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Construction and applications of Gaussian quadratures with nonclassical and exotic weight functions

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Abstract. In 1814 Carl Friedrich Gauß (1777–1855) developed his famous method of numerical integration which dramatically improves the earlier method of Isaac Newton (1643–1727) from 1676. Beside the some historical details in this survey, a formulation of this classical theory in modern terminology using theory of orthogonlity on real line, as well as the characterization, existence and uniqueness of these formulas, are presented. A special attention is devoted to the algorithms for constructing such quadrature formulas for nonclassical weight functions, their numerical stability and the corresponding software. Finally, some recent progress in this subject, as well as new important applications of these methods in several different directions (distributions in statistics and physics, summation of slowly convergent series, etc.) are presented.

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1. Introduction

Let $\mathcal{P}_n$ be the set of all algebraic polynomials of degree at most n, $\mathcal{P}$ be the set of all algebraic polynomials, and $\mathrm{d}\mu$ be a finite positive Borel measure on the real line $\mathbb{R}$ such that its support $\operatorname{supp}(\mathrm{d}\mu)$ is an infinite set, and all its moments $\mu_k = \int_{\mathbb{R}} t^k \,\mathrm{d}\mu$, $k = 0, 1, \ldots$, exist and are finite.

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The n-point quadrature formula

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\mu(t) = \sum_{k=1}^{n} A_k f(\tau_k) + R_n(f), \tag{1.1}$$

which is exact on the set $\mathcal{P}_{2n-1}$ ($R_n(\mathcal{P}_{2n-1}) = 0$) is known as the *Gauss-Christofell quadrature formula* (cf. [10, p. 29], [14, p. 324]). It is a quadrature formula of the maximal algebraic degree of exactness $d_{\max} = 2n - 1$. First formula of this type

$$\int_{0}^{1} f(t)\,\mathrm{d}t = \sum_{k=1}^{n} A_k f(\tau_k) + R_n(f), \tag{1.2}$$

was descovered by Carl Friedrich Gauss two centuries ago.

In this survey paper we give an account on this kind of quadrature rules and several their new applications. The paper is organized as follows. Starting with the famous idea of Gauss and some historical details, in Section 2 we give its formulation in modern terminology and a connection with orthogonal polynomials. Section 3 is devoted to constructive theory of orthogonal polynomials. Numerical construction of Gaussian quadratures with respect to strong non-classical weights and some exotic weight functions, as well as several applications of such rules in approximation theory, statistics, and summation of slowly convergent series are studied in Section 4. Special attention is paid to available software, which is based on recent progress in symbolic computation and variable precision arithmetic.

2. Two centuries of Gaussian rules

After Newton formula of numerical integration from 1676 (known as Newton-Cotes rules),

$$\int_{a}^{b} f(t)\,\mathrm{d}t \approx Q_n(f) = \sum_{k=1}^{n} A_k f(\tau_k), \tag{2.1}$$

obtained by an integration of the corresponding interpolation polynomal of $f(t)$ at n different fixed points (nodes), $\tau_1, \ldots, \tau_n$ (usually selected equidistantly on $[a,b]$), Gauss in 1814 developed his famous method [4][1], which dramatically improves the previous Newton method. While Newton-Cotes formula exact only for polynomials of degree at most $n-1$, Gauss' question was what is the maximum degree of exactness that can be achieved in (2.1) (i.e., in (1.2) supposing that $[a,b] = [0,1]$) if the nodes $\tau_1, \ldots, \tau_n$ are free.

Since in the quadrature sum

$$Q_n(f) = \sum_{k=1}^{n} A_k f(\tau_k)$$

there are $2n$ unknowns parameters: τ_k, A_k, $k = 1, \ldots, n$, Gauss started with the conjecture that the quadrature formula (1.2) could be exact for all algebraic polynomials of degree at most $2n-1$. Starting from the work of Newton and Cotes and using only

[1]Gauss submitted his manuscript on September 16, 1814.

his own result on continued fractions associated with hypergeometric series, Gauss proved this result. It is interesting to mention that Gauss determined numerical values of quadrature parameters, the nodes τ_k and the weights A_k, $k = 1, \ldots, n$, for all $n \le 7$, with almost 16 significant decimal digits[2]. This discovery was 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 these formulas was provided by Jacobi [13], and furher contributions by Mehler, Radau, Heine, etc. A significant generalization to arbitrary measures was given by Christoffel (see a nice survey of Gauss-Christoffel quadrature formulae written by Gautschi [6]). The error term and convergence were proved by Markov and Stieltjes, respectively. It was only in 1928 Uspensky gave the first proof for the convergence of Gaussian formula on unbounded intervals with the classical measures of Laguerre and Hermite.

As we mentioned in Section 1, these formulae with maximal degree of precision are known today as the Gauss-Christoffel quadrature formulae.

In modern terminology, the formulation of this classical theory can be given in the following form: *Let* $\mathrm{d}\mu(t)$ *is a positive measure on* $\mathbb{R}$ *with finite or unbounded support, for which all moments* $\mu_k = \int_{\mathbb{R}} t^k \,\mathrm{d}\mu(t)$ *exist and are finite, and* $\mu_0 > 0$. *Then, for each* $n \in \mathbb{N}$, *there exists the* n*-point Gauss-Christoffel quadrature formula* (1.1) *which is exact for all algebraic polynomials of degree* $\le 2n-1$, *i.e.,* $R_n(f) = 0$ *for each* $f \in \mathcal{P}_{2n-1}$.

The Gauss–Christoffel quadrature formula (1.1) 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

$$(p,q) = \int_{\mathbb{R}} p(t)q(t)\,\mathrm{d}\mu(t) \quad (p,q \in \mathcal{P}). \tag{2.2}$$

Therefore, orthogonal polynomials play an important role in the analysis and construction of quadrature formulas of the maximal, or nearly maximal, algebraic degree of exactness (cf. [10], [14], [9], [19]). The inner product (2.2) gives rise to a unique system of monic orthogonal polynomials $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,;\,\mathrm{d}\mu)$, such that

$$\pi_k(t) \equiv \pi_k(\,\mathrm{d}\mu; t) = t^k + \text{terms of lower degree}, \quad k = 0, 1, \ldots, \tag{2.3}$$

and

$$(\pi_k, \pi_n) = ||\pi_n||^2 \delta_{kn} = \begin{cases} 0, & n \ne k, \\ ||\pi_n||^2, & n = k. \end{cases}$$

The following theorem is due to Jacobi [13] (cf. [14, p. 297]).

Theorem 2.1. *Given a positive integer* m $(\le n)$, *the quadrature formula* (1.1) *has degree of exactness* $d = n - 1 + m$ *if and only if the following conditions are satisfied:*

1° *Formula* (1.1) *is interpolatory;*

2° *The node polynomial* $\omega_n(t) = (t-\tau_1)\cdots(t-\tau_n)$ *satisfies*

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

[2]Otherwise, τ_k, $k = 1, \ldots, n$, are zeros of the shifted Legendre polynomial $P_n(2x-1)$.

According to this theorem, the n-point quadrature formula (1.1) with respect to the positive measure $\mathrm{d}\mu(t)$ has the maximal algebraic degree of exactness $2n-1$, i.e., $m = n$ is optimal ($\omega_n = \pi_n$). 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.

2.1. *Fundamental three–term recurrence relation.* Because of the property $(tp, q) = (p, tq)$ of the inner product (2.2), the monic orthogonal polynomials (2.3) satisfy the three–term recurrence relation

$$\pi_{k+1}(t) = (t-\alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t), \quad k = 0, 1, 2\ldots, \tag{2.4}$$

with $\pi_0(t) = 1$ and $\pi_{-1}(t) = 0$, where $(\alpha_k) = (\alpha_k(\mathrm{d}\mu))$ and $(\beta_k) = (\beta_k(\mathrm{d}\mu))$ are sequences of recursion coefficients which depend on the measure $\mathrm{d}\mu$. The coefficient β_0 may be arbitrary, but is conveniently defined by $\beta_0 = \mu_0 = \int_{\mathbb{R}} \mathrm{d}\mu(t)$.

There are many reasons way the coefficients α_k and β_k in the three–term recurrence relation (2.4) are fundamental quantities in the constructive theory of orthogonal polynomials (for details see [7]).

First, α_k and β_k provide a compact way of representing and easily calculating orthogonal polynomials, their derivatives, and their linear combinations, requiring only a linear array of parameters.

The same recursion coefficients α_k and β_k appear in the *Jacobi continued fraction associated with the measure* $\mathrm{d}\mu$,

$$F(z) = \int_{\mathbb{R}} \frac{\mathrm{d}\mu(t)}{z-t} \sim \frac{\beta_0}{z-\alpha_0-}\,\frac{\beta_1}{z-\alpha_1-}\cdots,$$

which is known as the *Stieltjes transform* of the measure $\mathrm{d}\mu$ (for details see [10, p. 15], [14, p. 114]). For the n-th *convergent* of this continued fraction, it is easy to see that

$$\frac{\beta_0}{z-\alpha_0-}\,\frac{\beta_1}{z-\alpha_1-}\cdots\frac{\beta_{n-1}}{z-\alpha_{n-1}} = \frac{\sigma_n(z)}{\pi_n(z)}, \tag{2.5}$$

where σ_n are the so–called *associated polynomials*, defined by

$$\sigma_k(z) = \int_{\mathbb{R}} \frac{\pi_k(z) - \pi_k(t)}{z-t}\,\mathrm{d}\mu(t), \quad k \ge 0.$$

The associated polynomials satisfy the same fundamental relation (2.4), i.e.,

$$\sigma_{k+1}(z) = (z-\alpha_k)\sigma_k(z) - \beta_k\sigma_{k-1}(z), \quad k \ge 0,$$

only with starting values $\sigma_0(z) = 0$, $\sigma_{-1}(z) = -1$.

The function of the second kind,

$$\varrho_k(z) = \int_{\mathbb{R}} \frac{\pi_k(t)}{z-t}\,\mathrm{d}\mu(t), \quad k \ge 0,$$

where z is outside the spectrum of $\mathrm{d}\mu$, also satisfy the same three–term recurrence relation (2.4) and represent its *minimal solution*, normalized by $\varrho_{-1}(z) = 1$, as observed by Gautschi in [5].

It is easy to see that the rational function (2.5) has simple poles at the zeros $z=\tau_{n,k}$, $k=1,\dots,n$, of the polynomial $\pi_n(t)$. If by $\lambda_{n,k}$ we denote the corresponding residues of $\sigma_n(z)/\pi_n(z)$ at these poles, i.e.,

$$\lambda_{n,k}=\lim_{z\to\tau_{n,k}}(z-\tau_{n,k})\frac{\sigma_n(z)}{\pi_n(z)}=\frac{1}{\pi_n'(\tau_{n,k})}\int_{\mathbb{R}}\frac{\pi_n(t)}{t-\tau_{n,k}}\,\mathrm{d}\mu(t), \tag{2.6}$$

then for the continued fraction representation (2.5) we can get the following form

$$\frac{\sigma_n(z)}{\pi_n(z)}=\sum_{k=1}^{n}\frac{\lambda_{n,k}}{z-\tau_{n,k}}\,.$$

As we can see, the coefficients $\lambda_{n,k}$ are exactly the weight coefficients (Christoffel numbers) in the Gauss–Christoffel quadrature formula (1.1) and they can be expressed by the so–called Christoffel function $\lambda_n(\mathrm{d}\mu;t)$ (cf. [14, Chapters 2 & 5]) in the form

$$A_k=\lambda_n(\mathrm{d}\mu;\tau_k),\quad k=1,\dots,n,$$

and zeros of the polynomial $\pi_n(t)$ are the nodes of (1.1), i.e., $\tau_k=\tau_{n,k}$, $k=1,\dots,n$.

3. Constructive theory of orthogonal polynomials and quadratures

A classical approach in construction of Gauss-Christoffel quadrature rules is based on a computation of nodes by using Newton's method and then a direct application of some expressions derived from (2.6) for the weight coefficients (cf. Davis & Rabinowitz [3]).

However, a characterization of the Gaussian formula via an eigenvalue problem for one symmetric tridiagonal *Jacobi matrix*, of order n associated with the measure $\mathrm{d}\mu$,

$$J_n(\mathrm{d}\mu)=\begin{bmatrix}\alpha_0 & \sqrt{\beta_1} & & & \mathbf{O}\\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{n-1}}\\ \mathbf{O} & & & \sqrt{\beta_{n-1}} & \alpha_{n-1}\end{bmatrix}, \tag{3.1}$$

has become the basis of current methods for generating Gaussian quadratures. The most popular of them is the *Golub-Welsch procedure*, obtained by a simplification of QR algorithm, so that beside all eigenvalues only the first components of the eigenvectors are computed [12].

Theorem 3.1. *The nodes τ_k in the Gauss-Christoffel quadrature rule* (1.1) *are eigenvalues of the Jacobi matrix $J_n(\mathrm{d}\mu)$ given by* (3.1). *The weight coefficients A_k are given by*

$$A_k=\lambda_{n,k}=\beta_0 v_{k,1}^2,\quad k=1,\dots,n,$$

where $\beta_0=\mu_0=\int_{\mathbb{R}}\mathrm{d}\mu(t)$ and $v_{k,1}$ is the first component of the normalized eigenvector $\mathbf{v}_k$ $(=[v_{k,1}\ \dots\ v_{k,n}]^{\mathrm{T}})$ corresponding to the eigenvalue τ_k,

$$J_n(\mathrm{d}\mu)\mathbf{v}_k=\tau_k\mathbf{v}_k,\quad \mathbf{v}_k^{\mathrm{T}}\mathbf{v}_k=1,\quad k=1,\dots,n.$$

Therefore, if we know recursive coefficients α_k and β_k in the fundamental three-term recurrence relation (2.4), the problem of construction Gaussian rules can be easily solved by the Golub-Welsch procedure. This procedure is implemented in several packages including the most known `ORTPOL` given by Gautschi [8].

Unfortunately, the recursion coefficients are known explicitly only for some narrow classes of orthogonal polynomials, e.g. they are known for the so-called *very classical* orthogonal polynomials (Jacobi, the generalized Laguerre, and Hermite polynomials). Orthogonal polynomials for which the recursion coefficients are not known we call *strongly non–classical polynomials.* For these, if we know how to compute the first n recursion coefficients α_k and β_k, $k = 0, 1, \ldots, n-1$, then we can compute all orthogonal polynomials of degree at most n by a straightforward application of the three–term recurrence relation (2.4), construct the corresponding Gauss–Christoffel quadratures for any number of nodes less than or equal to n, etc.

An important progress for strongly non–classical measures was given by Walter Gautschi. In [7] he started with an arbitrary positive measure $\mathrm{d}\mu(t)$, which is given explicitly or implicitly via moment information, and considered the actual (numerical) construction of orthogonal polynomials as a basic computational problem: *For a given measure* $\mathrm{d}\mu$ *and for given* $n \in \mathbb{N}$, *generate the first coefficients* $\alpha_k(\mathrm{d}\mu)$ *and* $\beta_k(\mathrm{d}\mu)$, $k = 0, 1, \ldots, n-1$. In about two dozen papers, Gautschi developed the so–called *constructive theory of orthogonal polynomials on* $\mathbb{R}$, including effective algorithms for numerically generating orthogonal polynomials, a detailed stability analysis of such algorithms, the corresponding software implementation, etc. (cf. [8], [9], [10], [20], [21]).

Following [10] we mention here some basic facts in the constructive theory of orthogonal polynomials and Gaussian quadratures. We consider two tasks:

(a) *Construction of recursion coefficients* α_k, β_k, $k = 0, 1, \ldots, n-1$;

(b) *Construction of the Gauss-Christoffel quadrature* (1.1), i.e.,

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\mu(t) = \sum_{k=1}^{n} A_k f(\tau_k) + R_n(f). \tag{3.2}$$

The first construction (a) is, in fact, a map, in notation $\mathbf{K}_n : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$, of the first $2n$ moments to $2n$ recursive coefficients,

$$\boldsymbol{\mu} = (\mu_0, \mu_1, \ldots, \mu_{2n-1}) \;\mapsto\; \boldsymbol{\rho} = (\alpha_0, \ldots, \alpha_{n-1}, \beta_0, \ldots, \beta_{n-1}).$$

An important aspect in the numerical construction (a) is the sensitivity of this problem with respect to small perturbation in the data, i.e., perturbations in the first $2n$ moments μ_k, $k = 0, 1, \ldots, 2n-1$ (when we calculate coefficients for $k \le n-1$).

There is a simple algorithm, due to Chebyshev, which transforms the moments to desired recursion coefficients, but its viability is strictly dependent on the conditioning of this mapping. Usually it is severely ill conditioned so that these calculatios via moments, in finite precision on a computer, are quite ineffective, especially for measures on unbounded supports. The only salvation, in this case, is to either use symbolic computation, which however requires special resources and often is not possible, or else to use the explicit form of the measure. In the latter case, an appropriate discretization of the measure and subsequent approximation of the recursion coefficients is a viable alternative.

In his analysis, Gautschi introduced also another map $\mathbf{G}_n : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$, as a map of moments into the parameters of the Gauss-Christoffel quadrature (3.2),

$$\boldsymbol{\mu} = (\mu_0, \mu_1, \ldots, \mu_{2n-1}) \ \mapsto \ \boldsymbol{\gamma} = (A_1, \ldots, A_n, \tau_1, \ldots, \tau_n),$$

and represented it as a *composition* of two maps

$$\mathbf{K}_n = \mathbf{H}_n \circ \mathbf{G}_n,$$

where $\mathbf{H}_n : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ maps the Gaussian parameters into the recursion coefficients, $\boldsymbol{\gamma} \ \to \ \boldsymbol{\rho}$.

The map $\mathbf{H}_n$, as well as its inverse map $\mathbf{H}_n^{-1}$, are generally *well-conditioned*, and the condition of $\mathbf{K}_n$ is more or less the same as the condition of $\mathbf{G}_n$. Notice that an implementation of the map $\mathbf{H}_n^{-1}$ can be done by the Golub-Welsch procedure.

The map $\mathbf{G}_n$ is usually *ill-conditioned*, i.e., its condition number is much larger than one, $\operatorname{cond}\mathbf{G}_n \gg 1$. If the condition number is of order 10^m, it roughly means a loss of m decimal digits in results when the input data are perturbed by one units in the last digit. For example, if the working precision is d decimal digits, e.g., $d = 16$ and the condition number is 10^{14}, then results will be accurate to about $16 - 14 = 2$ digits!

The (absolute) condition number of the map $\mathbf{G}_n$ is defined as a norm of the Fréchet derivative of this map,

$$(\operatorname{cond}\mathbf{G}_n)(\boldsymbol{\mu}) = \left\| \frac{\partial \mathbf{G}_n(\boldsymbol{\mu})}{\partial \boldsymbol{\mu}} \right\|.$$

Otherwise, the Fréchet derivative is a linear transformation defined by the Jacobian matrix.

In order to determine $\operatorname{cond}\mathbf{G}_n$, Gautschi introduced the inverse map of $\mathbf{G}_n$ as $\mathbf{F}_n : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ ($\boldsymbol{\gamma} = (A_1, \ldots, A_n, \tau_1, \ldots, \tau_n) \to \boldsymbol{\mu}$), defined by

$$\mu_k = \sum_{\nu=1}^{n} A_\nu \tau_\nu^k, \quad k = 0, 1, \ldots, 2n-1. \tag{3.3}$$

In fact, (3.3) is a system of $2n$ non-linear equations obtained from (3.2) by taking $f(t) = t^k$, $k = 0, 1, \ldots, 2n-1$, for which the remainder term $R_n(f)$ is equal to zero. It is clear that

$$\frac{\partial \mathbf{G}_n(\boldsymbol{\mu})}{\partial \boldsymbol{\mu}} = \begin{bmatrix} \dfrac{\partial \mu_0}{\partial A_1} & \cdots & \dfrac{\partial \mu_0}{\partial A_n} & \dfrac{\partial \mu_0}{\partial \tau_1} & \cdots & \dfrac{\partial \mu_0}{\partial \tau_n} \\ \vdots & & & & & \\ \dfrac{\partial \mu_{2n-1}}{\partial A_1} & \cdots & \dfrac{\partial \mu_{2n-1}}{\partial A_n} & \dfrac{\partial \mu_{2n-1}}{\partial x\tau_1} & \cdots & \dfrac{\partial \mu_{2n-1}}{\partial \tau_n} \end{bmatrix} = \mathbf{T}\boldsymbol{\Lambda},$$

where $\mathbf{\Lambda} = \operatorname{diag}(1, \ldots, 1, A_1, \ldots, A_n)$ and $\mathbf{T}$ is a confluent Vandermonde matrix

$$\mathbf{T} = \begin{bmatrix} 1 & \cdots & 1 & 0 & \cdots & 0 \\ \tau_1 & \cdots & \tau_n & 1 & \cdots & 1 \\ \tau_1^2 & \cdots & \tau_n^2 & 2\tau_1 & \cdots & 2\tau_n \\ \vdots & & & & & \\ \tau_1^{2n-1} & \cdots & \tau_n^{2n-1} & (2n-1)\tau_1^{2n-1} & \cdots & (2n-1)\tau_n^{2n-1} \end{bmatrix}.$$

Since

$$\frac{\partial \mathbf{G}_n}{\partial \boldsymbol{\mu}} = \left(\frac{\partial \mathbf{F}_n}{\partial \boldsymbol{\gamma}}\right)^{-1} = \mathbf{\Lambda}^{-1}\mathbf{T}^{-1},$$

the following expression for calculating the condition number

$$(\operatorname{cond} \mathbf{G}_n)(\boldsymbol{\mu}) = \left\|\mathbf{\Lambda}^{-1}\mathbf{T}^{-1}\right\|$$

holds. Several estimates of $(\operatorname{cond} \mathbf{G}_n)(\boldsymbol{\mu})$ and examples for different measures can be found in [10]. As a rule, the conditional number grows exonentially fast with n (see Fig. 1).

Suppose that we have a numerical method for realizing the mapping $\mathbf{G}_n$ in an arithmetic with the working precision of d decimal digits. Then, the accuracy of results (here, the recursion coefficients α_k and β_k) depends on the working precision, but also on the condition number of this mapping. Roughly speaking, if we need the accuracy of ℓ decimal digits in results for each $k < n$, then the condition number $(\operatorname{cond} \mathbf{G}_n)$ must be less than 10^m, where $m = d - \ell$. For example, among the methods (A), (B), (C) (see Fig. 1), only the method (C) provides the required accuracy for a fixed $n = N$.

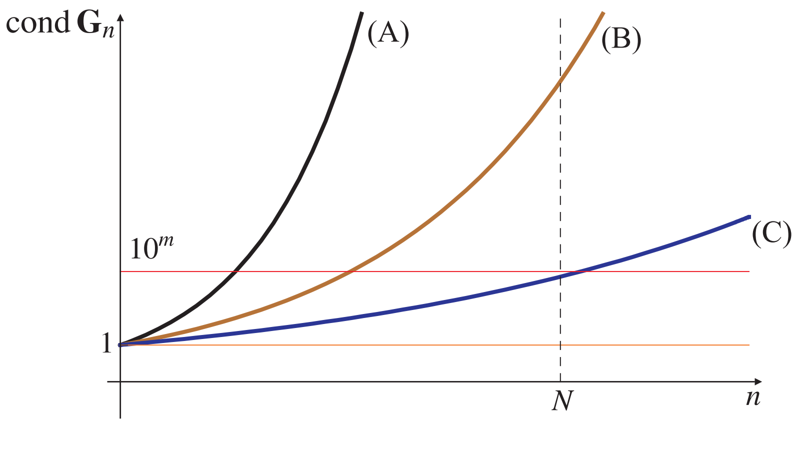

FIGURE 1. The condition number $\operatorname{cond} \mathbf{G}_n$ for three different methods of construction (A), (B) and (C)

There are three basic procedures for generating the recursion coefficients: (1) the *method of* (*modified*) *moments*, (2) the *discretized Stieltjes–Gautschi procedure*, (3) the *Lanczos algorithm*, and they play the central role in the constructive theory of orthogonal polynomials (cf. [7], [9], [10], [14]).

Recent progress in symbolic computation and variable-precision arithmetic now makes it possible to generate the recurrence coefficients α_k and β_k directly by using the original Chebyshev method of moments, but in a sufficiently high precision arithmetic, i.e., we should take the working precision to be $d = \ell + m$. Such an approach enables us to overcome the numerical instability!

Respectively symbolic/variable-precision software for orthogonal polynomials is available: Gautschi's package `SOPQ` in MATLAB and our MATHEMATICA package `OrthogonalPolynomials` (see [1] and [23]), which is downloadable from the web site `http://www.mi.sanu.ac.rs/~gvm/`.

All that is required is a procedure for symbolic calculation of the moments or their numerical calculation in variable-precision arithmetic. Details on applications this package to construction of recursive coefficients and parameters of Gaussian formulas will be done in the next section.

4. Construction of orthogonal polynomials and quadratures for some non-classical weights

4.1. Some distributions in physics

Bose-Einstein and Fermi-Dirac weights on $\mathbb{R}^+$ are defined by

$$\varepsilon(t) = \frac{t}{\mathrm{e}^t - 1} \quad \text{and} \quad \varphi(t) = \frac{1}{\mathrm{e}^t + 1}, \tag{4.1}$$

respectively. These functions and the corresponding quadratures are widely used in solid state physics, e.g., the total energy of thermal vibration of a crystal lattice can be expressed in the form $\int_0^{+\infty} f(t)\varepsilon(t)\,\mathrm{d}t$, where $f(t)$ is related to the phonon density of states. Integrals with $\varphi(t)$ are encountered in the dynamics of electrons in metals. Also, integrals of the previous type can be used for summation of slowly convergent series (see Section 5).

The moments of the functions (4.1) can be exactly calculated in terms of Riemann zeta function as

$$\mu_k(\varepsilon) = \int_0^{+\infty} \frac{t^{k+1}}{\mathrm{e}^t - 1}\,\mathrm{d}t = (k+1)!\zeta(k+2), \quad k \in \mathbb{N}_0,$$

and

$$\mu_k(\varphi) = \int_0^{+\infty} \frac{t^k}{\mathrm{e}^t + 1}\,\mathrm{d}t = \begin{cases} \log 2, & k = 0, \\ (1 - 2^{-k})k!\zeta(k+1), & k > 0, \end{cases}$$

respectively, and these moments are enough for constructing recursive coefficients in the corresponding three-term recurrence relations for orthogonal polynomials with respect to the weight functions (4.1).

For example, using our MATHEMATICA package `OrthogonalPolynomials` (see [1] and [23]) and executing the following commands (for Einstein's weight):

```
<< orthogonalPolynomials`
mEin =Table[(k+1)! Zeta[k+2], {k,0,100}];
{alE, beE} = aChebyshevAlgorithm[mEin, WorkingPrecision->55];
{alE1,beE1}=aChebyshevAlgorithm[mEin, WorkingPrecision -> 80];
N[Max[Abs[alE/alE1-1], Abs[beE/beE1-1]],3]
```

we obtain the first 50 recurrence coefficients with the maximal relative error 3.31×10^{-21}, using the working precision of 55 decimal digits. Notice that for calculating this maximal relative error in recursive coefficients we have to compute them with some better precision (in this case we used 80 decimal digits).

Now, we can calculate Gaussian parameters (nodes and weights) for each $n \leq 50$. For example, for $n = 10$ we have:

```
PGQ[n_] :=aGaussianNodesWeights[n,alE,beE,WorkingPrecision->25,
        Precision->20]
{n10, w10} = N[PGQ[10],20]

  {{0.17127645878001723630, 0.89167285640716281560,
    2.1546962419952769267, 3.9409621944320753085,
    6.2730549781202005837, 9.2198332084047489872,
    12.896129024261770678, 17.492620202296984539,
    23.375068766890757875, 31.480929908705477946},
   {0.40175819838719705508, 0.61781515020685988777,
    0.43092384916712431584, 0.16018318534772922234,
    0.031116001568317075487, 0.0030029502799063140584,
    0.00013244003563186081692, 2.2807340153227672644*10^-6,
    1.1114755872888526597*10^-8,6.6895094339315858173*10^-12}}
```

For details see [11], [20], [23].

4.2. Exotic exponential weights on $\mathbb{R}^+$

In this subsection we mention only the weight function of the form $w(t) = w^{(\alpha,\beta)}(x) = \exp(-t^{-\alpha} - t^{\beta})$ on $\mathbb{R}^+$, with parameters $\alpha > 0$ and $\beta > 1$.

In a simpler case when $\alpha = \beta$, we can determine the moments in an analytic form as

$$\mu_k^{(\beta,\beta)} = \int_0^{+\infty} t^k w^{(\beta,\beta)}(t)\,\mathrm{d}t = \frac{2}{\beta} K_{(k+1)/\beta}(2), \quad k \in \mathbb{N}_0, \tag{4.2}$$

where $K_r(z)$ is the modified Bessel function of the second kind.

The general case $w(t) = w^{(\alpha,\beta)}(x)$, $\alpha \neq \beta$, can be solved by the the so-called Meijer G function

$$G_{p,q}^{m,n}\left(z \,\middle|\, \begin{matrix} a_1,\ldots,a_p \\ b_1,\ldots,b_q \end{matrix}\right) \equiv G_{p,q}^{m,n}\left(z \,\middle|\, \begin{matrix} a_1,\ldots,a_n; a_{n+1},\ldots,a_p \\ b_1,\ldots,b_m; b_{m+1},\ldots,b_q \end{matrix}\right)$$

$$= \frac{1}{2\pi \mathrm{i}} \int_L \frac{\prod\limits_{\nu=1}^{m} \Gamma(b_\nu - s) \prod\limits_{\nu=1}^{n} \Gamma(1 - a_\nu + s)}{\prod\limits_{\nu=m+1}^{q} \Gamma(1 - b_\nu + s) \prod\limits_{\nu=n+1}^{p} \Gamma(a_\nu - s)} z^s \,\mathrm{d}s.$$

For some specific values of α i β we have (see [15])

$$\begin{aligned}
\mu_k^{(1,2)} &= \frac{1}{2^{k+2}\sqrt{\pi}}\, G_{2,4}^{3,1}\left(\frac{1}{4}\,\middle|\, \begin{matrix} -\,;\,- \\ -\frac{k+1}{2}, -\frac{k}{2}, 0; - \end{matrix}\right), \quad k \ge 0; \\
\mu_k^{(2,1)} &= \frac{2^k}{\sqrt{\pi}}\, G_{2,4}^{3,1}\left(\frac{1}{4}\,\middle|\, \begin{matrix} -\,;\,- \\ 0, \frac{k+1}{2}, \frac{k+2}{2}; - \end{matrix}\right), \qquad k \ge 0; \\
\mu_k^{(1,3)} &= \frac{1}{2\cdot 3^{k+3/2}\pi}\, G_{2,5}^{4,1}\left(\frac{1}{27}\,\middle|\, \begin{matrix} -\,;\,- \\ -\frac{k+1}{3}, -\frac{k}{3}, -\frac{k-1}{3}, 0; - \end{matrix}\right), \quad k \ge 0.
\end{aligned}$$

As an example we take $\alpha = \beta = 2$. In order to generate quadratures, for example, for $m \le n = 100$, we need the first two hundred moments $\mu_k^{(2,2)}$, given by (4.2). Using the Mathematica package `OrthogonalPolynomials`, with the following commands

```
<< orthogonalPolynomials`
mom = Table[BesselK[(k+1)/2, 2], {k,0,200}];
{al,be} = aChebyshevAlgorithm[mom, WorkingPrecision -> 120];
{al1,be1} = aChebyshevAlgorithm[mom, WorkingPrecision -> 140];
N[Max[Abs[al/al1 - 1], Abs[be/be1 - 1]], 3]
```

we obtain the first 100 recursive coefficients with relative errors less than 2.21×10^{-23}. As we can see, the calculation of the recursive coefficients in this case is a very sensitive process, which here, in the worst case, causes a loss of about 98 decimal digits!

The corresponding Gaussian quadrature formulas have an application in integration of functions which can *increase exponentially* at the endpoints 0 and $+\infty$. For the so-called "truncated" Gaussian quadratures the stability and convergence with the order of the best polynomial approximation in suitable function spaces are proved in [15].

4.3. Some distribution in statistics

Following Stoyanov [26, §7.1] we give an example with the inverse Gaussian distribution (IG) with "easy" parameters, say $(1, 1)$. Thus, we consider a random variable $\theta \sim \mathrm{IG}$, with density function

$$w_1(x) = \begin{cases} \dfrac{\mathrm{e}}{\sqrt{2\pi}}\, x^{-3/2} \exp\Big[-\dfrac{1}{2}\Big(x + \dfrac{1}{x}\Big)\Big], & \text{if } \ x > 0, \\ 0, & \text{if } \ x \le 0. \end{cases}$$

In terms of the modified Bessel function of the second kind, we have its moments as

$$\mu_k^{(1)} = \int_0^{+\infty} x^k w_1(x)\,\mathrm{d}x = \mathrm{e}\sqrt{\frac{2}{\pi}}\, K_{k-1/2}(1), \quad k \in \mathbb{N}_0.$$

Now, taking `WorkingPrecision -> WP` (WP=50) in the package `OrthogonalPolynomials`, we can obtain the first 50 recurrence coefficients for orthogonal polynomials with respect to this weight function $w_1(x)$, with the maximal relative error 1.88×10^{-25}.

If we consider a power transformation of θ, i.e., θ^r for a real r, for example $r = 3$, the density function of the random variable $X = \theta^3$ is given by (see [26, §7.1])

$$w_3(x) := \begin{cases} \dfrac{\mathrm{e}}{3\sqrt{2\pi}}\, x^{-7/6} \exp\Big[-\dfrac{1}{2}\Big(x^{1/3} + \dfrac{1}{x^{1/3}}\Big)\Big], & \text{if } x > 0, \\ 0, & \text{if } x \le 0, \end{cases}$$

and its moments are

$$\mu_k^{(3)} = \int_0^{+\infty} x^k w_3(x)\,\mathrm{d}x = \mathrm{e}\sqrt{\frac{2}{\pi}}\, K_{3k-1/2}(1), \quad k \in \mathbb{N}_0.$$

Now, the construction problem is slightly better conditioned. Namely, in this case in order to obtain the first 50 recurrence coefficients with a similar maximal relative error (3.84×10^{-26}) we need only WP=35, i.e, 15 digits less!

Graphs of previous weight functions w_1 and w_3 are displayed in Fig. 2.

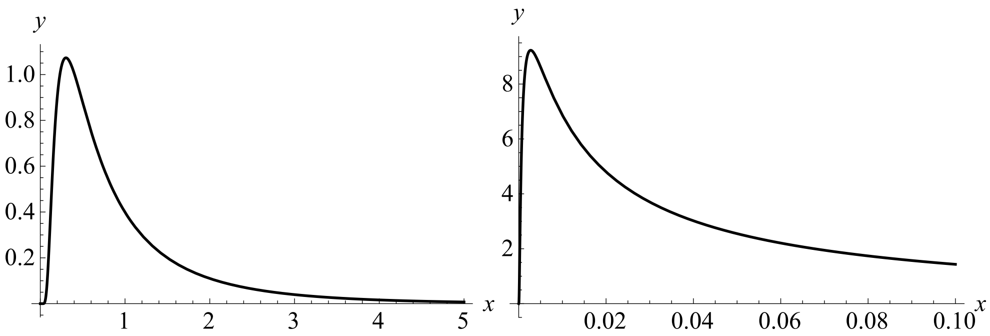

FIGURE 2. Graphs of $x \mapsto w_1(x)$ (left) and $\mapsto w_3(x)$ (right)

In order to calculate the following integral

$$\int_{\mathbb{R}} w_1(x) \cos x \,\mathrm{d}x = 0.5382958183103370411157777\ldots,$$

we apply n-point Gaussian quadratures obtained for each $n \le 50$ by the following commands

```
<< orthogonalPolynomials`
 f[x_] := Cos[x]; exact = 0.5382958183103370411157777;
 mom=Table[Exp[1] Sqrt[2/Pi] BesselK[k-1/2, 1], {k,0,99}];
 {alB,beB}=aChebyshevAlgorithm[mom, WorkingPrecision -> 50];
 PQ[n_] :=aGaussianNodesWeights[n, alB, beB,
           WorkingPrecision -> 25,Precision -> 20];
 ss = Table[N[PQ[n][[2]].f[PQ[n][[1]]], 20], {n,5,50,5}];
 err = Table[N[Abs[ss[[k]]/exact - 1], 3], {k, 1, 10}];
```

Gaussian approximations $Q_n(f;w_1)$ and the corresponding relative errors $\mathrm{err}(n)$ for $n=5(5)50$ are presented in Table 1. Numbers in parenthesis indicate the decimal exponents.

TABLE 1. Gaussian approximations $Q_n(f;w_1)$ and relative errors for $f(x)=\cos x$

n	$Q_n(f;w_1)$	err(n)
5	0.54279156780936401515	8.35(−3)
10	0.53844179972070903368	2.71(−4)
15	0.53829287281685621212	5.47(−6)
20	0.53829574913263199781	1.29(−7)
25	0.53829582036400719491	3.82(−9)
30	0.53829581835353617306	8.03(−11)
35	0.53829581830877861990	2.90(−12)
40	0.53829581831030650190	5.67(−14)
45	0.53829581831033828714	2.31(−15)
50	0.53829581831033706428	4.30(−17)

In this subsection we also mention a few distribution for which, using the MATHEMATICA package `OrthogonalPolynomials`, we can get the recursion coefficients for $k\le n$ in a symbolic form, where n is a finite number. Assuming these expressions as hypothesis, in some cases we can prove the analytic expressions for recurrence coefficients.

First, we consider the Stieltjes-Wigert weight function

$$w(x):=\begin{cases}\dfrac{1}{\sqrt{2\pi}\sigma x}\exp\Big[-\dfrac{\log^2(x)}{2\sigma^2}\Big], & \text{if } \ x>0,\\ 0, & \text{if } \ x\le 0,\end{cases}$$

for which the moments are given by

$$\mu_k=\int_0^{+\infty}x^k w(x)\,\mathrm{d}x=q^{k^2/2},\quad k\in\mathbb{N}_0\quad (q=\mathrm{e}^{\sigma^2}).$$

In this case, executing the following commands

```
<< orthogonalPolynomials`
mom = Table[q^(k^2/2), {k, 0, 39}];
{al, be} = aChebyshevAlgorithm[mom, Algorithm -> Symbolic]
```

we can obtain the first twenty coefficients in the three-term recurrence relation in an analytic form, and then prove that

$$\alpha_k=q^{k-1/2}\big(q^{k+1}+q^k-1\big);\quad \beta_0=1,\ \beta_k=q^{3k-2}\big(q^k-1\big),\quad k=0,1,\dots\ .$$

Similarly, for the weight function on $\mathbb{R}$ given by

$$w(x)=\frac{x^2\mathrm{e}^{-\pi x}}{(1-\mathrm{e}^{-\pi x})^2}=\Big(\frac{x}{2\sinh(\pi x/2)}\Big)^2=\frac{1}{4}[w^A(x/2)]^2,$$

where $w^A(x)$ is the Abel weight on $\mathbb{R}$ (see [14, p. 159]), we can determine the moments in terms of Bernoulli numbers

$$\mu_k = \begin{cases} 0, & k \text{ is odd}, \\ (-1)^{k/2} 2^{k+2} \dfrac{B_{k+2}}{\pi}, & k \text{ is even}. \end{cases}$$

Using the package package `OrthogonalPolynomials`, for the corresponding sequence $\{\beta_k\}_{k\geq 0}$ we obtain (see [22])

$$\left\{ \frac{2}{3\pi}, \frac{4}{5}, \frac{72}{35}, \frac{80}{21}, \frac{200}{33}, \frac{1260}{143}, \frac{784}{65}, \frac{1344}{85}, \frac{6480}{323}, \frac{3300}{133}, \frac{4840}{161}, \frac{20592}{575}, \frac{9464}{225}, \dots \right\}.$$

After some experiments, we conjectured and proved that

$$\beta_0 = \mu_0 = \frac{2}{3\pi}, \quad \beta_k = \frac{k(k+1)^2(k+2)}{(2k+1)(2k+3)}, \quad k \in \mathbb{N}.$$

Finally, for the weight function on $\mathbb{R}$, given by

$$w(x) = x^2 \frac{e^{\pi x/2} + e^{-\pi x/2}}{(e^{\pi x/2} - e^{-\pi x/2})^2} = 2\cosh\frac{\pi x}{2}\Big(\frac{x}{2\sinh(\pi x/2)}\Big)^2,$$

we get the moments (cf. [22])

$$\mu_k = \begin{cases} 0, & k \text{ is odd}, \\ \dfrac{2^{k+3}}{\pi}(2^{k+2}-1)|B_{k+2}|, & k \text{ is even}. \end{cases}$$

In this case we have that

$$\beta_0 = \mu_0 = \frac{4}{\pi}, \quad \beta_k = \begin{cases} (k+1)^2, & k \text{ is odd}, \\ k(k+2), & k \text{ is even}. \end{cases}$$

5. Summation of slowly convergent series

There are many methods for fast summation of slowly convergent series. In this section we consider only the so-called *summation/integration* procedures. The basic idea in such procedures is to transform the sum to an integral with respect to some weight function on $\mathbb{R}$ (or $\mathbb{R}_+$), and then to approximate this integral by a finite quadrature sum,

$$\sum_{k=1}^{+\infty} (\pm 1)^k f(k) = \int_{\mathbb{R}} g(x) w(x)\, dx \approx \sum_{\nu=1}^{N} A_\nu g(x_\nu),$$

where the function g is connected with f in some way. Thus, these procedures need two steps:

(a) Methods of transformation $\sum \Rightarrow \int$;

(b) Construction of Gaussian quadratures

$$\int_{\mathbb{R}} g(x) w(x)\, dx = \sum_{\nu=1}^{N} A_\nu g(x_\nu) + R_n(f),$$

where w is a *non-classical* weight.

5.1. Laplace transformation method

In this subsection we mention only the basic idea of the *Laplace transform method.*

Suppose that the general term of series is expressible in terms of the Laplace transform, or its derivative, of a known function.

Let $f(s) = \int_0^{+\infty} \mathrm{e}^{-st} g(t)\,\mathrm{d}t$, $\operatorname{Re} s \geq 1$. Then

$$T = \sum_{k=1}^{+\infty} f(k) = \sum_{k=1}^{+\infty} \int_0^{+\infty} \mathrm{e}^{-kt} g(t)\,\mathrm{d}t = \int_0^{+\infty} \left(\sum_{k=1}^{+\infty} \mathrm{e}^{-kt} \right) g(t)\,\mathrm{d}t,$$

i.e.,

$$T = \int_0^{+\infty} \frac{\mathrm{e}^{-t}}{1-\mathrm{e}^{-t}}\, g(t)\,\mathrm{d}t = \int_0^{+\infty} \frac{t}{\mathrm{e}^t - 1} \frac{g(t)}{t}\,\mathrm{d}t.$$

Thus, the *summation of series* is now transformed to an *integration problem* with respect to the Bose-Einstein weight function $\varepsilon(t) = t/(\mathrm{e}^t - 1)$ on $\mathbb{R}^+$, which is considered in Subsection 4.1.

Similarly, for "alternating" series, we have

$$S = \sum_{k=1}^{+\infty} (-1)^k f(k) = \int_0^{+\infty} \frac{1}{\mathrm{e}^t + 1} (-g(t))\,\mathrm{d}t, \tag{5.1}$$

where the Fermi-Dirac weight function on $\mathbb{R}^+$, $\varphi(t) = 1/(\mathrm{e}^t + 1)$, is appeared on the right-hand side in (5.1).

For details and examples see [11], [18], [22].

5.2. Hyperbolic weight functions and $\sum \Rightarrow \int$ transformation

In this subsection we consider an alternative summation/integration procedure for the series

$$T_{m,n} = \sum_{k=m}^{n} f(k) \quad \text{and} \quad S_{m,n} = \sum_{k=m}^{n} (-1)^k f(k), \tag{5.2}$$

where $m, n \in \mathbb{Z}$ $(m < n \leq +\infty)$ and the function f is holomorphic in the region

$$\big\{ z \in \mathbb{C} \;\big|\; \operatorname{Re} z \geq \alpha,\; m-1 < \alpha < m \big\}. \tag{5.3}$$

Our method of transformation "sum" to "integral" requires the indefinite integral F of f chosen so as to satisfy the following decay properties (see [16], [14]),

(C1) *F is a holomorphic function in the region* (5.3);

(C2) $\displaystyle\lim_{|t| \to +\infty} \mathrm{e}^{-c|t|} F(x + \mathrm{i}t/\pi) = 0$, *uniformly for* $x \geq \alpha$;

(C3) $\displaystyle\lim_{x \to +\infty} \int_{\mathbb{R}} \mathrm{e}^{-c|t|} \left| F(x + \mathrm{i}t/\pi) \right| \mathrm{d}t = 0$,

where $c = 2$ or $c = 1$, when we consider $T_{m,n}$ or $S_{n,m}$, respectively.

Let $m - 1 < \alpha < m$, $n < \beta < n + 1$, $\delta > 0$, and

$$G = \left\{ z \in \mathbb{C} \,:\, \alpha \leq \operatorname{Re} z \leq \beta,\; |\operatorname{Im} z| \leq \frac{\delta}{\pi} \right\}.$$

Using contour integration of a product of functions $z \mapsto f(z)g(z)$ over the rectangle $\Gamma = \partial G$ in the complex plane, where $g(z) = \pi/\tan\pi z$ and $g(z) = \pi/\sin\pi z$, by Cauchy's residue theorem, we obtain

$$T_{m,n} = \frac{1}{2\pi \mathrm{i}} \oint_\Gamma f(z) \frac{\pi}{\tan\pi z}\,\mathrm{d}z \quad \text{and} \quad S_{m,n} = \frac{1}{2\pi \mathrm{i}} \oint_\Gamma f(z) \frac{\pi}{\sin\pi z}\,\mathrm{d}z.$$

After integration by parts, these formulas reduce to

$$T_{m,n} = \frac{1}{2\pi \mathrm{i}} \oint_\Gamma \left(\frac{\pi}{\sin\pi z}\right)^2 F(z)\,\mathrm{d}z, \quad S_{m,n} = \frac{1}{2\pi \mathrm{i}} \oint_\Gamma \left(\frac{\pi}{\sin\pi z}\right)^2 \cos\pi z\, F(z)\,\mathrm{d}z,$$

where F is an integral of f.

Finally, setting $\alpha = m-1/2$, $\beta = n+1/2$, and letting $\delta \to +\infty$, under conditions (C1), (C2), and (C3), the previous integrals over Γ reduce to the weighted integrals over $(0,+\infty)$, giving transformations

$$\sum_{k=m}^{+\infty} f(k) = \int_0^{+\infty} w_1(t)\Phi\left(m - \frac{1}{2}, \frac{t}{\pi}\right)\mathrm{d}t \tag{5.4}$$

and

$$\sum_{k=m}^{+\infty} (-1)^k f(k) = (-1)^m \int_0^{+\infty} w_2(t)\Psi\left(m - \frac{1}{2}, \frac{t}{\pi}\right)\mathrm{d}t, \tag{5.5}$$

where the weight functions are given by

$$w_1(t) = \frac{1}{\cosh^2 t} \quad \text{and} \quad w_2(t) = \frac{\sinh t}{\cosh^2 t}, \tag{5.6}$$

respectively. Here F is an integral of f, as well as

$$\Phi(x,y) = -\frac{1}{2}\left[F(x+\mathrm{i}y) + F(x-\mathrm{i}y)\right] = -\mathrm{Re}\, F(x+\mathrm{i}y)$$

and

$$\Psi(x,y) = \frac{1}{2\mathrm{i}}\left[F(x+\mathrm{i}y) - F(x-\mathrm{i}y)\right] = \mathrm{Im}\, F(x+\mathrm{i}y).$$

The second our task is a numerical construction of Gaussian quadratures with respect to the hyperbolic weights w_1 and w_2, given in (5.6),

$$\int_0^{+\infty} g(t)w_s(t)\,\mathrm{d}t = \sum_{\nu=1}^{N} A_{\nu,s}^N g(\tau_{\nu,s}^N) + R_{N,s}(g) \quad (s = 1,2), \tag{5.7}$$

with weights $A_{\nu,s}^N$ and nodes $\tau_{\nu,s}^N$, $\nu = 1,\ldots,N$ $(s = 1,2)$, which are exact for all $g \in \mathcal{P}_{2N-1}$.

The moments of the hyperbolic weights w_1 and w_2 can be expressed in explicit form (see [22])

$$\mu_k^{(1)} = \int_0^{+\infty} t^k w_1(t)\,\mathrm{d}t = \begin{cases} 1, & k = 0, \\ \log 2, & k = 1, \\ (2^{k-1}-1)k!/4^{k-1}\zeta(k), & k \geq 2; \end{cases}$$

and

$$\mu_k^{(2)} = \int_0^{+\infty} t^k w_2(t)\,\mathrm{d}t = \begin{cases} 1, & k=0,\\ k\left(\dfrac{\pi}{2}\right)^k |E_{k-1}|, & k\,(\text{odd}) \geq 1,\\ \dfrac{2k}{4^k}\left[\psi^{(k-1)}(\tfrac{1}{4}) - \psi^{(k-1)}(\tfrac{3}{4})\right], & k\,(\text{even}) \geq 2, \end{cases}$$

where $\zeta(k)$ is the Riemann zeta function, E_k are Euler's numbers, defined by the generating function

$$\frac{2}{\mathrm{e}^t + \mathrm{e}^{-t}} = \sum_{k=0}^{+\infty} E_k \frac{t^k}{k!},$$

and $\psi(z)$ is the so-called digamma function, i.e., the logarithmic derivative of the gamma function, $\psi(z) = \Gamma'(z)/\Gamma(z)$. Mathematica evaluates derivatives $\psi^{(n)}(z)$ to arbitrary numerical precision, using the function `PolyGamma[n,z]`.

In order to construct Gaussian rules with respect to the weight $w_2(t)$ on $(0, +\infty)$ for $N \leq 50$, we need the recursion coefficients α_k and β_k for $k \leq N-1 = 49$, i.e., the moments for $k \leq 2N-1 = 99$. Taking the `WorkingPrecision` to be 100, and executing the following commands:

```
<< orthogonalPolynomials`
   mom2=Join[{1},Table[If[OddQ[k],k(Pi/2)^k Abs[EulerE[k-1]],
       2k/4^k(PolyGamma[k-1,1/4]-PolyGamma[k-1,3/4])],{k,1,99}]];
   {al,be}=aChebyshevAlgorithm[mom2, WorkingPrecision -> 100];
```

we obtain the first 50 recursion coefficients α_k and β_k, with the relative errors less than 6.18×10^{-60}.

In construction the corresponding recursion coefficients for the weight $w_1(t)$ on $(0, +\infty)$ for $N \leq 50$, the second line in the previous commands should be replaced by

```
mom1=Join[{1,Log[2]},Table[(2^(k-1)-1)k!/4^(k-1)Zeta[k],{k,2,99}]];
```

In this case, the first 50 recursion coefficients are obtained with slightly better accuracy (precisely, with the maximal relative error 3.65×10^{-63}).

These 50 recursive coefficients are enough for constructing Gaussian formulas (5.7) for each $N \leq 50$ and $s = 1, 2$.

Example 5.1. Now we consider a typical slowly convergent series

$$T(p) = \sum_{k=1}^{+\infty} \frac{1}{k^{1/p}(k+1)}, \quad p \geq 1, \tag{5.8}$$

which can be also represented in the form, by extracting a finite number of terms,

$$T(p) = \sum_{k=1}^{m-1} \frac{1}{k^{1/p}(k+1)} + \sum_{k=m}^{+\infty} \frac{1}{k^{1/p}(k+1)}. \tag{5.9}$$

Then, we apply our integral transformation (5.4) to the second (infinity) series in (5.9). Thus, using Gaussian quadrature formula (5.7) with respect to the weight $w_1(t) =$

$1/\cosh^2 t$ on $\mathbb{R}_+$, we obtain

$$T(p) \approx Q_m^{(N)}(p) = \sum_{k=1}^{m-1} \frac{1}{k^{1/p}(k+1)} + \sum_{\nu=1}^{N} A_{\nu,1}^N \Phi_p(m-1/2, \tau_{\nu,1}^N/\pi), \tag{5.10}$$

with $\Phi_p(x,y) = -\frac{1}{2}\left[F_p(x+\mathrm{i}y) + F_p(x-\mathrm{i}y)\right]$, where $\tau_{\nu,1}^N$ and $A_{\nu,1}^N$ are nodes and weights of the N-point Gaussian rule (5.7) ($s=1$).

Taking different values for m, we can notice the change rate of convergence of this quadrature processes. Namely, the rapidly increasing of convergence of the summation process as m increases is due to the singularities (poles) of $\Phi_p(m-1/2, z/\pi)$ moving away from the real line (see [20] and [22]). Here, $f_p(z) = 1/(z^{1/p}(z+1))$ and

$$F_1(z) = \log(z) - \log(z+1), \qquad F_2(z) = 2\arctan\left(\sqrt{z}\right) - \pi,$$

$$F_3(z) = \frac{1}{2}\log\frac{z+1}{\left(\sqrt[3]{z}+1\right)^3} + \sqrt{3}\arctan\left(\frac{2\sqrt[3]{z}-1}{\sqrt{3}}\right) - \frac{\pi\sqrt{3}}{2}, \quad \text{etc.}$$

For $p=2$ the series $T(2)$ appears in a study of spirals (cf. [2]) and defines the well-known *Theodorus constant*,

$$T(2) = \sum_{k=1}^{+\infty} \frac{1}{\sqrt{k}(k+1)} = 1.8580\ldots.$$

The first 10^6 terms of $T(2)$ give the result $T(2) \approx 1.86$ (only 3-digit accuracy).

For larger values of p, the corresponding series $T(p)$ is slower. For example, for $p=6$ an accuracy with only 3 digits in $T(6)$ by a direct summation needs 10^{18} terms. However, our summation/integration formula (5.10) for $p=6$ and $m=10$ gives approximations $Q_{10}^{(N)}(6)$, $N = 5(10)45$, which are presented in Table 2. In each entry the first digit in error is underlined.

Table 2. Gaussian approximations $Q_{10}^{(N)}(6)$ for $N = 5(10)45$

N	$Q_{10}^{(N)}(6)$
5	$5.69941177638356\underline{3}0$
15	$5.6994117763835619667430485043356\underline{4}1$
25	$5.69941177638356196674304850433562773287204829\underline{0}3$
35	$5.6994117763835619667430485043356277328720482911358004 9\underline{9}7$
45	$5.699411776383561966743048504335627732872048291135800493867761\underline{0}6$

As we can see, this method is very efficient; the quadrature formula with only $N = 45$ nodes gives more than 60 exact digits in the sum $T(6)$!

For details and other applications see [16], [17], and [22].

6. Construction of some perfectly symmetric cubature rules

Using the MATHEMATICA package `OrthogonalPolynomias` we can construct some perfectly symmetric two-dimensional cubature formulas in $D \subset \mathbb{R}^2$ with minimal number of nodes,

$$I(f) = \iint_D w(x,y) f(x,y)\,\mathrm{d}x\,\mathrm{d}y = \sum_{i=1}^{N} A_i f(P_i) + R_N(f). \tag{6.1}$$

Such a cubature formula has the nodes of the form $(\pm x_j, \pm y_j)$ and $(\pm y_j, \pm x_j)$ with the same weights. Regarding [25] we call it as a "good" formula if all of its weights are positive.

For completely symmetric weight functions $w(x,-y) = w(-x,y) = w(x,y) \geq 0$, the typical domains D are the square with vertices $(\pm 1, \pm 1)$, the unit circle, and the entire plane $\mathbb{R}^2$.

We recall that a two-dimensional cubature rule of degree d integrates exactly all monomials $x^i y^j$, i.e., $R_N(x^i y^j) = 0$, for which $i + j \leq d$.

In order to obtain "good" cubature rules for some weights $w(x,y)$ of degree $d \leq 7$, Stroud and Secrest [28] used the nodes whose "generators" are of the form $(0,0)$, $(\alpha,0)$, (β,β). For rules of degree $d \geq 8$, it is necessary to include nodes whose "generators" are of the form (γ,δ). Each of them generates eight nodes of the form: $(\pm\gamma, \pm\delta)$, $(\pm\delta, \pm\gamma)$ with the same weight, while $(\alpha,0)$ and (β,β) generate only four nodes: $(\pm\alpha, 0)$, $(0, \pm\alpha)$ and $(\pm\beta, \pm\beta)$, respectively. Of course, $(0,0)$ gives only one node $(0,0)$.

Following [25], the method of construction needs integrals

$$\begin{cases} I(x^{2k}) \ \text{ and } \ I(x^{2j}y^{2k}) \\ k = 0, 1 \ldots, [N/2]; \\ 1 \leq j \leq k; \ j + k = 2, \ldots, [N/2], \end{cases}$$

as well as the following "special moments", i.e., integrals of the form

$$\begin{aligned} \mu_{jk} &= I\big[(x^2 - y^2)^2 (x^2 y^2)^j (x^2 + y^2)^k\big] \\ &= \int_0^{+\infty}\!\!\int_0^{+\infty} w(x,y)(x^2 - y^2)^2 (x^2 y^2)^j (x^2 + y^2)^k \,\mathrm{d}x\,\mathrm{d}y, \end{aligned} \tag{6.2}$$

where $j \geq 1$, $k \geq 0$. The corresponding system of nonlinear equations $R_N(x^i y^j) = 0$, $i + j \leq d$, can be separated in a few systems of the Gaussian type (3.3), which can be solved using the MATHEMATICA package `OrthogonalPolynomials`.

In this section we show only construction of cubature formulas (6.1) on $D = \mathbb{R}^2$, with respect to the complete symmetric weight function of the form $w(x,y) = w_\nu(x,y)$, $\nu = 1, 2, 3$, where

$$w_1(x,y) = \mathrm{e}^{-(x^2+y^2)}, \quad w_2(x,y) = \mathrm{e}^{-\sqrt{x^2+y^2}}, \quad w_3(x,y) = \mathrm{e}^{-(|x|+|y|)}.$$

The special moments for the previous weight functions w_1 and w_2 can be calculated in an analytic form as

$$\mu_{jk}^{(1)} = \frac{(2j+k+2)!\pi}{2^{4j+3}(j+1)}\binom{2j}{j} \qquad \text{and} \qquad \mu_{jk}^{(2)} = \frac{(4j+2k+5)!\pi}{2^{4j+2}(j+1)}\binom{2j}{j},$$

respectively. In the third case it can be expressed by the following integral

$$\mu_{jk}^{(3)} = \frac{(4j+2k+5)!}{2^{4j+k+1}}\int_0^1 \sqrt{z}\,(1-z)^{2j}(1+z)^k\,\mathrm{d}z,$$

or in terms of hypergeometric functions as

$$\begin{aligned}\mu_{jk}^{(3)} \;&=\; \frac{(4j+2k+5)!}{2^{k-2}(2j+1)\binom{4(j+1)}{2(j+1)}}\left\{{}_2F_1\left(-\frac{1}{2},-k;2j+\frac{5}{2};-1\right)\right.\\ &\qquad\left.+\frac{k-2j-1}{2(j+1)}\,{}_2F_1\left(\frac{1}{2},-k;2j+\frac{5}{2};-1\right)\right\}.\end{aligned}$$

Example 6.1. In order to construct 44-point cubature formulas of degree $d=15$ with respect to the weight $w(x,y)=w_3(x,y)=\exp(-|x|-|y|)$ on $\mathbb{R}^2$, we use the following generators:

$$(u_i,0),\ i=1,2,3,4;\quad (v_i,v_i),\ j=1,2,3;\quad (w_i,z_i),\ i=1,2.$$

Generator P_i	Weight A_i	Number of points
$(u_i,0)$	a_i	4
(v_i,v_i)	b_i	4
(w_i,z_i)	c_i	8

Then the corresponding system of equations is given by

$$\sum_i c_i(w_i^2-z_i^2)^2(w_i^2z_i^2)^j(w_i^2+z_i^2)^k = \frac{1}{8}\,\mu_{jk}$$

$$j=1,\ldots,\left[\frac{m-2}{2}\right];\quad k=0,1,\ldots,m-2j-2.$$

Using the Mathematica package `OrthogonalPolynomials` for the "generator nodes" in this 44-point cubature formula of degree $d=15$ we obtain:

```
{{16.75517334835192,0}, {9.520295794790188,0},
{4.451284933071043,0}, {1.326612922551803,0},
{10.40246868263913,10.40246868263913},
{6.307197292644404,6.307197292644404},
{2.533316709591005,2.533316709591005},
{13.16709143114937,3.265192228507983},
{6.770241049738993,2.369872911188105}},
```

and for the corresponding weight coefficients the following values:

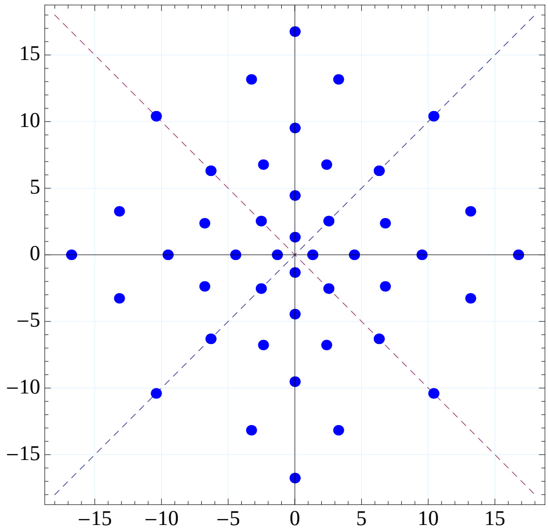

FIGURE 3. Distribution of nodes in 44-point cubature formula of degree $d = 15$ for the weight function w_3

```
{8.186694686950403*(10^-7), 0.0006529201474967032,
0.06663038092243385, 0.8569723144924805,
6.812119062461652*(10^-8), 0.00007773406088317548,
0.07219519187714604, 2.913841882561950*(10^-6),
0.001732372012567657}.
```

Finally, the distribution of nodes in this cubature formula ($N = 44$ and $d = 15$) is displayed in in Fig. 3.

Remark 6.2. Cubature formulas (6.1) with the exponential weights w_ν, $\nu = 1, 2, 3$, have been recently used in [24] and [27].

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