-1$, i.e., for each $f \in \mathcal{P}_{n-1}$. In modern terminology, given n distinct points τ_k and corresponding values $f(\tau_k)$, Newton constructs the unique polynomial $P \in \mathcal{P}_{n-1}$, which at the points τ_k assumes the same values as f, i.e., $P(\tau_k) = f(\tau_k)$, $k = 1, 2, \ldots, n$, expressing this interpolation polynomial in terms of divided differences. Evidently, for the interpolation error $r_n(f;t) := f(t) - P(t)$ we have $r_n(f;t) = 0$ for all $f \in \mathcal{P}_{n-1}$. Subsequently, integrating this polynomial over $[a,b]$, Newton obtains (1). Here, we give it in a more convenient (Lagrange) form. Namely, the interpolation polynomial P can be expressed in terms of the so-called fundamental polynomials

$$\ell_k(t) = \frac{\omega_n(t)}{\omega_n'(\tau_k)(t-\tau_k)}, \quad k = 1, \ldots, n, \qquad (2)$$

where $\omega_n(t) = \prod_{k=1}^n (t - \tau_k)$, and therefore $A_k = I(\ell_k)$, $k = 1, 2, \ldots, n$, and $R_n(f) = I(f) - Q_n(f) = I(r_n(f;\,\cdot\,))$. Obviously, the remainder term $R_n(f) = 0$ for each $f \in \mathcal{P}_{n-1}$. The quadrature formula obtained in this way is known as *interpolatory* and it has *degree of exactness* at least $n-1$. We write $d = d(Q_n) \geq n-1$.

Starting from the work of Newton and Cotes and combining it with his earlier work on the hypergeometric series, Gauss in 1814 (see [23]) develops his famous method of numerical integration which dramatically improves the earlier method of Newton and Cotes. Namely, Gauss' question was what is the maximum degree of exactness that can be achieved if the nodes τ_k are free. He started with the conjecture that $\max_{\tau_k, A_k} d(Q_n) = 2n-1$, since there are $2n$ unknowns in (1): τ_k, A_k, $k = 1, \ldots, n$, and $2n$ conditions $R_n(t^\nu) = 0$, $\nu = 0, 1, \ldots, 2n-1$. To simplify consideration, we put $(a,b) = (-1,1)$.

Since

$$R_n\left(\frac{1}{z-\cdot}\right)=\sum_{\nu=0}^{+\infty}\frac{R_n(t^\nu)}{z^{\nu+1}},\quad |z|>1\geq|t|,$$

the problem can be reduced to

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

On other hand

$$I\left(\frac{1}{z-\cdot}\right)=\int_{-1}^{1}\frac{dt}{z-t}=\log\frac{1+z^{-1}}{1-z^{-1}}$$

can be expressed as a continued function

$$I\left(\frac{1}{z-\cdot}\right)=\cfrac{2}{z-\cfrac{1/3}{z-\cfrac{2^2/(3\cdot5)}{z-\cfrac{3^2/(5\cdot7)}{z-\cfrac{4^2/(7\cdot9)}{z-\ddots}}}}},$$

which was well known to Gauss (see [23]). Also, Gauss knew that the n-th rational convergent of the previous continued function, $R_{n-1,n}(z)=p_{n-1}(z)/q_n(z)$ ($\deg p_{n-1}=n-1$, $\deg q_n=n$), satisfies

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

Expanding $R_{n-1,n}(z)$ in partial fractions and taking poles (zeros of $q_n(z)$) as the nodes of the quadrature formula (1), Gauss obtains

$$R_{n-1,n}(z)=\sum_{k=1}^{n}\frac{A_k}{z-\tau_k},\quad \text{with}\ \ A_k=\operatorname*{Res}_{z=\tau_k}R_{n-1,n}(z),\ k=1,\dots,n.$$

By such a quadrature formula Q_n, defined by $Q_n(1/(z-\cdot)):=R_{n-1,n}(z)$, it follows that

$$R_n\left(\frac{1}{z-\cdot}\right)=I\left(\frac{1}{z-\cdot}\right)-Q_n\left(\frac{1}{z-\cdot}\right)=I\left(\frac{1}{z-\cdot}\right)-R_{n-1,n}(z),$$

i.e.,

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

Thus, $d(Q_n) = 2n - 1$. Gauss expressed the denominator and numerator polynomials (q_n and p_{n-1}) in terms of his hypergeometric series. Otherwise, these polynomial are known now as Legendre polynomials of the first and second kind.

No doubt that Gauss' discovery is the most significant event of the 19th century in the field of numerical integration and perhaps in all of numerical analysis. An elegant alternative derivation of this famous method was provided by Jacobi, and a significant generalization to arbitrary measures was given by Christoffel. The error term and convergence were proved by Markov and Stieltjes, respectively. Today these formulae with maximal degree of precision are known as the *Gauss-Christoffel quadrature formulae*. A nice survey of Gauss-Christoffel quadrature formulae was written by Gautschi [24].

In modern terminology, the formulation of this classical theory can be given in the following form: *Let $d\mu$ be a finite positive Borel measure on the real line $\mathbb{R}$ such that its support is an infinite set, and all its moments $\mu_k = \int_{\mathbb{R}} t^k \, d\mu(t)$, $k = 0, 1, \ldots$, exist and are finite. Then, for each $n \in \mathbb{N}$, there exists the n-point Gauss-Christoffel quadrature formula*

$$\int_{\mathbb{R}} f(t) \, d\mu(t) = \sum_{k=1}^{n} A_k f(\tau_k) + R_n(f), \tag{3}$$

which is exact for all algebraic polynomials of degree $\leq 2n-1$, i.e., $R_n(f) = 0$ for each $f \in \mathcal{P}_{2n-1}$.

The Gauss-Christoffel quadrature formula can be characterized as an interpolatory formula for which its *node polynomial* $\omega_n(t) = \prod_{k=1}^{n}(t - \tau_k)$ is orthogonal to $\mathcal{P}_{n-1}$ with respect to the inner product defined by

$$(f, g) = \int_{\mathbb{R}} f(t) g(t) \, d\mu(t) \quad (f, g \in L^2(d\mu)). \tag{4}$$

Thus, the nodes in (3) are zeros of the monic orthogonal polynomial $\omega_n(t) = \pi_n(d\mu; t)$. The corresponding weights A_k (Christoffel numbers) can be expressed by the so-called Christoffel function $\lambda_n(d\mu; t)$ (cf. [53, Chapters 2 & 5]) in the form $A_k = \lambda_n(d\mu; \tau_k)(> 0)$, $k = 1, \ldots, n$. In the special case $d\mu(t) = dt$ on $[-1, 1]$ considered by Gauss, the nodes are zeros of the Legendre polynomial P_n.

If μ is an absolutely continuous function, then we say that $\mu'(t) = w(t)$ is a *weight function* and the measure $d\mu$ can be expressed as $d\mu(t) = w(t) \, dt$, where the weight function w is non-negative and measurable in Lebesgue's

sense for which all moments exist and $\mu_0 > 0$. If the support of the measure (weight) is $\operatorname{supp}(w) = [a, b]$, where $-\infty < a < b < +\infty$, we have Gaussian quadratures (and the corresponding orthogonal polynomials) on the finite interval $[a, b]$.

In the general case, the function μ can be written in the form $\mu = \mu_{\mathrm{ac}} + \mu_{\mathrm{s}} + \mu_{\mathrm{j}}$, where μ_{ac} is absolutely continuous, μ_{s} is singular, and μ_{j} is a jump function.

One of the most important uses of orthogonal polynomials is in the construction of quadrature formulas of the maximal, or nearly maximal, algebraic degree of exactness for integrals involving a positive measure $d\mu$. The following theorem is due to Jacobi [44] (cf. [53, p. 297]).

Theorem 1. *Given a positive integer m ($\leq n$), the quadrature formula* (3) *has degree of exactness $d = n - 1 + m$ if and only if the following conditions are satisfied:*

1° *Formula* (3) *is interpolatory;*

2° *The node polynomial ω_n satisfies*

$$(\forall p \in \mathcal{P}_{m-1}) \qquad (p, \omega_n) = \int_{\mathbb{R}} p(t) q_n(t)\, d\mu(t) = 0.$$

According to Theorem 1, an n-point quadrature formula (3) with respect to the positive measure $d\mu(t)$ has the maximal algebraic degree of exactness $2n - 1$, i.e., $m = n$ is optimal. The higher m ($> n$) is impossible. Indeed, according to 2°, the case $m = n + 1$ requires the orthogonality $(p, \omega_n) = 0$ for all $p \in \mathcal{P}_n$, which is impossible when $p = \omega_n$.

The cases $m = n-1$ and $m = n-2$ lead to the Gauss-Radau (one of the endpoints a or b is included in the set of nodes) and Gauss-Lobatto formulas ($\tau_1 = a$ and $\tau_n = b$), respectively.

3. *Gauss-Christoffel quadrature rules for classical and non-classical weights*

We start this section with monic polynomials

$$\pi_k(d\mu; t) = \pi_k(t) = t^k + \text{ lower degree terms},$$

$k = 0, 1, \ldots$, which are orthogonal with respect to the inner product (4). Because of the property $(tf, g) = (f, tg)$, these polynomials satisfy the three-term recurrence equation

$$\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t), \qquad k = 0, 1, 2, \ldots, \tag{5}$$

$$\pi_0(t) = 0, \quad \pi_{-1}(t) = 0,$$

where $(\alpha_k) = (\alpha_k(d\mu))$ and $(\beta_k) = (\beta_k(d\mu))$ are sequences of recursion coefficients. The coefficient β_0 which is multiplied by $\pi_{-1}(x) = 0$ in (5) may be arbitrary. Sometimes, it is convenient to define it by $\beta_0 = \mu_0 = \int_{\mathbb{R}} d\mu(x)$. Then the norm of π_n can be expressed in the form $\|\pi_n\| = \sqrt{(\pi_n, \pi_n)} = \sqrt{\beta_0\beta_1 \cdots \beta_n}$.

For generating Gauss-Christoffel quadrature rules there are numerical methods, which are computationally much better than a computation of nodes by using Newton's method and then a direct application of Christoffel's expressions for the weights (see e.g. Davis and Rabinowitz [18]). The characterization of the Gauss-Christoffel quadratures via an eigenvalue problem for the Jacobi matrix has become the basis of current methods for generating these quadratures. The most popular of them is one due to Golub and Welsch [43]. Their method is based on determining the eigenvalues and the first components of the eigenvectors of a symmetric tridiagonal Jacobi matrix.

Theorem 2. *The nodes τ_k in the Gauss-Christoffel quadrature rule* (3)*, with respect to a positive measure $d\mu$, are the eigenvalues of the n-th order Jacobi matrix*

$$J_n(d\mu) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & \mathrm{O} \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{n-1}} \\ \mathrm{O} & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{bmatrix}, \tag{6}$$

where α_ν and β_ν, $\nu = 0, 1, \ldots, n-1$, are the coefficients in the three-term recurrence relation (5) *for the monic orthogonal polynomials $\pi_\nu(d\mu; \cdot)$. The weights A_k are given by*

$$A_k = \beta_0 v_{k,1}^2, \qquad k = 1, \ldots, n,$$

where $\beta_0 = \mu_0 = \int_{\mathbb{R}} d\mu(t)$ and $v_{k,1}$ is the first component of the normalized eigenvector $\mathbf{v_k}$ corresponding to the eigenvalue x_k,

$$J_n(d\mu)\mathbf{v_k} = \mathbf{x_k}\mathbf{v_k}, \qquad \mathbf{v_k}^{\mathrm{T}}\mathbf{v_k} = \mathbf{1}, \qquad \mathbf{k} = \mathbf{1}, \ldots, \mathbf{n}.$$

Simplifying QR algorithm so that only the first components of the eigenvectors are computed, Golub and Welsch [43] gave an efficient procedure

for constructing the Gaussian quadrature rules. This procedure was implemented in several programming packages including the most known `ORTHPOL` given by Gautschi [31] (see also our package `OrthogonalPolynomials` realized in `Mathematica` [13]).

According to Theorem 2, we need the recursion coefficients α_k and β_k, $k \leq m-1$, for the monic polynomials $\pi_\nu(d\mu;\,\cdot\,)$, in order to construct the n-point Gauss-Christofell quadrature formula (3), with respect to a positive measure $d\mu$, for each $n \leq m$. In the case of the classical orthogonal polynomials, i.e., Jacobi, generalized Laguerre and Hermite polynomials (cf. [53, Section 2.3]), these coefficients are known explicitly[1] and the construction problem of Gaussian quadratures is completely solved by Theorem 2. However, in the case of strong non-classical polynomials (see [53, Subsection 2.4.7]), we need an additional numerical construction of recursion coefficients (see [53, Subsection 2.4.8]).

In the sequel we mention some non-classical measures $d\mu(x) = w(x)\,dx$ for which the recursion coefficients $\alpha_k(d\mu)$, $\beta_k(d\mu)$, $k = 0, 1, \ldots, n-1$, have been provided in the literature and used in the construction of Gaussian quadratures.

1° *One-sided Hermite weight* $w(x) = \exp(-x^2)$ on $[0, c]$, $0 < c \leq +\infty$. This distribution $w(x)\,dx$ is known as the *Maxwell* (*velocity*) *distribution*. The cases $c = 1$, $n = 10$ and $c = +\infty$, $n = 15$ were considered by Steen, Byrne and Gelbard [96] (see also Gautschi [30]).

2° *Logarithmic weight* $w(x) = x^\alpha \log(1/x)$, $\mu > -1$ on $(0, 1)$. Piessens and Branders [79] considered cases when $\alpha = 0, \pm 1/2, \pm 1/3, -1/4, -1/5$ (see also Gautschi [29]).

3° *Airy weight* $w(x) = \exp(-x^3/3)$ on $(0, +\infty)$. The inhomogeneous Airy functions $\mathrm{Hi}(x)$ and $\mathrm{Gi}(x)$, arise in theoretical chemistry (e.g. in harmonic oscillator models for large quantum numbers) and their integral representations (see Lee [50]) are given by

$$\begin{aligned} \mathrm{Hi}(t) &= \frac{1}{\pi}\int_0^{+\infty} w(x)e^{xt}\,dx, \\ \mathrm{Gi}(t) &= -\frac{1}{\pi}\int_0^{+\infty} w(x)e^{-xt/2}\cos\Big(\frac{\sqrt{3}}{2}\,xt + \frac{2\pi}{3}\Big)\,dx. \end{aligned}$$

These functions can effectively be evaluated by the Gaussian quadrature relative to the Airy weight $w(x)$. It needs orthogonal polynomials with

[1] Also, there are a few non-classical cases for which the recursion coefficients are known explicitly (see [53, Section 2.4]).

respect to this weight. Gautschi [27] computed the recursion coefficients for $n = 15$ with 16 decimal digits after the decimal point (D).

4° *Reciprocal gamma function* $w(x) = 1/\Gamma(x)$ on $(0, +\infty)$. Gautschi [26] determined the recursion coefficients for $n = 40$ with 20 significant decimal digits (S). This function could be useful as a probability density function in reliability theory (see Fransén [21]).

5° *Einstein's* and *Fermi's weight functions* on $(0, +\infty)$,

$$w_1(x) = \varepsilon(x) = \frac{x}{e^x - 1} \qquad \text{and} \qquad w_2(x) = \varphi(x) = \frac{1}{e^x + 1}\,.$$

These functions arise in solid state physics. Integrals with respect to the measure $d\mu(x) = \varepsilon(x)^r\,dx$, $r = 1$ and $r = 2$, are widely used in phonon statistics and lattice specific heats and occur also in the study of radiative recombination processes. Similarly, integrals with $\varphi(x)$ are encountered in the dynamics of electrons in metals. For $w_1(x)$, $w_2(x)$, $w_3(x) = \varepsilon(x)^2$ and $w_4(x) = \varphi(x)^2$, Gautschi and Milovanović [36] gave the first systematic investigation on the derivation of quadrature rules with high-precision, determined the recursion coefficients α_k and β_k, $k < n = 40$, and gave an application of the corresponding Gauss-Christoffel quadratures to the summation of slowly convergent series, whose general term is expressible in terms of a Laplace transform or its derivative. We call such a summation the *method of Laplace transform*.

In the numerical construction for the measure $d\mu(x) = [\varepsilon(x)]^r\,dx$ on $(0, +\infty)$, $r \geq 1$, we used the discretized Stieltjes procedure based on the Gauss-Laguerre quadratures, so that

$$\begin{aligned}\int_0^{+\infty} P(x)\,d\mu(x) &= \frac{1}{r}\int_0^{+\infty} P(x/r)\left(\frac{x/r}{1-e^{-x/r}}\right)^r e^{-x}\,dx \\ &\approx \sum_{k=1}^{N} \frac{A_k^L}{r}\left(\frac{x_k^L/r}{1-e^{-x_k^L/r}}\right)^r P(x_k^L/r),\end{aligned}$$

where $P \in \mathcal{P}$ and $N \gg n$. The Gauss-Laguerre nodes x_k^L (zeros of the standard Laguerre polynomial $L_N(x)$) and the weights A_k^L can be easily computed for an arbitrary N by the Golub-Welsch algorithm.

6° *The hyperbolic weights* on $(0, +\infty)$,

$$w_1(x) = \frac{1}{\cosh^2 x} \qquad \text{and} \qquad w_2(x) = \frac{\sinh x}{\cosh^2 x}\,.$$

The recursion coefficients α_k, β_k, for $k < 40$ were obtained by Milovanović [56]. The main application of these quadratures is the summation of slowly convergent series, with the general term $a_k = f(k)$. Such a method known as the *method of contour integration* was given in [56] (for further applications see [57]).

If F is an integral of f and

$$\Phi(x, y) = -\frac{1}{2}[F(x + iy) + F(x - iy)],$$

then, under certain conditions,

$$\begin{aligned} T_m = \sum_{k=m}^{+\infty} a_k &= \int_0^{+\infty} \Phi(m - 1/2, t/\pi) w_1(t)\, dt \\ &= \sum_{\nu=1}^{n} A_\nu \Phi(m - 1/2, \tau_\nu/\pi) + R_n(\Phi). \end{aligned}$$

As an illustration, we consider only the series

$$T_1(a) = \sum_{k=1}^{+\infty} \frac{1}{\sqrt{k}(k + a)}\,, \tag{7}$$

which appeared (for $a = 1$) in a study of spirals (see Davis [17]) and defines the "Theodorus constant." The first 1 000 000 terms of the series $T_1(1)$ give the result $1.8580\ldots$, i.e., $T_1(1) \approx 1.86$ (only 3-digit accuracy). Using the *method of Laplace transform*, as a increases, the convergence of the Gauss quadrature formula (with Einstein's weight) slows down considerably. For example, when $a = 8$, we get results with relative errors $1.4{\times}10^{-1}$, $2.3{\times}10^{-2}$, 1.5×10^{-3}, 1.9×10^{-4}, 2.5×10^{-5}, 2.1×10^{-6}, 2.5×10^{-7}, and 2.6×10^{-8}, for $n = 5(5)40$, respectively.

Now, we directly apply the *method of contour integration* to (7) with

$$F(z) = \frac{2}{\sqrt{a}} \left(\arctan \sqrt{\frac{z}{a}} - \frac{\pi}{2} \right),$$

where the integration constant is taken so that $F(\infty) = 0$.

We can represent (7) in the form

$$T_1(a) = \sum_{k=1}^{m-1} \frac{1}{\sqrt{k}(k + a)} + T_m(a), \qquad T_m(a) = \sum_{k=m}^{+\infty} \frac{1}{\sqrt{k}(k + a)}, \tag{8}$$

and then use the Gaussian quadrature formula (with the hyperbolic weight w_1) to calculate $T_m(a)$. Relative errors in approximations for $T_1(a)$, when $a \geq 1/2$ and $m = 4$ are less than 10^{-18} with only $n = 10$ nodes. The method is very efficient. Moreover, its convergence is slightly faster if the parameter a is larger. Taking $n = 25$ nodes in our quadratures, we obtain the exact sum $T_1(1) = 1.86002507922119030718069591572\ldots$ (to 30 significant digits).

An approach to summation formulas due to Plana, Lindelöf and Abel was recently given by Dahlquist [14, 15, 16].

Here we also mention an interesting application of Gaussian type formulas in the so-called *moment-preserving spline approximation* of a given function f on $[0, +\infty)$ (or on a finite interval, e.g. $[0, 1]$). Such kind of problems appeared in the physics literature, for example in the approximation of the Maxwell velocity distribution by a linear combination of Dirac δ-functions (see Laframboise and Stauffer [49]) or in the corresponding approximation by a linear combination of Heaviside step functions (see Calder and Laframboise [8]). The authors used some classical methods, which are very sensitive to rounding errors, and therefore their computations require a high-precision arithmetic. In order to get a stable method for this kind of approximation, Gautschi and Milovanović [38] found new applications of Gaussian type of quadratures.

Let f be a given function defined on the positive real line $\mathbb{R}_+ = [0, +\infty)$ and $s_{n,m}$ be a spline of the form

$$s_{n,m}(t) = \sum_{\nu=1}^{n} a_\nu (t_\nu - t)_+^m, \quad 0 \leq t < +\infty, \tag{9}$$

where the plus sign on the right is the cutoff symbol, $u_+ = u$ if $u > 0$ and $u_+ = 0$ if $u \leq 0$, $0 < t_1 < \cdots < t_n$, $a_\nu \in \mathbb{R}$. We considered the moment-preserving spline approximation $f(t) \approx s_{n,m}(t)$ such that

$$\int_0^{+\infty} s_{n,m}(t) t^j \, dV = \int_0^{+\infty} f(t) t^j \, dV, \quad j = 0, 1, \ldots, 2n-1,$$

where dV is the volume element depending on the geometry of the problem. In some concrete applications in physics, up to unimportant numerical factors, $dV = t^{d-1} \, dt$, where $d = 1, 2$, and 3 for rectilinear, cylindric, and spherical geometry, respectively.

For fixed $n, m \in \mathbb{N}$, $d \in \{1, 2, 3\}$ and certain conditions on f we proved in [38] that the spline function $s_{n,m}$ exists uniquely if and only if the measure

$$d\lambda_m(t) = \frac{(-1)^{m+1}}{m!} t^{m+d} f^{(m+1)}(t) \, dt \quad \text{on} \quad [0, +\infty)$$

admits an n-point Gauss-Christoffel quadrature formula

$$\int_0^{+\infty} g(x)\,d\lambda_m(x) = \sum_{\nu=1}^{n} \lambda_\nu^{(n)} g(\tau_\nu^{(n)}) + R_n(g; d\lambda_m), \tag{10}$$

with distinct positive nodes $\tau_\nu^{(n)}$, where $R_n(g; d\lambda_m) = 0$ for all $g \in \mathcal{P}_{2n-1}$. In that event, the knots t_ν and weights a_ν in (9) are given by

$$t_\nu = \tau_\nu^{(n)}, \quad a_\nu = t_\nu^{-(m+d)} \lambda_\nu^{(n)}, \quad \nu = 1, \ldots, n.$$

The approximation error $e_{n,m}(t) := f(t) - s_{n,m}(t)$ can be expressed by the remainder term of (10), i.e., $e_{n,m}(t) = R_n(\sigma_t; d\lambda_m)$, where $\sigma_t(x) = x^{-(m+d)}(x-t)_+^m$, $x, t > 0$.

Note that for $m = 0$, (9) reduces to linear combination of Heaviside step functions. The case with Dirac δ-functions can be formally obtained putting $m = -1$.

Approximation on a compact interval was considered by Frontini, Gautschi and Milovanović [22].

On the end of this section we mention that there are several other extensions and generalizations, e.g. the so-called *optimal quadratures*, *Radau* and *Lobatto quadratures*, *Kronrod quadratures*, etc. An account of the role played by moments and modified moments in the construction of interpolatory quadrature rules, especially weighted Newton-Cotes and Gaussian rules, is given by Gautschi [33].

4. *Quadratures with multiple node*

More than hundred years after the famous Gauss method of approximate integration, there appeared the idea of numerical integration involving multiple nodes Chakalov [9, 10, 11], Turán [99], Popoviciu [81], Ghizzetti and Ossicini [40, 41], etc.

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. Interpolation quadrature formulae of a general form

$$I(f) = \int_{\mathbb{R}} f(t)\,d\mu(t) \cong Q(f),$$

where

$$Q(f) = \sum_{\nu=1}^{n} \sum_{i=0}^{n_\nu - 1} A_{i,\nu} f^{(i)}(\tau_\nu) + \sum_{\nu=1}^{m} \sum_{i=0}^{m_\nu - 1} B_{i,\nu} f^{(i)}(\eta_\nu), \tag{11}$$

with an algebraic degree of exactness at least $M+N-1$, were investigated by D. D. Stancu [88, 91, 98].

Using fixed and free nodes we introduce two polynomials

$$q_M(t) := \prod_{\nu=1}^{m}(t-\eta_\nu)^{m_\nu} \quad \text{and} \quad Q_N(t) := \prod_{\nu=1}^{n}(t-\tau_\nu)^{n_\nu}, \tag{12}$$

where $M=\sum_{\nu=1}^{m} m_\nu$ and $N=\sum_{\nu=1}^{n} n_\nu$. Choosing the free nodes to increase the degree of exactness leads to so-called Gaussian type of quadratures. If the free (or *Gaussian*) nodes $\tau_1,\dots,\tau_n$ 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*. D.D. Stancu [93] proved that $\tau_1,\dots,\tau_n$ *are the Gaussian nodes if and only if*

$$\int_{\mathbb{R}} t^k Q_N(t) q_M(t)\,d\mu(t)=0 \tag{13}$$

for $k=0,1,\dots,n-1$. Under some restrictions of node polynomials $q_M(t)$ and $Q_N(t)$ on the support interval of the measure $d\mu(t)$ we can give sufficient conditions for the existence of Gaussian nodes (cf. Stancu [93] and [42]). For example, *if the multiplicities of the Gaussian nodes are odd, e.g.,* $n_\nu=2s_\nu+1$, $\nu=1,\dots,n$, *and if the polynomial with fixed nodes* $q_M(t)$ *does not change its sign in the support interval of the measure* $d\mu(t)$, *then, in this interval, there exist real distinct nodes* τ_ν, $\nu=1,\dots,n$.

The last condition for the polynomial $q_M(t)$ means that the multiplicities of the internal fixed nodes must be even. Defining a new (nonnegative) measure $d\hat{\mu}(t)$ by $d\hat{\mu}(t)=\gamma q_M(t)\,d\mu(t)$ ($\gamma=\operatorname{sgn}(q_M(t))$, the "orthogonality conditions" (13) can be expressed in the simpler form

$$\int_{\mathbb{R}} t^k Q_N(t)\,d\hat{\mu}(t)=0, \quad k=0,1,\dots,n-1.$$

This means that the general quadrature problem (11), under these conditions, can be reduced to a problem with only Gaussian nodes, but with respect to another modified measure. Computational methods for this purpose are based on Christoffel's theorem and described in details in [32] (see also [42] and [47]).

Let $\pi_n(t) := \prod_{\nu=1}^{n}(t-\tau_\nu)$. Since $Q_N(t)/\pi_n(t)=\prod_{\nu=1}^{n}(t-\tau_\nu)^{2s_\nu}\geq 0$ over the support interval, we can make an additional reinterpretation of the "orthogonality conditions" (13) in the form

$$\int_{\mathbb{R}} t^k \pi_n(t)\,d\mu(t)=0, \quad k=0,1,\dots,n-1, \tag{14}$$

where

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

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 the support interval. As we see 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 [20, pp. 214–226]). This polynomial $\pi_n(t)$ belongs to the class of so-called *σ-orthogonal polynomials* $\{\pi_{n,\sigma}(t)\}_{n\in\mathbb{N}_0}$, which correspond to the sequence $\sigma = (s_1, s_2, \ldots)$ connected with multiplicities of Gaussian nodes. Namely, $\pi_n(t) = \pi_{n,\sigma}(t)$. If $\sigma = (s, s, \ldots)$, these polynomials reduce to the *s-orthogonal polynomials*. (For details see Milovanović [59].)

Quadratures with only Gaussian nodes ($m = 0$),

$$\int_{\mathbb{R}} f(t)\,d\lambda(t) = \sum_{\nu=1}^{n}\sum_{i=0}^{2s_\nu} A_{i,\nu} f^{(i)}(\tau_\nu) + R(f), \tag{15}$$

which are exact for all algebraic polynomials of degree at most $d_{\max} = 2\sum_{\nu=1}^{n} s_\nu + 2n - 1$, are known as *Chakalov-Popoviciu quadrature formulas* (see [9, 10, 11], [81]). A deep theoretical progress in this subject was made by Stancu (see [98] and [86]–[95]). In the special case of the Legendre measure on $[-1, 1]$, when all multiplicities are mutually equal, these formulas reduce to the well-known *Turán quadrature* [99]. The case with a weight function $d\mu(t) = w(t)dt$ on $[a, b]$ has been investigated by Italian mathematicians Ossicini, Ghizzetti, Guerra, Rosati, and also by Chakalov, Stroud, Stancu, Ionescu, Pavel, etc. (see Milovanović [59] for references).

At the Third Conference on Numerical Methods and Approximation Theory (Niš, August 18–21, 1987) (see [54]) we presented a stable method with quadratic convergence for numerically constructing s-orthogonal polynomials, which zeros are nodes of Turán quadratures. The basic idea for our method to numerically construct s-orthogonal polynomials with respect to the measure $d\mu(t)$ on the real line $\mathbb{R}$ is a reinterpretation of the *s-orthogonality* in terms of implicitly defined standard orthogonality. Further progress in this direction was made by Gautschi and Milovanović [39]. After our survey [59] (published in series "Numerical Analysis in the 20th Century"), where we gave a connection between quadratures, s and σ-orthogonality and moment-preserving approximation with defective splines, the interest for this subject rapidly increases (Gautschi, Yang, Shi, Yang & Wang, Gout & Guessab, Shi & Xu, etc.). A very efficient method for

constructing quadratures with multiple nodes was given recently by Milovanović, Spalević and Cvetković [74].

The error analysis and estimates of the remainder term in quadratures on $[-1,1]$ with multiple nodes have been treated recently in the class of analytic functions in the interior of a simple closed curve Γ in the complex plane surrounding the interval $[-1,1]$. Two choices of the contour Γ have been widely used: 1° a circle with center at origin and radius ϱ (>1), and 2° an ellipse with foci at ± 1. In several papers Milovanović and Spalević (see [68, 69, 70, 71, 72, 73]) developed a few methods for error estimates and obtained very exact L^1- and L^∞-estimates of the remainder term for the generalized Chebyshev weights.

Another type of quadratures with multiple nodes are the so-called *Birkhoff quadratures*. Roughly speaking their quadrature sums do not include all derivatives. We mention here only a very special case of Birkhoff quadratures – the generalized $(0,m)$ quadrature problem

$$\int_{\mathbb{R}} f(x)\,d\mu(x) = \sum_{k=1}^{n} \Big[v_k f(x_k) + w_k f^{(m)}(x_k) \Big] + R(f) \tag{16}$$

of highest degree of precision, which first was stated in 1974 by Turán for $d\mu(x) = dx$ on $[-1,1]$, $m=2$, and nodes as zeros of the polynomial $\Pi_n(x) := (1-x^2)P'_{n-1}(x)$, where P_k is the Legendre polynomial of degree k (cf. [100]). For some particular results on (16) see [101], [19], [75], [51].

We mention also two nice recent books by Shi [83, 84].

Further extensions dealing with quadratures with multiple nodes for ET (Extended Tschebycheff) systems were given by [45], [2], [4], [3], etc.

5. *Orthogonality with respect to a moment functional and corresponding quadratures*

In the previous sections the inner product was always positive definite provided the existence of the corresponding orthogonal polynomials with real zeros in the support of the measure. Such zeros appeared as the nodes of the Gaussian formulas. However, there are a more general concept of orthogonality with respect to a given linear moment functional L on the linear space $\mathcal{P}$ of all algebraic polynomials. Because of linearity, the value of the linear functional L at every polynomial is known if the values of L are known at the set of all monomials, i.e., if we know $L(x^k) = \mu_k$, for each $k \in \mathbb{N}_0$. In that case we can introduce a system of orthogonal polynomials

$\{\pi_k\}_{k=0\in\mathbb{N}_0}$ with respect to the functional L if for all nonnegative integers k and n (cf. Chihara [12, p. 7]),

- $\pi_k(x)$ is polynomial of degree k,
- $L(\pi_k(x)\pi_n(x)) = 0$, if $k \neq n$,
- $L(\pi_n^2(x)) \neq 0$.

If the sequence of orthogonal polynomials exists for a given linear functional L, then L is called quasi-definite or regular linear functional. Under the condition $L(\pi_n^2(x)) > 0$, $n \in \mathbb{N}_0$, the functional L is called positive definite. The necessary and sufficient conditions for the existence of a sequence of orthogonal polynomials with respect to the linear functional L are that for each $n \in \mathbb{N}$ the Hankel determinants

$$\Delta_n = \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-1} \\ \mu_1 & \mu_2 & & \mu_n \\ \vdots & & & \\ \mu_{n-1} & \mu_n & & \mu_{2n-2} \end{vmatrix} \neq 0. \tag{17}$$

This concept of orthogonality enables us to consider also the quadratures of Gaussian type with respect to the functional L, even in the cases when the weight is a complex function. In the next subsections we mention only the two such cases.

5.1. *Orthogonality on the semicircle and quadratures.* Let w be a weight function which is positive and integrable on the open interval $(-1, 1)$, though possibly singular at the endpoints, and which can be extended to a function $w(z)$ holomorphic in the half disc $D_+ = \{z \in \mathbb{C} : |z| < 1,\ \mathrm{Im}\ z > 0\}$. Consider the following "inner product"

$$(f, g) = \int_\Gamma f(z)g(z)w(z)(iz)^{-1}\,dz = \int_0^\pi f(e^{i\theta})g(e^{i\theta})w(e^{i\theta})\,d\theta, \tag{18}$$

where Γ is the circular part of ∂D_+ and all integrals are assumed to exist (possibly) as appropriately defined improper integrals. The "inner product" is not Hermitian; we deliberately did not conjugate the second factor g and did not integrate with respect to the measure $|w(e^{i\theta})|\,d\theta$. The existence of the corresponding orthogonal polynomials $\{\pi_n\}_{n\in\mathbb{N}_0}$, therefore, is not guaranteed.

The case $w = 1$ was considered by Gautschi and Milovanović [37]. The existence and uniqueness of polynomials orthogonal on the unit semicircle were proved via moment determinants.

A more general case of the complex weight was considered by Gautschi, Landau and Milovanović [35]. Under the condition

$$\operatorname{Re}\,(1,1) = \operatorname{Re}\,\int_0^\pi w(e^{i\theta})\,d\theta \neq 0,$$

they proved that the orthogonal polynomials $\{\pi_n\}_{n\in\mathbb{N}_0}$ exist uniquely and they can be represented in the form $\pi_n(z) = p_n(z) - i\theta_{n-1}p_{n-1}(z)$, where

$$\theta_{n-1} = \theta_{n-1}(w) = \frac{\mu_0 p_n(0) + iq_n(0)}{i\mu_0 p_{n-1}(0) - q_{n-1}(0)}.$$

Here, p_k are standard (real) polynomials orthogonal with respect to the inner product

$$[f,g] = \int_{-1}^{1} f(x)\overline{g(x)}w(x)\,dx,$$

and q_k are the corresponding associated polynomials of the second kind,

$$q_k(z) = \int_{-1}^{1} \frac{p_k(z) - p_k(x)}{z - x} w(x)\,dx.$$

In the previous mentioned papers, we obtained several results for the polynomials π_n, including the three-term recurrence relation, zero distribution, and a linear differential equation. Also, we gave a few applications in numerical differentiation and numerical integration.

In [55] the Gegenbauer case $w(z) = (1-z^2)^{\lambda-1/2}$, $\lambda > -1/2$, on $[-1,1]$, was investigated, for which $\mu_0 = \pi$. The explicit expressions for θ_n in terms of gamma function enabled us to propose a stable construction of Gauss-Christoffel quadratures on the semicircle

$$\int_0^\pi f(e^{i\theta})w(e^{i\theta})\,d\theta = \sum_{\nu=1}^{n} \sigma_\nu f(\zeta_\nu) + R_n(f).$$

The nodes $\zeta_\nu = \zeta_\nu^{(n)}$ are precisely the zeros of $\pi_n(z)$. In order to determine the weights $\sigma_\nu = \sigma_\nu^{(n)}$, we consider an eigenvalue problem for the Jacobi

matrix

$$J_n = \begin{bmatrix} i\alpha_0 & \theta_0 & & & \mathrm{O} \\ \theta_0 & i\alpha_1 & \theta_1 & & \\ & \theta_1 & i\alpha_2 & \ddots & \\ & & \ddots & \ddots & \theta_{n-2} \\ \mathrm{O} & & & \theta_{n-2} & i\alpha_{n-1} \end{bmatrix}.$$

Using some matrix transformations (see [55]) we reduce this complex matrix to a real nonsymmetric tridiagonal matrix given by

$$A_n = -iD_n^{-1} J_n D_n = \begin{bmatrix} \alpha_0 & \theta_0 & & & \mathrm{O} \\ -\theta_0 & \alpha_1 & \theta_1 & & \\ & -\theta_1 & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \theta_{n-2} \\ \mathrm{O} & & & -\theta_{n-2} & \alpha_{n-1} \end{bmatrix},$$

whose eigenvalues are $\eta_\nu = -i\zeta_\nu$. Denote by V_n the matrix of the eigenvectors of this matrix A_n, each normalized so that the first component is equal to 1. Putting $\mathbf{v} = [\sigma_\mathbf{1}\ \sigma_\mathbf{2}\ \ldots\ \sigma_\mathbf{n}]^\mathbf{T}$, we can get a system of linear equations for finding the weight coefficients

$$V_n \mathbf{v} = \pi \mathbf{e_1},$$

where $\mathbf{e_1} = [\mathbf{1}\ \mathbf{0}\ \ldots\ \mathbf{0}]^\mathbf{T}$ (the first coordinate vector).

The zeros ζ_ν of π_n are located symmetrically with respect to the imaginary axis and for $n \geq 2$ all zeros are contained in D_+. For the general Jacobi weight $w(z) = (1-z)^\alpha (1+z)^\beta$, $\alpha, \beta > -1$, we conjectured that all zeros are also contained in the upper unit half disc D_+ (see [35]). This was verified numerically for many values of parameters α and β.

5.2. *Orthogonal polynomials for oscillatory weights.* Let w be a given weight function on $[-1,1]$ and $d\mu(x) = xw(x)e^{i\zeta x}\,dx$, where $\zeta \in \mathbb{R}$. In this subsection we consider the existence of the orthogonal polynomials π_n with respect to the functional

$$L(p) = \int_{-1}^{1} p(x)\,d\mu(x), \quad \mu_k = L(x^k),\ k \in \mathbb{N}_0. \tag{19}$$

Two cases are intensively studied.

1° *Case* $w(x) = 1$, $\zeta = m\pi$, $m \in \mathbb{Z} \setminus \{0\}$.

The existence and uniqueness for polynomials π_n were proved via moment determinants (see [61]). Namely, *for each integer $m \neq 0$, the orthogonal polynomials with respect to the measure $d\mu(x) = xe^{im\pi x}\,dx$ on $-1, 1]$ exist uniquely and satisfy the three-term recurrence relation*

$$\pi_{n+1}(x) = (x - i\alpha_n)\pi_n(x) - \beta_n\pi_{n-1}(x), \quad n \geq 0,$$

with $\pi_0(x) = 1$ and $\pi_{-1}(x) = 0$.

From the Hankel determinants it is clear that the recursion coefficients are rational functions in $\zeta = m\pi$. Using our software package [13] we can generate coefficients even in symbolic form for some reasonable values of n (e.g. $n \leq 20$) and state the following conjecture: *Let $a_n(z)$ and $c_n(z)$ be algebraic polynomials with integer coefficients of degree r_n and s_n, respectively, i.e., $a_n(z) = A_n z^{r_n} + \cdots$ and $c_n(z) = z^{s_n} + \cdots$. If $\zeta = m\pi$ and $n \geq 2$, then*

$$\alpha_n = \frac{a_n(\zeta^2)}{\zeta\, c_{n-1}(\zeta^2)c_n(\zeta^2)}\,, \qquad \beta_n = B_n\,\frac{c_{n-2}(\zeta^2)c_n(\zeta^2)}{\zeta^2\, c_{n-1}(\zeta^2)^2}\,,$$

where

$$A_n = \begin{cases} -\dfrac{n^2-1}{4} & (n \text{ odd}), \\ \dfrac{n^2+10n+8}{4} & (n \text{ even}), \end{cases} \qquad B_n = \begin{cases} 1 & (n \text{ odd}), \\ -n^2 & (n \text{ even}), \end{cases}$$

and

$$r_n = \frac{n(n+1)}{2}\,, \qquad s_n = \begin{cases} \dfrac{(n+1)^2}{4} & (n \text{ odd}), \\ \dfrac{n(n+2)}{4} & (n \text{ even}). \end{cases}$$

The complexity of expressions for α_n and β_n increases exponentially with n. On the other side, there is an efficient algorithm for their numerical construction [61].

The corresponding Gaussian quadratures can also be constructed. A possible application of these quadratures is in numerical calculation of integrals involving highly oscillatory integrands, in particular for calculation of the Fourier coefficients,

$$\begin{aligned} C_m(f) + iS_m(f) = \int_{-1}^{1} f(x)e^{im\pi x}\,dx &= \int_{-1}^{1} \frac{f(x) - f(0)}{x}\,d\mu(x) \\ &\approx \sum_{\nu=1}^{n} \frac{A_\nu^n}{x_\nu^n}(f(x_\nu^n) - f(0)), \end{aligned}$$

where x_ν^n are zeros of π_n, and A_k^n are the corresponding weight coefficients.

Taking $f(x) = \dfrac{x}{x^2+1/4}$ we have

$$S_m(f) = \int_{-1}^{1} \frac{x}{x^2+1/4} \sin(m\pi x)\, dx \approx G_n(f) = \operatorname{Im} \left\{ \sum_{\nu=1}^{n} \frac{A_\nu^n}{(x_\nu^n)^2+1/4} \right\}.$$

For example, for $m = 100$ and $n = 10$ we get

$$S_{100}(f) \approx G_{10}(f) = -0.00509295801381218410374386537 08.$$

If we increase m, the convergence of $G_n(f)$ is rather faster, e.g., for $m = 10^6$, the relative error in $G_{10}(f)$ is smaller than 10^{-60}. The integrand for $m = 200$ is presented in Figure .

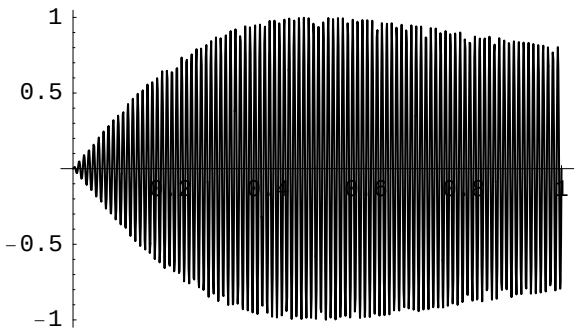

Figure 1. Integrand for $m = 200$

2° *Case* $w(x) = 1/\sqrt{1-x^2}$, $\zeta \in \mathbb{R}$. This case was considered recently by Milovanović and Cvetković [62]. We showed that the corresponding moments can be expressed in terms of Bessel functions J_0 and J_1 as

$$\mu_k = \frac{i\pi}{(i\zeta)^k}(P_k(\zeta^2)J_1(\zeta) + \zeta Q_k(\zeta^2)J_0(\zeta)), \quad k \in \mathbb{N}_0,$$

where P_k and Q_k are algebraic polynomials with integer coefficients of degrees $2[k/2]$ and $2[(k-1)/2]$, respectively, and satisfy the following recurrence relation

$$y_{k+2} = -(k+2)y_{k+1} - \zeta^2 y_k - (k+1)\zeta^2 y_{k-1},$$

with initial conditions

$$\begin{aligned} P_0 &= 1, \quad P_1 = -1, \quad P_2 = 2 - \zeta^2, \\ Q_0 &= 0, \quad Q_1 = 1, \qquad Q_2 = -1. \end{aligned}$$

When ζ is a positive zero of J_0, we proved that polynomials π_n orthogonal with respect to the functional (19) exist uniquely and satisfy the three-term recurrence relation, for which coefficients we found the asymptotic formulae. Moreover, we proved that the essential spectrum of the associated Jacobi operator created using three-term recurrence coefficients α_k and β_k, $k \in \mathbb{N}_0$, is $[-1, 1]$.

6. *Nonstandard quadratures of Gaussian type*

All previous quadrature rules use the information on the integrand only at some selected points x_k, $k = 1, \ldots, n$ (the values of the function f and its derivatives in the cases of rules with multiple nodes). Such quadratures will be called the *standard quadrature formulae*. However, in many cases in physics and technics it is not possible to measure the exact value of the function f at points x_k, so that a standard quadrature cannot be applied. On the other side, some other information on f can be available, as

1° the averages

$$\frac{1}{2h_k} \int_{I_k} f(x)\, dx$$

of this function over some non-overlapping subintervals I_k, with length of I_k equals $2h_k$, and their union which is a proper subset of $\operatorname{supp}(d\mu)$;

2° a fixed linear combination of the function values, e.g.

$$af(x-h) + bf(x) + cf(x+h)$$

at some points x_k, where a, b, c are constants and h is sufficiently small positive number, etc.

The last example is gained from communications. Namely, supposing that we are receiving a signal with an interference, then the measurements provide linear combinations of the function values rather than single function values. In another words, for signals (functions) which depend on time in a discrete sense, averaging can be given with respect to a discrete measure, with some jumps at $x_k - h$, x_k, $x_k + h$, in our simple example. The same problem appears when a signal f passes through a digital filter.

Suppose now that we want to find the value of the integral of the signal f with respect to some positive measure μ, i.e., to calculate $\int_{\mathbb{R}} f(x)\,d\mu(x)$, and that we know only values of the signal after passing through some digital filter, i.e., we know the values $g_k = af(x_k - h) + bf(x_k) + cf(x_k + h)$, $k = 1, \ldots, n$.

In this very simple example, using the initial conditions, in general, we can state a system of linear equations and calculate the values $f(x_k)$ from the values g_k, and then we apply the quadrature rule. Unfortunately, very often the system of linear equations is ill-conditioned and such a procedure significantly disturbs the final result of computations. Therefore, it is much better to use directly the values g_k instead of $f(x_k)$ if it is possible. This idea leads to the so-called *nonstandard quadratures* (see [67]).

Thus, if the information data $\{f(x_k)\}_{k=1}^n$ in the standard quadrature is replaced by $\{(\mathcal{A}^{h_k} f)(x_k)\}_{k=1}^n$, where $\mathcal{A}^h$ is an extension of some linear operator $\mathcal{A}^h : \mathcal{P} \to \mathcal{P}$, $h \geq 0$, we get a non-standard quadrature formula

$$\int_{\mathbb{R}} f(x)\,d\mu(x) = \sum_{k=1}^{n} w_k(\mathcal{A}^{h_k} f)(x_k) + R_n(f). \tag{20}$$

This kind of quadratures is based on operator values for a general family of linear operators $\mathcal{A}^h$, acting of the space of algebraic polynomials, such that the degrees of polynomials are preserved.

As a typical example for such operators is the *average* (*Steklov*) *operator* mentioned before in 1°, i.e.,

$$(\mathcal{A}^h p)(x) = \frac{1}{2h} \int_{x-h}^{x+h} p(x)\,dx, \qquad h > 0,\ p \in \mathcal{P}. \tag{21}$$

The first idea on so-called *interval quadratures*, which are an example of non-standard quadrature rules, appeared a few decades ago. In 1976 Omladič, Pahor and Suhadolc [78] considered quadratures with the average operator (21) (see also Pitnauer and Reimer [80]). Some further investigations were given by Kuz'mina [48], Sharipov [82], Babenko [1], and Motornyi [76].

Let $h_1, \ldots, h_n$ be nonnegative numbers such that

$$a < x_1 - h_1 \leq x_1 + h_1 < x_2 - h_2 \leq x_2 + h_2 < \cdots < x_n - h_n \leq x_n + h_n < b, \tag{22}$$

and let $w(x)$ be a given weight function on $[a, b]$. Using the previous inequalities it is obvious that we have $2(h_1 + \cdots + h_n) < b - a$.

Recently, Bojanov and Petrov [5] proved that the Gaussian interval quadrature rule of the maximal algebraic degree of exactness $2n-1$ exists, i.e.,

$$\int_a^b f(x)w(x)\,dx = \sum_{k=1}^{n} \frac{w_k}{2h_k} \int_{x_k-h_k}^{x_k+h_k} f(x)w(x)\,dx + R_n(f), \tag{23}$$

where $R_n(f) = 0$ for each $f \in \mathcal{P}_{2n-1}$. Under conditions $h_k = h$, $1 \le k \le n$, they also proved the uniqueness of (23). Moreover, in [6] Bojanov and Petrov proved the uniqueness of (23) for the Legendre weight ($w(x) = 1$) for any set of lengths $h_k \ge 0$, $k = 1, \ldots, n$, satisfying the condition (22). The question of the existence for bounded $[a, b]$ is proved in [5] in much broader context for a given Chebyshev system of functions.

Recently in [60], using properties of the topological degree of non-linear mappings, it was proved that Gaussian interval quadrature formula is unique for the Jacobi weight function $w(x) = (1-x)^\alpha(1+x)^\beta$, $\alpha, \beta > -1$, on $[-1, 1]$ and an algorithm for numerical construction was proposed. For the special case of the Chebyshev weight of the first kind and the special set of lengths an analytic solution can be given ([60]). Interval quadrature rules of Gauss-Radau and Gauss-Lobatto type with respect to the Jacobi weight functions are considered in [**?**].

Recently, Bojanov and Petrov [7] proved the existence and uniqueness of the weighted Gaussian interval quadrature formula for a given system of continuously differentiable functions, which constitute an ET system of order two on $[a, b]$.

The cases with interval quadratures on unbounded intervals with the classical generalized Laguerre and Hermite weights have been recently investigated by Milovanović and Cvetković in [63] and [66].

In meantime we considered the nonstandard quadratures (20) with some special operators of the form (see [67])

$$(\mathcal{A}^h p)(x) = \frac{1}{2h} \int_{x-h}^{x+h} p(t)\,dt,$$

$$(\mathcal{A}^h p)(x) = \sum_{k=-m}^{m} a_k p(x+kh) \quad \text{or} \quad (\mathcal{A}^h p)(x) = \sum_{k=-m}^{m-1} a_k p\left(x + (k+\frac{1}{2})h\right),$$

and

$$(\mathcal{A}^h p)(x) = \sum_{k=0}^{m} \frac{b_k h^k}{k!} \mathcal{D}^k p(x),$$

where m is a fixed natural number and $\mathcal{D}^k = d^k/dx^k$, $k \in \mathbb{N}_0$.

7. *Gaussian quadrature for Müntz systems*

Gaussian integration can be extended in a natural way to non-polynomial functions, taking a system of linearly independent functions

$$\{P_0(x), P_1(x), P_2(x), \ldots\} \qquad (x \in [a,b]), \tag{24}$$

usually chosen to be complete in some suitable space of functions. If $d\sigma(x)$ is a given nonnegative measure on $[a,b]$ and the quadrature rule

$$\int_a^b f(x)d\sigma(x) = \sum_{k=1}^{n} A_k f(x_k) + R_n(f) \tag{25}$$

is such that it integrates exactly the first $2n$ functions in (24), we call the rule (25) *Gaussian with respect to the system* (24). The existence and uniqueness of a Gaussian quadrature rule (25) with respect to the system (24), or shorter a *generalized Gaussian formula*, is always guaranteed if the first $2n$ functions of this system constitute a Chebyshev system on $[a,b]$. Then, all the weights $A_1, \ldots, A_n$ in (25) are positive. In the terms of moment spaces, the Gaussian rule corresponds to the unique *lower principal representation* of the measure $d\sigma(x)$ (see Karlin and Studden [46]).

The generalized Gaussian quadratures for Müntz systems goes back to Stieltjes [97] in 1884. Taking $P_k(x) = x^{\lambda_k}$ on $[a,b] = [0,1]$, where $0 \le \lambda_0 < \lambda_1 < \cdots$, Stieltjes showed the existence of Gaussian formulae. In his short note he considered also Gauss-Radau formulae.

A numerical algorithm for constructing the generalized Gaussian quadratures was recently investigated by Ma, Rokhlin and Wandzura [52]. They take a Chebyshev system of functions $\{P_0, P_1, \ldots, P_{2n-1}\}$ on $[a,b]$ with certain additional properties (Extended Hermite (EH) system). Their procedure requires the construction of the functions

$$\xi_i(x) = \sum_{j=1}^{2n} \alpha_{ij} P_{j-1}(x), \qquad \eta_i(x) = \sum_{j=1}^{2n} \beta_{ij} P_{j-1}(x) \qquad (i = 1, \ldots, n), \tag{26}$$

such that

$$\begin{cases} \xi_i(x_k) = 0, \\ \xi_i'(x_k) = \delta_{ik}, \end{cases} \qquad \begin{cases} \eta_i(x_k) = \delta_{ik}, \\ \eta_i'(x_k) = 0, \end{cases} \tag{27}$$

for all $i = 1, \ldots, n$ and all $k = 1, \ldots, n$. The algorithm is ill conditioned (see [52, Remark 6.2]). In order to obtain the double precision results (REAL*8),

the authors have performed the computations in extended precision (Q-arithmetic – REAL*16) for generating Gaussian quadratures up to order 20, and in MATHEMATICA (120 digits operations) for generating Gaussian quadratures of higher orders ($n \leq 40$). In particular, they considered the following important cases of EH systems:

$$\{1, \log x, x, x \log x, \ldots, x^{n-1}, x^{n-1} \log x\} \tag{28}$$

and

$$\{1, x^s, x, x^{s+1}, \ldots, x^{n-1}, x^{s+n-1}\} \tag{29}$$

for $s = 1/3$, $s = -1/3$, $s = -2/3$.

In [64], Milovanović and Cvetković presented an alternatively numerical method for constructing the generalized Gaussian quadrature (25) for Müntz polynomials, which is exact for each

$$f \in M_{2n-1}(\Lambda) = \operatorname{span}\{x^{\lambda_0}, x^{\lambda_1}, \ldots, x^{\lambda_{2n-1}}\}.$$

Beside the properties of orthogonal Müntz polynomials on $(0, 1)$ and their connection with orthogonal rational functions, we gave also a method for numerical evaluation of such generalized polynomials (see [58]). Our method is rather stable and simpler than the previous one, since it is based on orthogonal Müntz systems. It performs calculations in double precision arithmetics in order to get double precision results.

As it is well-known the Gaussian quadrature rule is unique provided the measure σ has nonnegative absolutely continuous part and has finitely many atoms on $[0, 1]$. Such quadratures possess several properties of the classical Gaussian formulae (for polynomial systems), such as positivity of the weights, rapid convergence, etc. They can be applied to the wide class of functions, including smooth functions, as well as functions with end-point singularities, such as those appeared in the boundary-contact value problems, integral equations, complex analysis, potential theory, and several other fields (see [52]).

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