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Methods for the computation of slowly convergent series and finite sums based on Gauss-Christoffel quadratures[†]

Gradimir V. Milovanović

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Abstract

In this paper we give an account on summation/integration methods for the computation of slowly convergent series and finite sums. The methods are based on Gauss-Christoffel quadrature rules with respect to some nonclassical weight functions over $\mathbb{R}$ or $\mathbb{R}_+$. For constructing such rules we use the recent progress in symbolic computation and variable-precision arithmetic, as well as our Mathematica package `OrthogonalPolynomials` [4, 26]. Together with our own results, we are also taking into consideration the use of other known results, especially the classical summation formulae of Euler-Maclaurin and Abel-Plana, in order to apply them afterwards in the computational techniques that we have developed recently. We present the Laplace transform method [15] and the contour integration method [21, 23], and give several numerical examples in order to illustrate the efficiency of different summation/integration methods.

Keywords: Summation, Gaussian quadratures, weight function, three-term recurrence relation, convergence, Laplace transform, contour integration.

MSC: Primary 65B10; Secondary 40A25, 41A55, 65B15, 65D30, 65D32, 30E20, 33C90.

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§1. Introduction

For slowly convergent series and finite sums, which appear in many problems in mathematics, physics and other sciences, there are several numerical methods based on linear and nonlinear transformations. In general, starting from the sequence of partial sums of the series, these transformations give other sequences with a faster convergence to the sum of the series. There is a rich literature on this subject (cf. references in Mastroianni and Milovanović [19]).

In this paper we give an account on some summation processes for series ($n = \infty$) and finite sums,

$$\sum_{k=1}^{n} (\pm 1)^k f(k), \tag{1.1}$$

with a given function $z \mapsto f(z)$ with certain properties with respect to the variable z, based on ideas related to Gauss-Christoffel quadratures. In a general case, the function f can depend on other parameters, e.g., $f(z; x, \ldots)$, so that these summation processes can be applied also to some classes of functional series, not only to numerical series.

The basic idea in our methods is to transform the sum (1.1) to an integral with respect to some measure $d\mu$ on $\mathbb{R}$ (or $\mathbb{R}_+$), and then to approximate this integral by a finite quadrature sum,

$$\sum_{k=1}^{n} (\pm 1)^k f(k) = \int_{\mathbb{R}} g(t)\, d\mu(t) \approx \sum_{\nu=1}^{N} A_\nu g(x_\nu), \tag{1.2}$$

where the function g is connected with f in some way, and the weights $A_\nu \equiv A_\nu^{(n)}$ and abscissae $x_\nu \equiv x_\nu^{(n)}$, $\nu = 1, \ldots, N$, are chosen in such a way as to approximate closely the sum (1.1) for a large class of functions with a relatively small number $N \ll n$. In our approach we take the Gaussian quadrature sums as the sum on the right-hand side in (1.2). Together with our own results, we also consider some other known results, in particular the classical summation formulae of Euler-Maclaurin and Abel-Plana, in order to combine them with the computational techniques that we have developed recently.

For the construction of Gaussian quadratures with respect to nonstandard measures $d\mu$ on $\mathbb{R}$ or $\mathbb{R}_+$ we use the recent progress in symbolic computation and variable-precision arithmetic and our Mathematica package `OrthogonalPolynomials` [4, 26]. The approach enables us to overcome the numerical instability in generating coefficients of the three-term recurrence relation for the corresponding orthogonal polynomials with respect to the measure $d\mu$.

The paper is organized as follows. Section 2 is devoted to the classical summation formulae of Euler-Maclaurin and Abel-Plana. Recurrence coefficients for some orthogonal polynomial systems on

$\mathbb{R}$ and $\mathbb{R}_+$ are studied in Section 3. For some of them, these coefficients can be expressed in an explicit form. In Sections 4 and 5 we present the Laplace transform method and the contour integration method, respectively. Finally, in order to illustrate the efficiency of different summation/integration methods we give a few numerical examples in Section 6.

§2. Summation formulae of Euler-Maclaurin and Abel-Plana

The first result on summation/integration methods was the well-known Euler-Maclaurin formula, discovered by Leonard Euler (1707–1783) in 1732 in connection with the so-called *Basel problem* (or in modern terminology, for the Riemann zeta function, with *determining* $\zeta(2)$),

$$\sum_{k=m}^{n} f(k) = \int_m^n f(x)dx + \frac{1}{2}(f(m)+f(n)) + \sum_{j=1}^{r} \frac{B_{2j}}{(2j)!}\left[f^{(2j-1)}(n) - f^{(2j-1)}(m)\right] + E_r(f), \qquad (2.1)$$

which holds for any $m \in \mathbb{N}_0$, $n, r \in \mathbb{N}$, $m < n$, and $f \in C^{2r}[m,n]$, where B_{2j} are the Bernoulli numbers. This formula was also found independently by Colin Maclaurin (1698–1746) in 1738, who used (2.1) for calculating integrals. Bernoulli numbers are defined by the generating function

$$\frac{t}{e^t - 1} = \sum_{j=0}^{\infty} \frac{B_j t^j}{j!}.$$

For example, $B_0 = 1$, $B_1 = -1/2$, $B_2 = 1/6$, $B_3 = 0$, $B_4 = -1/30$, $B_5 = 0$, $B_6 = 1/42$, etc.

The error term $E_r(f)$ in (2.1) can be expressed in different forms (cf. [24]); e.g., if $f \in C^{2r+2}[m,n]$ then there exists $\eta \in (m,n)$ such that

$$E_r(f) = (n-m)\,\frac{B_{2r+2}}{(2r+2)!} f^{(2r+2)}(\eta). \qquad (2.2)$$

A history of this formula was given by Barnes [2], and some details can be found in [28, 1, 12, 13, 3, 24].

Alternatively, the Euler-Maclaurin summation formula (2.1) is related to the so-called composite trapezoidal rule,

$$T_{m,n}f := \sum_{k=m}^{n}{}'' f(k) = \frac{1}{2}f(m) + \sum_{k=m+1}^{n-1} f(k) + \frac{1}{2}f(n).$$

Namely, the error of this rule can be expressed in terms of the Euler-Maclaurin formula (2.1),

$$T_{m,n}f - \int_m^n f(x)dx = \sum_{j=1}^{r} \frac{B_{2j}}{(2j)!}\left[f^{(2j-1)}(n) - f^{(2j-1)}(m)\right] + E_r^T(f). \tag{2.3}$$

In other words, it means that the trapezoial sum $T_{m,n}f$ can be improved by values of derivatives at the end points of the interval of integration, through corrections terms in the form presented on the right hand side in (2.3). The Euler-Maclaurin summation formula is a standard formula and it is implemented in the package MATHEMATICA as the function `NSum` with option `Method -> Integrate`.

There is also another summation formula, the Abel-Plana formula, which is not so well known like the Euler-Maclaurin formula. In 1820 Giovanni (Antonio Amedeo) Plana (1781–1864) obtained the summation formula

$$\sum_{k=0}^{+\infty} f(k) - \int_0^{+\infty} f(x)dx = \frac{1}{2}\, f(0) + i\int_0^{+\infty} \frac{f(iy) - f(-iy)}{e^{2\pi y} - 1}dy, \tag{2.4}$$

which holds for analytic functions, f in $\Omega = \big\{z \in \mathbb{C} \,:\, \Re z \ge 0\big\}$, that satisfy the conditions:

$$\lim_{|y|\to+\infty} e^{-|2\pi y|}|f(x \pm iy)| = 0,$$

uniformly in x on every finite interval, and such that

$$\int_0^{+\infty} |f(x+iy) - f(x-iy)|e^{-|2\pi y|}dy$$

exists for every $x \ge 0$ and tends to zero when $x \to +\infty$. This formula was also proved by Niels Henrik Abel (1802–1829) in 1823. In addition, Abel also proved an interesting *"alternating series version"*, under the same conditions, namely,

$$\sum_{k=0}^{+\infty}(-1)^k f(k) = \frac{1}{2}\, f(0) + i\int_0^{+\infty} \frac{f(iy) - f(-iy)}{2\sinh \pi y}dy. \tag{2.5}$$

For the finite sum $S_{n,m}f = \displaystyle\sum_{k=m}^{n}(-1)^k f(k)$, it becomes

$$S_{n,m}f = \frac{1}{2}\big[(-1)^m f(m) + (-1)^n f(n+1)\big] + \int_{-\infty}^{+\infty} \big[\psi_{n+1}(y) - \psi_m(y)\big]w^A(y)dy, \tag{2.6}$$

where the *Abel weight* on $\mathbb{R}$, $\omega^A(x)$, and the function $\psi_m(y)$ are given by

$$w^A(x) = \frac{x}{2\sinh \pi x} \quad \text{and} \quad \psi_m(y) = (-1)^m \frac{f(m+iy) - f(m-iy)}{2iy}. \tag{2.7}$$

Let $m, n \in \mathbb{N}$, $m < n$, and $C(\varepsilon)$ be a closed rectangular contour with vertices at $m \pm ib$, $n \pm ib$, $b > 0$ (see Figure 1), and with semicircular indentations of radius ε around m and n. Let f be an analytic function in the strip $\Omega_{m,n} = \{z \in \mathbb{C} : m \leq \Re z \leq n\}$ and suppose that for every $m \leq x \leq n$,

$$\lim_{|y| \to +\infty} e^{-|2\pi y|} |f(x \pm iy)| = 0 \quad \text{uniformly in } x,$$

and that

$$\int_0^{+\infty} |f(x+iy) - f(x-iy)| e^{-|2\pi y|} dy$$

exists.

The integral

$$\int_{C(\varepsilon)} \frac{f(z)}{e^{-i2\pi z} - 1} dz,$$

with $\varepsilon \to 0$ and $b \to +\infty$, leads to the *Abel-Plana formula* in the form

$$T_{m,n} f - \int_m^n f(x) dx = \int_{-\infty}^{+\infty} \big(\phi_n(y) - \phi_m(y)\big) w^P(y) dy, \tag{2.8}$$

where

$$\phi_m(y) = \frac{f(m+iy) - f(m-iy)}{2iy} \quad \text{and} \quad w^P(y) = \frac{|y|}{e^{|2\pi y|} - 1}. \tag{2.9}$$

Practically, the Abel-Plana formula (2.8) gives the error of the composite trapezoidal formula (like the Euler-Maclaurin formula).

In order to find the moments of the *Plana* weight function $x \mapsto w^P(x)$ on $\mathbb{R}$, we note first that if k is odd, the moments are zero, i.e.,

$$\mu_k(w^P) = \int_{\mathbb{R}} x^k w^P(x) dx = \int_{\mathbb{R}} x^k \frac{|x|}{e^{|2\pi x|} - 1} dx = 0.$$

For even k, we have

$$\mu_k(w^P) = 2 \int_0^{+\infty} \frac{x^{k+1}}{e^{2\pi x} - 1} dx = \frac{2}{(2\pi)^{k+2}} \int_0^{+\infty} \frac{t^{k+1}}{e^t - 1} dt,$$

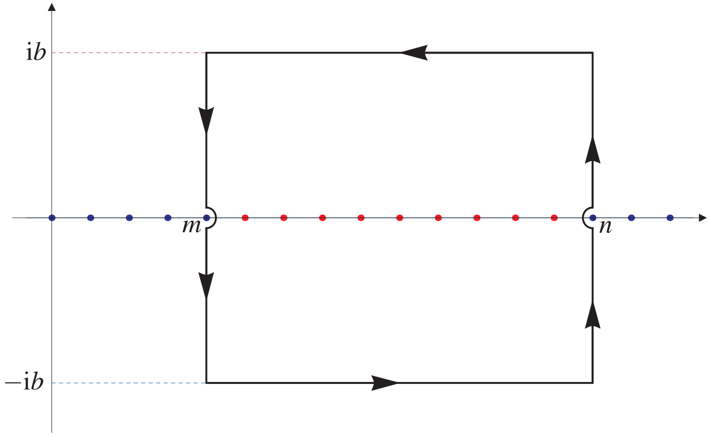

Figure 1: Rectangular contour $C(\varepsilon)$

which can be exactly expressed in terms of the Riemann zeta function $\zeta(s)$,

$$\mu_k(w^P) = \frac{2(k+1)!\zeta(k+2)}{(2\pi)^{k+2}} = (-1)^{k/2}\frac{B_{k+2}}{k+2},$$

because the number $k+2$ is even.

Thus, in terms of Bernoulli numbers, the moments are

$$\mu_k(w^P) = \begin{cases} 0, & k \text{ is odd}, \\ (-1)^{k/2}\dfrac{B_{k+2}}{k+2}, & k \text{ is even}. \end{cases} \tag{2.10}$$

Now, by the Taylor expansion for $\phi_m(y)$ (and $\phi_n(y)$) on the right-hand side in (2.8),

$$\phi_m(y) = \frac{f(m+iy) - f(m-iy)}{2iy} = \sum_{j=1}^{+\infty} \frac{(-1)^{j-1}y^{2j-2}}{(2j-1)!} f^{(2j-1)}(m),$$

and using the moments (2.10), the Abel-Plana formula (2.8) reduces to the Euler-Maclaurin formula,

$$T_{m,n}f - \int_m^n f(x)dx \quad = \quad \sum_{j=1}^{+\infty} \frac{(-1)^{j-1}}{(2j-1)!}\mu_{2j-2}(w^P)\left(f^{(2j-1)}(n) - f^{(2j-1)}(m)\right)$$

$$= \sum_{j=1}^{+\infty} \frac{B_{2j}}{(2j)!} \left(f^{(2j-1)}(n) - f^{(2j-1)}(m) \right),$$

because of $\mu_{2j-2}(w^P) = (-1)^{j-1} B_{2j}/(2j)$ (for more details see Dahlquist [5, 6, 7]).

A similar summation formula is the so-called *midpoint summation formula*. It can be obtained by combining two Plana formulas for $f(z-1/2)$ and $f((z+m-1)/2)$. Namely,

$$T_{m,2n-m+2} f\Big(\frac{z+m-1}{2}\Big) - T_{m,n+1} f\Big(z - \frac{1}{2}\Big) = \sum_{k=m}^{n} f(k),$$

i.e.,

$$\sum_{k=m}^{n} f(k) - \int_{m-1/2}^{n+1/2} f(x)dx = \int_{-\infty}^{+\infty} \left[\phi_{m-1/2}(y) - \phi_{n+1/2}(y)\right] w^M(y)dy,$$

where the *midpoint weight function* is given by

$$w^M(x) = w^P(x) - w^P(2x) = \frac{|x|}{e^{|2\pi x|} + 1}$$

and $\phi_{m-1/2}$ and $\phi_{n+1/2}$ are defined in (2.9), taking $m := m - 1/2$ and $m := n + 1/2$, respectively.

There are also several other summation formulas. For example, the *Lindelöf* formula for alternating series is

$$\sum_{k=m}^{+\infty} (-1)^k f(k) = (-1)^m \int_{-\infty}^{+\infty} f(m - 1/2 + iy) \frac{dy}{2\cosh \pi y},$$

where the *Lindelöf* weight function is given by

$$w^L(x) = \frac{1}{2\cosh \pi y} = \frac{1}{e^{\pi x} + e^{-\pi x}}.$$

All these weights are even functions on $\mathbb{R}$. As we mentioned in Section 1, a summation problem can be also transformed into the integration with respect to a weight function defined on the half line $\mathbb{R}_+$.

In the sequel we present some of the most important weight functions on $\mathbb{R}$ and $\mathbb{R}_+$, including their moments. The recursion coefficients β_k for the weights on $\mathbb{R}$ are also presented.

§3. Recurrence coefficients for some orthogonal polynomial systems on $\mathbb{R}$ and $\mathbb{R}_+$

We denote the space of all algebraic polynomials defined on $\mathbb{R}$ by $\mathbb{P}$, and by $\mathbb{P}_N \subset \mathbb{P}$ the space of polynomials of degree at most N ($N \in \mathbb{N}$). Suppose that for a given weight function w all moments $\mu_k = \int_{\mathbb{R}} x^k w(x)dx$, $k \geq 0$, exist, are finite and $\mu_0 > 0$. Then, for each $N \in \mathbb{N}$, there exists the N-point Gauss-Christoffel quadrature rule

$$\int_{\mathbb{R}} f(x)w(x)dx = \sum_{\nu=1}^{N} A_\nu^{(N)} f(x_\nu^{(N)}) + R_N(f), \tag{3.1}$$

which is exact for all polynomials of degree $\leq 2N-1$ ($f \in \mathbb{P}_{2N-1}$).

The Gauss-Christoffel quadrature formula (3.1) can be characterized as an interpolatory formula for which its *node polynomial* $\pi_N(x) = \prod_{\nu=1}^{N}\bigl(x - x_\nu^{(N)}\bigr)$ is *orthogonal* to $\mathbb{P}_{N-1}$ with respect to the inner product defined by

$$(p,q) = \int_{\mathbb{R}} p(x)q(x)w(x)dx \quad (p,q \in \mathbb{P}).$$

Because of the property $(xp,q) = (p,xq)$, these (monic) orthogonal polynomials π_k satisfy the fundamental *three–term recurrence relation*

$$\pi_{k+1}(x) = (x-\alpha_k)\pi_k(x) - \beta_k\pi_{k-1}(x), \quad k = 0,1,\ldots, \tag{3.2}$$

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

For even weights on $\mathbb{R}$, the coefficients α_k are zero, so that the recurrence relation (3.2) becomes

$$\pi_{k+1}(x) = x\pi_k(x) - \beta_k\pi_{k-1}(x), \quad k = 0,1,\ldots \tag{3.3}$$

The quadrature *nodes* $x_\nu^{(N)}$, $\nu = 1,\ldots,N$, are eigenvalues of the *Jacobi* matrix

$$J_n(w) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & \mathbf{0} \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{N-1}} \\ \mathbf{0} & & & \sqrt{\beta_{N-1}} & \alpha_{N-1} \end{bmatrix},$$

and the first components of the corresponding normalized eigenvectors $\mathbf{v}_\nu = [v_{\nu,1} \ \ldots \ v_{\nu,N}]^{\mathrm{T}}$ (with $\mathbf{v}_\nu^{\mathrm{T}}\mathbf{v}_\nu = 1$) give the *Christoffel numbers*, $A_\nu^{(N)} = \lambda_{N,\nu} = \beta_0 v_{\nu,1}^2$, $\nu = 1, \ldots, N$.

Unfortunately, the recursion coefficients are known explicitly only for some narrow classes of orthogonal polynomials, as e.g. for the classical orthogonal polynomials (Jacobi, the generalized Laguerre, and Hermite polynomials). However, for a large class of the so-called *strongly non-classical polynomials* these coefficients can be constructed numerically. Basic procedures for generating these coefficients are the *method of (modified) moments*, the *discretized Stieltjes–Gautschi procedure* and the *Lanczos algorithm*, and they play a central role in the so-called *constructive theory of orthogonal polynomials*, which was developed by Walter Gautschi in the eighties on the last century. In [9] he starts with an arbitrary positive measure $d\mu(t)$, which is given explicitly, or implicitly via moment information, and considers the basic computational problem: *for a given measure* $d\mu$ *and for a given* $n \in \mathbb{N}$*, generate the first* n *coefficients* $\alpha_k(d\mu)$ *and* $\beta_k(d\mu)$ *for* $k = 0, 1, \ldots, n-1$. The problem is very sensitive with respect to small perturbations in the data. The basic references are [9, 11, 19, 25].

Recent progress in *symbolic computation* and *variable-precision arithmetic* now makes possible to generate the recurrence coefficients α_k and β_k directly by using the original Chebyshev method of moments in sufficiently high precision. The corresponding software for such a purpose, as well as many other calculations with orthogonal polynomials and different quadrature rules, is now available: Gautschi's package `SOPQ` in MATLAB, and our MATHEMATICA package `OrthogonalPolynomials` (see [4] and [26]). These packages are downloadable from the web sites `http://www.cs.purdue.edu/archives/2002/wxg/codes/` and `http://www.mi.sanu.ac.rs/~gvm/`, respectively. Thus, all that is required is a procedure for the symbolic calculation of moments or their calculation in variable-precision arithmetic.

3.1. The weight functions on $\mathbb{R}$

In this part we give an account of some of the most important (even) weight functions on $\mathbb{R}$, including their moments and the coefficients β_k in the three-term recurrence relation (3.3) for the corresponding orthogonal polynomials. For a given sequence of moments (`mom`), our MATHEMATICA package `OrthogonalPolynomials` enables us to get recurrence coefficients `{al,be}` in a symbolic form,

```
{al,be}=aChebyshevAlgorithm[mom, Algorithm -> Symbolic];
```

Graphics of these weight functions are displayed in figures 2 and 3.

Sonin-Markov weight: $w^{SM}(x) = |x|^\beta \exp(-x^2)$**,** $\beta > -1$

The corresponding orthogonal polynomials $\{\pi_k\}_{k=0}^{+\infty}$ are known as the Sonin-Markov or generalized Hermite polynomials. They can be expressed in terms of the generalized (monic) Laguerre polynomials,

$$\pi_{2k}(x) = \hat{L}_k^\alpha(x^2), \quad \pi_{2k+1}(x) = x\hat{L}_k^{\alpha+1}(x^2) \quad (\alpha = (\beta-1)/2).$$

Using [19, p. 102, theorems 2.2.11 and 2.2.12], we have the following equations for the coefficients β_k in (3.3),

$$\beta_{2k} + \beta_{2k+1} = \alpha_k^{(1)} = 2k + \alpha + 1, \quad \beta_{2k-1}\beta_{2k} = \beta_k^{(1)} = k(k+\alpha)$$

and

$$\beta_{2k+1} + \beta_{2k+2} = \alpha_k^{(2)} = 2k + \alpha + 2, \quad \beta_{2k}\beta_{2k+1} = \beta_k^{(2)} = k(k+\alpha+1),$$

where $\alpha_k^{(\nu)}$ and $\beta_k^{(\nu)}$, $\nu = 1, 2$, are the recurrence coefficients for the generalized monic Laguerre polynomials $\hat{L}_k^\alpha$ and $\hat{L}_k^{\alpha+1}$, respectively. From the previous equations we get

$$\beta_k = \begin{cases} \dfrac{k+\beta}{2}, & k \text{ odd}, \\ \dfrac{k}{2}, & k \text{ even}, \end{cases}$$

and $\beta_0 = \mu_0 = \int_{\mathbb{R}} w^{SM}(x)dx = \Gamma((\beta+1)/2)$.

In the special case $\beta = 0$, this weight function reduces to the well-known *Hermite weight* $w^H(x) = \exp(-x^2)$. This is the most popular (classical) weight function on the real line. The recurrence coefficients of the classical Hermite polynomials orthogonal with respect to this weight function on $\mathbb{R}$ are

$$\beta_0 = \sqrt{\pi}, \quad \beta_k = \frac{k}{2}, \quad k = 1, 2, \ldots$$

Remark 3.1. There are several generalizations of the Sonin-Markov weight function. For example, the *Freud weight* is defined by $w^F(x) = \exp(-|x|^\alpha)$, $\alpha \geq 1$, or, in general, $w(x) = \exp(-2Q(x))$, where Q is a function (e.g., a polynomial in a special case) with some properties.

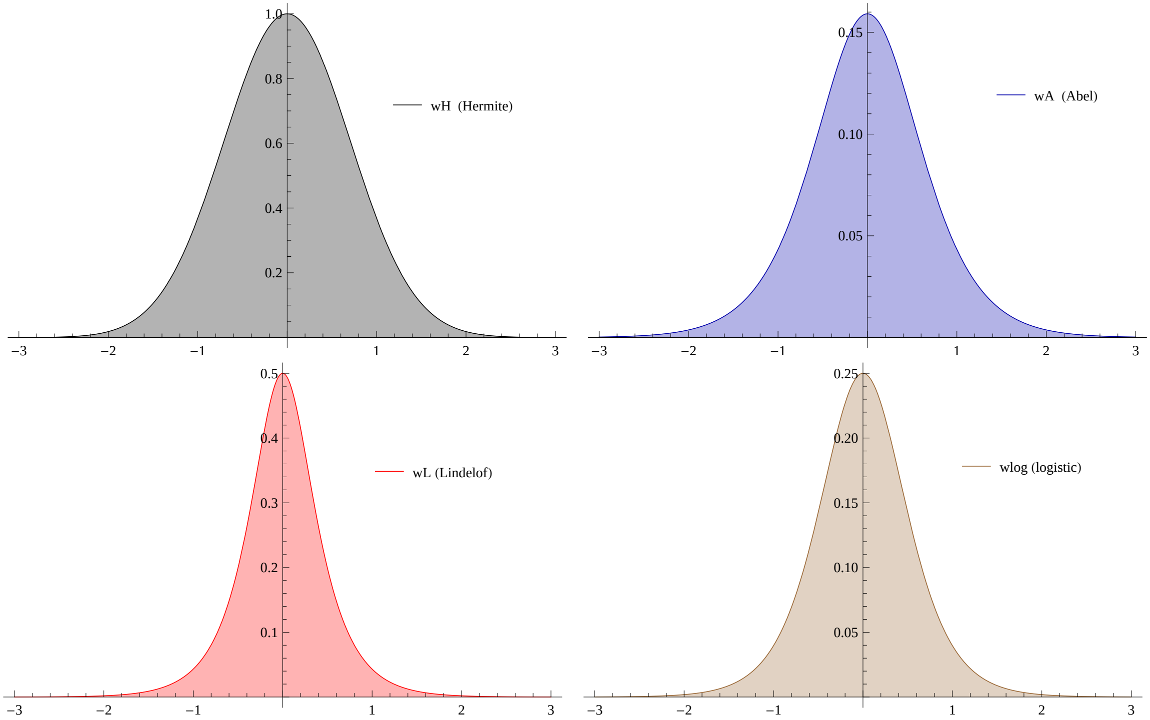

Figure 2: Weight functions on $\mathbb{R}$: Cases $1°$–$4°$

Abel weight: $w^A(x) = x/(2\sinh(\pi x))$

The moments for this weight are

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

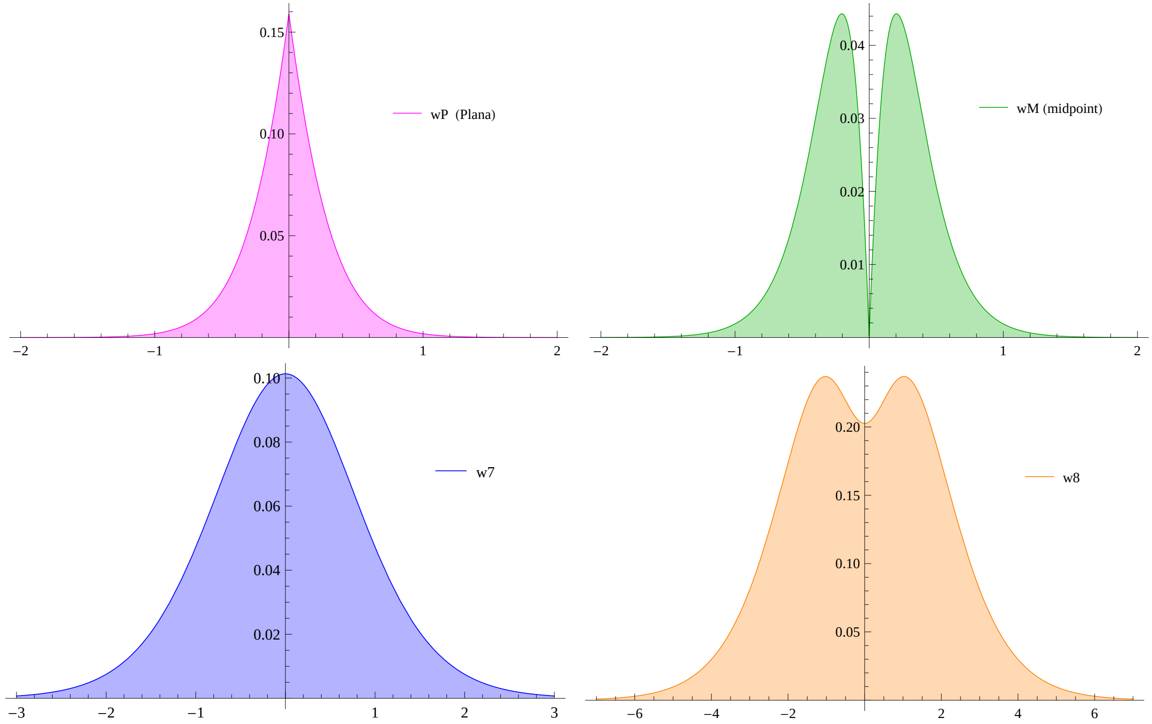

Figure 3: Weight functions on $\mathbb{R}$: Cases $5°$–$8°$

and the coefficients in the three-term recurrence relation (3.3) for the corresponding orthogonal polynomials are known explicitly (see [19, p. 159]),

$$\beta_0 = \mu_0 = \frac{1}{4}, \quad \beta_k = \frac{k(k+1)}{4}, \quad k = 1, 2, \ldots$$

Lindelöf weight: $w^L(x) = 1/(2\cosh(\pi x))$

The moments for this weight are

$$\mu_k = \begin{cases} 0, & k \text{ odd}, \\ 2(4\pi)^{-k-1}k!\left[\zeta\left(k+1,\frac{1}{4}\right) - \zeta\left(k+1,\frac{3}{4}\right)\right], & k \text{ even}, \end{cases}$$

where $\zeta(s,a)$ is the generalized Riemann zeta function, defined by

$$\zeta(s,a) = \sum_{\nu=0}^{+\infty}(\nu+a)^{-s}.$$

The recurrence coefficients are known explicitly (see [19, p. 159]),

$$\beta_0 = \mu_0 = \frac{1}{2}, \quad \beta_k = \frac{k^2}{4}, \quad k = 1,2,\ldots$$

Logistic weight: $w^{\log}(x) = e^{-\pi x}/(1+e^{-\pi x})^2 = 1/(2\cosh(\pi x/2))^2 = [w^L(x/2)]^2$

The moments for this weight are

$$\mu_k = \begin{cases} 0, & k \text{ odd}, \\ \dfrac{2}{\pi}(-1)^{k/2-1}\left(2^{k-1}-1\right)B_k, & k \text{ even} \end{cases}$$

and the coefficients in the three-term recurrence relation (3.3) for the corresponding orthogonal polynomials are also known explicitly (see [19, p. 159]),

$$\beta_0 = \mu_0 = \frac{1}{\pi}, \quad \beta_k = \frac{k^4}{4k^2-1}, \quad k = 1,2,\ldots$$

Plana weight: $w^P(x) = |x|/(e^{|2\pi x|}-1)$

The moments for this weight function are given in (2.10), and our package `OrthogonalPolynomials` gives the sequence of recurrence coefficients $\{\beta_k\}_{k\geq 0}$ in the rational form:

$$\left\{\frac{1}{12}, \frac{1}{10}, \frac{79}{210}, \frac{1205}{1659}, \frac{262445}{209429}, \frac{33461119209}{18089284070}, \frac{361969913862291}{137627660760070}, \frac{85170013927511392430}{24523312685049374477},\right.$$

$$\frac{1064327215185988443814288995130}{2361552627563909211512391211 53}, \frac{2867899822547647571956750038701379556971 17}{5124643566492103168870569541234299064785 0},$$

$$\frac{152276258891366439896107174348030272403756344528080810 47}{2212147521291103911193549528920437912200375980011300650},$$

$$\left.\frac{58794344175474628397213864982194855427387844746923385269740181414841088 5}{71529318090286333175985287358122471724664434392542372273400541405857921}, \dots\right\}.$$

Midpoint weight: $w^M(x) = |x|/(e^{|2\pi x|} + 1)$

The moments for this weight are given by

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

The sequence $\{\beta_k\}_{k\geq 0}$ in rational form is

$$\left\{\frac{1}{24}, \frac{7}{40}, \frac{2071}{5880}, \frac{999245}{1217748}, \frac{21959166635}{18211040276}, \frac{108481778600414331}{55169934195679160}, \frac{2083852396915648173441543}{813782894744588335008520},\right.$$

$$\left.\frac{2569854383739095757141180926630813 5}{711653688516943358642628591888266 2}, \frac{2022217398360507246593127286050156180973495554 85}{457883445996331837976313744446948175389676295 98}, \dots\right\}.$$

The weight $w_7(x) = \dfrac{x^2 e^{-\pi x}}{(1 - e^{-\pi x})^2} = \left(\dfrac{x}{2\sinh(\pi x/2)}\right)^2 = \dfrac{1}{4}[w^A(x/2)]^2$

In this case the moments are

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

For the corresponding sequence $\{\beta_k\}_{k\geq 0}$ we obtain

$$\left\{\frac{2}{3\pi}, \frac{4}{5}, \frac{72}{35}, \frac{80}{21}, \frac{200}{33}, \frac{1260}{143}, \frac{784}{65}, \frac{1344}{85}, \frac{6480}{323}, \frac{3300}{133}, \frac{4840}{161}, \frac{20592}{575}, \frac{9464}{225}, \frac{12740}{261}, \frac{50400}{899}, \frac{21760}{341}, \dots\right\}.$$

After some experiments, we conjectured and proved that

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

The weight $w_8(x) = x^2 \dfrac{e^{\pi x/2} + e^{-\pi x/2}}{(e^{\pi x/2} - e^{-\pi x/2})^2} = 2\cosh(\pi x/2)\Big(\dfrac{x}{2\sinh(\pi x/2)}\Big)^2$

In this case the moments are

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

Also, in this case we proved that

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

3.2. Weight functions on $\mathbb{R}_+$

In this part we mention four important weight functions defined on $\mathbb{R}_+$.

Bose-Einstein and Fermi-Dirac weights: $\varepsilon(t) = \dfrac{t}{e^t - 1}$ **and** $\varphi(t) = \dfrac{1}{e^t + 1}$**, respectively**

These functions and the corresponding quadratures with respect to them are widely used in solid state physics.

The moments can be exactly calculated in terms of Riemann zeta function,

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

and

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

Hyperbolic weights on $\mathbb{R}_+$

Consider the hyperbolic weights

$$w_1(t) = \frac{1}{\cosh^2 t} \quad \text{and} \quad w_2(t) = \frac{\sinh t}{\cosh^2 t}. \tag{3.4}$$

The moments for these weights can be expressed in the form:

$$\mu_k^{(1)} = \int_0^{+\infty} t^k w_1(t)dt = \begin{cases} 1, & k=0, \\ \log 2, & k=1, \\ \dfrac{2^{k-1}-1}{4^{k-1}} k!\zeta(k), & k \ge 2 \end{cases}$$

and

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

respectively, where E_k are Euler's numbers and $\psi(z)$ is the so-called digamma function, i.e., the logarithmic derivative of the gamma function, $\psi(z) = \Gamma'(z)/\Gamma(z)$.

In the cases studied in this subsection, the recurrence coefficients α_k and β_k in (3.2) are not rational numbers, so that the option `Algorithm -> Symbolic` in their construction (by the procedure `aChebyshevAlgorithm` in our MATHEMATICA package `OrthogonalPolynomials`) cannot be applied. Therefore, in these cases, we use the variable-precision arithmetic to overcome the numerical instability in the numerical construction of α_k and β_k, by setting `WorkingPrecision` to be sufficiently large. For example, if we want to construct the first 50 recursion coefficients, with `WorkingPrecision->80`, we only need to execute the following commands:

```
<< OrthogonalPolynomials`
momBE=Table[(k+1)!Zeta[k+2],{k,0,199}];
{al,be}=aChebyshevAlgorithm[momBE, WorkingPrecision->80];
```

Taking larger `WorkingPrecision`, for example `100`,

```
{al1,be1}=aChebyshevAlgorithm[momBE, WorkingPrecision->100];
N[Max[Abs[al/al1-1],Abs[be/be1-1]],3]
```

we get the maximal relative error in the previous recurrence coefficients `{al,be}` to be 1.61×10^{-43}.

§4. Laplace transform method

Consider the two series

$$T = \sum_{k=1}^{+\infty} a_k \quad \text{and} \quad S = \sum_{k=1}^{+\infty} (-1)^k a_k. \tag{4.1}$$

Suppose that the general term of the series in (4.1) is expressible in terms of the Laplace transform, or its derivative, of a known function.

Let

$$f(s) = \int_0^{+\infty} e^{-st} g(t) dt, \quad \Re s \geq 1.$$

Then for $a_k = f(k)$, we have

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

i.e.,

$$T = \sum_{k=1}^{+\infty} f(k) = \int_0^{+\infty} \frac{g(t)}{t} \cdot \frac{t}{e^t - 1} dt. \tag{4.2}$$

Similarly, for "alternating" series, we have

$$S = \sum_{k=1}^{+\infty} (-1)^k f(k) = \int_0^{+\infty} (-g(t)) \frac{1}{e^t + 1} dt. \tag{4.3}$$

Also, if $a_k = f'(k)$, we can get

$$\sum_{k=1}^{+\infty} f'(k) = -\sum_{k=1}^{+\infty} \int_0^{+\infty} t e^{-kt} g(t) dt = \int_0^{+\infty} (-g(t)) \frac{t}{e^t - 1} dt$$

and

$$\sum_{k=1}^{+\infty} (-1)^k f'(k) = \sum_{k=1}^{+\infty} (-1)^{k-1} \int_0^{+\infty} t e^{-kt} g(t) dt = \int_0^{+\infty} (t g(t)) \frac{1}{e^t + 1} dt.$$

Thus, the *summation of series* is now transformed to an equivalent *integration problem.*

The first idea for the numerical integration of these integrals is the application of the Gauss-Laguerre quadrature, but its convergence can be very slow because of the presence of poles on the imaginary axis at the points $\pm 2\pi i$, $\pm 4\pi i$, $\ldots$ (in the case of integrals for T) and $\pm \pi i$, $\pm 3\pi i$, $\ldots$ (in the case of integrals for S).

Another approach for the integration over $(0, +\infty)$,

$$\int_0^{+\infty} h(t)w(t)dt = \sum_{\nu=1}^{N} A_\nu h(x_\nu) + R_N(h), \tag{4.4}$$

with respect to the weight functions $w(t) = \varepsilon(t)$ (Bose-Einstein weight) and $w(t) = \varphi(t)$ (Fermi-Dirac weight), was developed by Gautschi and Milovanović [15] (see also [10] and [23]).

§5. Contour integration method

An alternative summation/integration procedure for the series (4.1) with $a_k = f(k)$, when the function f is analytic in the region

$$\big\{z \in \mathbb{C} \ \big| \ \Re z \geq \alpha, \ m-1 < \alpha < m\big\} \tag{5.1}$$

was considered in [21] (see also [22] and [23]). This method requires the indefinite integral F of f chosen so as to satisfy certain decay properties.

Here we consider a more general version of this method which can be applied also to finite sums. In fact, we consider the series

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

with an analytic (holomorphic) function f in

$$G = \Big\{z \in \mathbb{C} \, : \, \alpha \leq \Re z \leq \beta, \, |\Im z| \leq \frac{\delta}{\pi}\Big\},$$

where $m, n \in \mathbb{Z}$, $m < n \leq +\infty$, and $m-1 < \alpha < m$, $n < \beta < n+1$, $\delta > 0$, $\Gamma = \partial G$.

By contour integration of a product of functions $z \mapsto f(z)g(z)$ over the rectangle Γ in the complex plane, where $g(z) = \pi/\tan \pi z$ and $g(z) = \pi/\sin \pi z$, we are able to reduce the summation of the series $T_{m,n}$ and $S_{m,n}$ to a problem of numerical integration with Gaussian quadrature rules on $(0, +\infty)$, respectively, with respect to the first and second hyperbolic weight functions of (3.4). The moments of these weights are given in subsection 3.2.

For a holomorphic function f in G, by Cauchy's residue theorem, we obtain

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

After integration by parts, these formulas reduce to

$$T_{m,n} = \frac{1}{2\pi i}\oint_\Gamma \Big(\frac{\pi}{\sin \pi z}\Big)^2 F(z)dz \quad \text{and} \quad S_{m,n} = \frac{1}{2\pi i}\oint_\Gamma \Big(\frac{\pi}{\sin \pi z}\Big)^2 \cos \pi z\, F(z)dz, \tag{5.3}$$

where F is an integral of f.

Assume now the following conditions for the function F (cf. [18, p. 57]):

(C1) F *is a holomorphic function in the region (5.1),*

(C2) $\lim\limits_{|t|\to+\infty} e^{-c|t|}F\left(x+it/\pi\right)=0$, *uniformly for* $x \geq \alpha$,

(C3) $\lim\limits_{x\to+\infty} \int_{-\infty}^{+\infty} e^{-c|t|}\left|F\left(x+it/\pi\right)\right| dt = 0$,

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

Setting $\alpha = m-1/2$, $\beta = n+1/2$ and letting $\delta \to +\infty$, we can prove that the integrals in (5.3) over Γ reduce to integrals along the lines $z=\alpha+iy$ and $z=\beta+iy$ ($-\infty<y<+\infty$). Namely, under condition (C2), the integrals on the lines $z = x \pm i(\delta/\pi)$, $\alpha \leq x \leq \beta$, tend to zero when $\delta\to+\infty$. In the case $n=\infty$, the condition (C3) implies that the integrals over the line $z=\beta+iy$, when $\delta\to+\infty$ and $\beta\to+\infty$, also tend to zero. Thus,

$$T_{m,n} = \int_0^{+\infty} \Phi_{m,n}(t)w_1(t)dt \quad \text{and} \quad S_{m,n} = \int_0^{+\infty} \Psi_{m,n}(t)w_2(t)dt, \tag{5.4}$$

where w_1 and w_2 are hyperbolic weight functions defined in (3.4) and the functions $t\mapsto\Phi_{m,n}(t)$ and $t\mapsto\Psi_{m,n}(t)$ can be expressed in terms of the real and imaginary parts of the function $F(z)$.

Formulas (5.4) suggest to apply Gaussian quadrature to the integrals on the right, using the weight functions w_1 and w_2, respectively, i.e.,

$$\int_0^{+\infty} g(t)w_s(t)dt = \sum_{\nu=1}^{N} A_{\nu,s}^N g(\tau_{\nu,s}^N) + R_{N,s}(g) \qquad (s=1,2), \tag{5.5}$$

where $A_{\nu,s}^N$ and $\tau_{\nu,s}^N$, $\nu = 1, \ldots, N$ $(s = 1, 2)$, are parameters of these quadratures and the remainders $R_{N,s}(g) = 0$ $(s = 1, 2)$ for all $g \in \mathbb{P}_{2N-1}$. The required recursion coefficients for the corresponding orthogonal polynomials (in the numerical construction of Gaussian quadratures (5.5)) can be computed using the moments which are given in subsection 3.2 (last case).

In this way we obtain the following statements (cf. [21, 23]):

Theorem 5.1. *Let F be an integral of f such that conditions* (C1)–(C3) *are satisfied with $c = 2$. If $A_{\nu,1}^N$ and $\tau_{\nu,1}^N$, $\nu = 1, \ldots, N$, are the weights and nodes of the N-point Gaussian quadrature rule* (5.5) *with respect to the weight function $w_1(t) = 1/\cosh^2 t$ on $\mathbb{R}_+$, then*

$$T_{m,n} = \sum_{k=m}^{n} f(k) = \sum_{\nu=1}^{N} A_{\nu,1}^N \Phi_{m,n}\Big(\frac{\tau_{\nu,1}^N}{\pi}\Big) + R_{N,1}(\Phi_{m,n}),$$

where

$$\Phi_{m,n}(t) = \Phi\Big(m - \frac{1}{2}, \frac{t}{\pi}\Big) - \Phi\Big(n + \frac{1}{2}, \frac{t}{\pi}\Big)$$

and $\Phi(x, y)$ is defined by

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

Theorem 5.2. *Let F be an integral of f such that conditions* (C1)–(C3) *are satisfied with $c = 1$. If $A_{\nu,2}^N$ and $\tau_{\nu,2}^N$, $\nu = 1, \ldots, N$, are the weights and nodes of the N-point Gaussian quadrature rule* (5.5) *with respect to the weight function $w_2(t) = \sinh t/\cosh^2 t$ on $\mathbb{R}_+$, then*

$$S_{m,n} = \sum_{k=m}^{n} (-1)^k f(k) = \sum_{\nu=1}^{N} A_{\nu,2}^N \Psi_{m,n}\Big(\frac{\tau_{\nu,2}^N}{\pi}\Big) + R_{N,2}(\Psi_{m,n}),$$

where

$$\Psi_{m,n}(t) = (-1)^m \Psi\Big(m - \frac{1}{2}, \frac{t}{\pi}\Big) + (-1)^n \Psi\Big(n + \frac{1}{2}, \frac{t}{\pi}\Big)$$

and $\Psi(x, y)$ is defined by

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

At the end of this section we mention an integral representation of the well-known (generalized) Mathieu series

$$S_m(r)=\sum_{n\geq 1}\frac{2n}{(n^2+r^2)^{m+1}}\quad\text{and}\quad \widetilde{S}_m(r)=\sum_{n\geq 1}(-1)^{n-1}\frac{2n}{(n^2+r^2)^{m+1}},$$

obtained by applying the previous transformation [27]:

Theorem 5.3. *For each $m\in\mathbb{N}$ and $r>0$ we have*

$$S_m(r)=\frac{\pi}{m}\int_0^{\infty}\frac{\sum\limits_{j=0}^{[m/2]}(-1)^j\binom{m}{2j}\left(r^2-x^2+\frac{1}{4}\right)^{m-2j}x^{2j}}{\left[\left(x^2-r^2+\frac{1}{4}\right)^2+r^2\right]^m}w_1(\pi x)\,dx$$

and

$$\widetilde{S}_m(r)=\frac{\pi}{m}\int_0^{\infty}\frac{\sum\limits_{j=0}^{[(m-1)/2]}(-1)^j\binom{m}{2j+1}\left(r^2-x^2+\frac{1}{4}\right)^{m-2j-1}x^{2j+1}}{\left[\left(x^2-r^2+\frac{1}{4}\right)^2+r^2\right]^m}w_2(\pi x)\,dx,$$

where w_1 and w_2 are the hyperbolic weights given in (3.4).

By means of these newly established integral forms of generalized Mathieu series, we have also obtained a new integral expression for the *Bessel function of the first kind of half integer order* $J_{m-1/2}$, solving a related *Fredholm integral equation of the first kind* with nondegenerate kernel (see [27]).

The series $S_1(r)$ was introduced and studied for the first time by Émile Leonard Mathieu (1835–1890) in his book devoted to the elasticity of solid bodies [20].

§6. Numerical examples

Example 6.1. Consider two simple series

$$T=\sum_{k=1}^{+\infty}\frac{1}{(k+1)^2}=\frac{\pi^2}{6}-1\qquad\text{and}\qquad S=\sum_{k=1}^{+\infty}\frac{(-1)^k}{(k+1)^2}=\frac{\pi^2}{12}-1.$$

Summation of the series T

(a) *Application of the Plana formula*

We first apply the formula (2.8), with $n=\infty$, to the series T, using m as an integer parameter. In that case we have

$$\begin{aligned} T=\sum_{k=1}^{+\infty} f(k) &= \sum_{k=1}^{m} f(k)-\frac{1}{2}f(m)+T_{m,\infty} \\ &= \sum_{k=1}^{m} f(k)-\frac{1}{2}f(m)+\int_m^{+\infty} f(x)dx-\int_{\mathbb{R}}\phi_m(y)w^P(x)dy \\ &= U_m(f)-\int_{\mathbb{R}}\phi_m(y)w^P(x)dy, \end{aligned}$$

where $\phi_m(y)$ and $w^P(x)$ are defined in (2.9),

$$U_m(f)=\sum_{k=1}^{m} f(k)-\frac{1}{2}f(m)+\int_m^{+\infty} f(x)dx$$

and $f(x)=1/(x+1)^2$.

For the integral $I(\phi_m)=\int_{\mathbb{R}}\phi_m(y)w^P(x)dy$, we construct the Gaussian quadratures with the Plana weight $w^P(x)$, $Q_N(\phi_m)=\sum\limits_{\nu=1}^{N} A_\nu^{(N)}\phi_m(x_\nu^{(N)})$, for $N=5(5)50$ (that is to say for N from 5 to 50 with step 5, we use this notation later with the same sense) and `Precision->50`, using our Mathematica package:

```
<< orthogonalPolynomials`
moments=Table[If[OddQ[k],0,(-1)^(k/2)BernoulliB[k+2]/(k+2)], {k,0,99}];
{al,be}=aChebyshevAlgorithm[moments, Algorithm -> Symbolic];
pq[n_]:=aGaussianNodesWeights[n,al,be,WorkingPrecision->55, Precision->50];
nw=Table[pq[n], {n,5,50,5}];
```

The corresponding nodes and weights are the elements of the list `nw` in the Mathematica code. For example, for $N=15$ the nodes are `nw[[3]][[1]]` and the weights are `nw[[3]][[2]]` (the lengths of these lists are 15).

N	$m=1$	$m=2$	$m=3$	$m=4$	$m=5$	$m=0$	BEQ
5	2.0(−6)	2.4(−8)	8.1(−10)	5.4(−11)	5.7(−12)	1.1(−5)	3.0(−4)
10	2.7(−8)	4.4(−11)	2.5(−13	3.4(−15)	8.7(−17)	1.5(−8)	1.1(−8)
15	1.7(−9)	7.1(−13)	1.1(−15	4.5(−18)	3.6(−20)	3.4(−10)	3.2(−13)
20	2.2(−10)	3.3(−14)	1.9(−17)	3.0(−20)	9.5(−23)	1.9(−12)	8.0(−18)
25	4.4(−11)	2.9(−15)	7.5(−19)	5.3(−22)	7.9(−25)	3.1(−14)	1.8(−22)
30	1.2(−11)	3.9(−16)	5.1(−20)	1.8(−23)	1.4(−26)	2.1(−15)	3.9(−27)
35	3.7(−12)	6.9(−17)	5.1(−21)	1.0(−24)	4.7(−28)	6.8(−17)	8.2(−32)
40	1.4(−12)	1.5(−17)	6.9(−22)	8.4(−26)	2.3(−29)	2.6(−18)	1.7(−36)
45	5.7(−13)	4.0(−18)	1.1(−22)	9.1(−27)	1.6(−30)	8.6(−19)	3.3(−41)
50	2.6(−13)	1.2(−18)	2.3(−23)	1.2(−27)	1.4(−31)	1.2(−19)	6.5(−46)

Table 1: Applications of Plana formula and Laplace transform method to the series T. Relative errors in the Gaussian approximation (numbers in parentheses indicate decimal exponents).

The relative errors in the Gaussian approximations $T \approx T^{(N,m)} = U_m(f) - Q_N(\phi_m)$,

$$r_{N,m} = \left| \frac{T^{(N,m)} - T}{T} \right| = \left| \frac{I(\phi_m) - Q_N(\phi_m)}{T} \right|,$$

are given in Table 1 for $N = 5(5)50$ and $m = 1(1)5$. The rapid speed of convergence of the Gaussian rule (with the Plana weight) as m increases is due to the poles $\pm i(m+1)$ (second order!) of the function

$$y \mapsto \phi_m(y) = -\frac{2(m+1)}{[(m+1)^2 + y^2]^2}$$

moving away from the real line.

This influence of the poles to the convergence can be also reduced if the integration is performed only over the semiaxis $\mathbb{R}_+$. For example, if we apply the original Plana formula (2.4), where the integration is over $\mathbb{R}_+$ (practically, with respect to the Bose-Einstein function), i.e.,

$$T = \sum_{k=1}^{+\infty} f(k) = \int_0^{+\infty} f(x)dx - \frac{1}{2}f(0) - \frac{1}{2\pi^2}\int_0^{+\infty} \phi_0\left(\frac{t}{2\pi}\right) \cdot \frac{t}{e^t - 1}dt,$$

the relative errors in the corresponding Gaussian approximation are presented in the penultimate column of the same table (with $m = 0$).

(b) *Application of the Laplace transform method*

In the last column of Table 1 (BEQ) we give the relative errors in N-point Gaussian approximation (w.r.t. the Bose-Einsten weight) in the case of the Laplace transform method. In that case, for $f(s) = (s+1)^{-2}$ we have $g(t) = te^{-t}$, so that, according to (4.2) and (4.4),

$$T = \sum_{k=1}^{+\infty} \frac{1}{(k+1)^2} = \int_0^{+\infty} e^{-t} \frac{t}{e^t - 1} dt \approx \sum_{\nu=1}^{N} A_\nu \exp(-x_\nu),$$

where x_ν and A_ν, $\nu = 1, \ldots, N$, are nodes and weights in (4.4) when $w(t) = \varepsilon(t) = t/(e^t - 1)$.

It is interesting to note that the previous trick of "moving m" with the Laplace transform method does not lead to acceleration of convergence. For example, in this case we have that

$$T = \sum_{k=1}^{m-1} \frac{1}{(k+1)^2} + \sum_{k=1}^{+\infty} \frac{1}{(k+m)^2} = \sum_{k=1}^{m-1} \frac{1}{(k+1)^2} + \int_0^{+\infty} e^{-mt} \frac{t}{e^t - 1} dt.$$

The convergence of the corresponding quadrature process (as m increases) slows down considerably (see [21]). The reason for this is the behavior of the function $t \mapsto e^{-mt}$, which tends to a discontinuous function when $m \to +\infty$. On the other hand, the function is entire, which explains the ultimately much better results for $m = 1$.

(c) *Application of the contour integration method*

We put

$$T = \sum_{k=1}^{m-1} \frac{1}{(k+1)^2} + \sum_{k=m}^{+\infty} \frac{1}{(k+1)^2} = \sum_{k=1}^{m-1} \frac{1}{(k+1)^2} + T_{m,\infty},$$

where the first sum on the right-hand side for $m = 1$ is empty. We apply now the Gaussian rule with respect to the hyperbolic weight $w_1(t) = 1/\cosh^2 t$ to the second sum, $T_{m,\infty}$,

$$T_{m,\infty} = \int_0^{+\infty} w_1(t) \Phi\Big(m - \frac{1}{2}, \frac{t}{\pi}\Big) dt \approx Q_{N,1}(\Phi_{m,\infty}) = \sum_{\nu=1}^{N} A_{\nu,1}^N \Phi\Big(m - \frac{1}{2}, \frac{\tau_{\nu,1}^N}{\pi}\Big),$$

where $f(z) = 1/(z+1)^2$, $F(z) = -1/(z+1)$ (the integration constant being zero on account of the condition (C3)), and

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

Notice that $\Phi_{m,\infty}(t) = \Phi(m - 1/2, t/\pi)$ because $\lim\limits_{n \to +\infty} \Phi(n + 1/2, t/\pi) = 0$.

N	$m=1$	$m=2$	$m=3$	$m=4$	$m=5$
5	1.3(−7)	5.4(−9)	1.9(−10)	8.6(−12)	3.7(−13)
10	1.1(−10)	1.1(−13)	1.7(−16)	7.9(−18)	2.0(−19)
15	1.1(−13)	3.8(−17)	3.7(−20)	1.1(−22)	3.8(−25)
20	1.4(−15)	4.0(−20)	1.2(−24)	1.9(−27)	2.3(−29)
25	6.2(−18)	1.1(−22)	2.0(−27)	2.6(−30)	2.5(−33)
30	2.6(−19)	1.4(−25)	1.1(−31)	2.0(−33)	8.1(−37)
35	5.6(−21)	3.2(−27)	2.3(−32)	2.3(−36)	2.5(−40)
40	1.3(−22)	3.6(−30)	1.5(−34)	3.8(−39)	1.6(−43)
45	4.2(−24)	4.0(−31)	6.5(−38)	4.2(−42)	3.4(−46)
50	1.9(−25)	6.5(−33)	6.6(−39)	2.8(−44)	1.2(−48)

Table 2: Application of the contour integration method to the series T. Relative errors in the Gaussian approximation.

The relative errors in the Gaussian approximations,

$$T \approx T^{(N,m)} = \sum_{k=1}^{m-1} \frac{1}{(k+1)^2} + Q_{N,1}(\Phi_{m,\infty}),$$

can be expressed in the form $r_{N,m} = |(T^{(N,m)} - T)/T|$ and they are presented in Table 2 for $N = 5(5)50$ and $m = 1(1)5$. As we can see, the convergence is very fast!

Summation of the series S

According to (2.6) (for $n = \infty$), the series S can be expressed in the form

$$\begin{aligned} S &= \sum_{k=1}^{+\infty}(-1)^k f(k) = \sum_{k=1}^{m-1}(-1)^k f(k) + \sum_{k=1}^{+\infty}(-1)^k f(k) \\ &= \sum_{k=1}^{m-1}(-1)^k f(k) + \frac{1}{2}(-1)^m f(m) - \int_{\mathbb{R}} \psi_m(y) w^A(y)\,dy, \end{aligned}$$

where the function $y \mapsto \psi_m(y)$ and the Abel weight $w^A(y)$ are defined in (2.7). The recurrence coefficients for the orthogonal polynomials in this case are known explicitly and given in subsection

3.1 (Abel weight), so that we can calculate the parameters of the corresponding Gaussian formula in the following way:

```
<< orthogonalPolynomials`
al = Table[0, {k,0,49}]; be = Join[{1/4}, Table[k(k+1)/4, {k,1,49}]];
pq[n_]:=aGaussianNodesWeights[n,al,be,WorkingPrecision->55, Precision->50];
nw=Table[pq[n], {n,5,50,5}];
```

Relative errors in Gaussian approximations for $N = 5(5)50$ and $m = 1$, $m = 2$, and $m = 3$, are presented in Table 3.

Applying the Gaussian quadrature rule with respect to the Fermi-Dirac weight function $\varphi(t) = 1/(e^t+1)$ to the integral on the right side in (4.3), we obtain approximations with relative errors given also in Table 3 (FDQ-column).

N	Gauss-Abel formula (2.6)			Eq. (4.3)	Theorem 5.2				
	$m=1$	$m=2$	$m=3$	FDQ	$m=1$	$m=2$	$m=3$	$m=4$	$m=5$
5	1.9(−3)	5.7(−5)	3.4(−6)	1.2(−3)	1.1(−4)	1.9(−6)	2.2(−7)	1.5(−8)	4.5(−10)
10	2.3(−4)	2.3(−6)	4.7(−8)	6.5(−8)	3.5(−7)	1.9(−9)	2.3(−12)	1.0(−12)	1.1(−14)
15	6.0(−5)	2.9(−7)	3.0(−9)	2.1(−12)	5.0(−9)	8.1(−13)	1.9(−15)	3.2(−16)	9.2(−18)
20	2.2(−5)	6.5(−8)	3.9(−10)	5.5(−17)	8.9(−11)	6.6(−14)	1.1(−16)	6.2(−19)	7.6(−21)
25	1.0(−5)	1.9(−8)	7.7(−11)	1.3(−21)	3.4(−12)	6.2(−16)	6.8(−19)	2.5(−21)	1.3(−23)
30	5.3(−6)	7.2(−9)	2.0(−11)	3.0(−26)	2.4(−13)	2.4(−18)	9.7(−21)	1.2(−24)	1.3(−26)
35	3.0(−6)	3.1(−9)	6.5(−12)	6.4(−31)	2.0(−14)	1.1(−19)	4.3(−23)	1.3(−25)	2.1(−28)
40	1.9(−6)	1.5(−9)	2.4(−12)	1.3(−35)	1.5(−15)	5.6(−21)	1.3(−24)	1.1(−27)	9.8(−31)
45	1.2(−6)	7.6(−10)	9.9(−13)	2.7(−40)	4.2(−17)	8.3(−23)	6.7(−26)	3.8(−30)	2.0(−32)
50	8.2(−7)	4.2(−10)	4.5(−13)	5.4(−45)	1.1(−17)	1.7(−23)	2.6(−27)	4.1(−31)	8.9(−35)

Table 3: Application of summation/integration methods to the series S. Relative errors in Gaussian approximation.

Finally, applying the contour integration method to the series S (see Theorem 5.2), for $N = 5(5)50$ nodes and $m = 1(1)5$, we get the Gaussian approximations,

$$S \approx S^{(N,m)} = \sum_{k=1}^{m-1} \frac{(-1)^k}{(k+1)^2} + Q_{N,2}(\Psi_{m,\infty}),$$

where

$$Q_{N,2}(\Psi_{m,\infty}) = \sum_{\nu=1}^{N} A_{\nu,2}^{N} \Psi\Big(m - \frac{1}{2}, \frac{\tau_{\nu,2}^{N}}{\pi}\Big).$$

The relative errors, $r_{N,m} = |(S^{(N,m)} - S)/S|$, are presented in the last five columns in Table 3.

As we can see the Laplace transform method is most efficient in this case.

Example 6.2. We consider now the series

$$T_1(a) = \sum_{k=1}^{+\infty} \frac{1}{\sqrt{k}(k+a)} \qquad (a \geq 0).$$

$T_1(1)$ appears in a study of spirals and defines the well-known *Theodorus constant* (see Davis [8]). The series is slowly convergent. The first 1 000 000 terms of $T_1(1)$ give the result $T_1(1) = 1.8580\ldots \approx 1.86$ (only 3-digit accuracy).

In 1991 Gauutschi [10] calculated $T_1(a)$ by using the method of the Laplace transform for different values of a (≤ 32). As a increases, the convergence of the Gauss quadrature formula slows down considerably. For example, when $a = 8$, the corresponding quadrature with $N = 40$ nodes gives a result with relative error 2.6×10^{-8}.

In a special case for $a = 1$, Gautschi [14] has recently proved that

$$T_1(1) = \frac{2}{\sqrt{\pi}} \int_0^{+\infty} \frac{D(\sqrt{t})}{\sqrt{t}}\, w(t)dt,$$

where D is Dawson's integral $D(x) = e^{-x^2} \displaystyle\int_0^x e^{t^2} dt$ and w is the corresponding weight function given by $w(t) = t^{-1/2}\varepsilon(t) = \sqrt{t}/(e^t - 1)$. In the construction of Gaussian quadratures with respect to this weight, the moments are

$$\mu_k = \int_0^{+\infty} \frac{t^{k+1/2}}{e^t - 1} dt = \Gamma\Big(k + \frac{3}{2}\Big)\zeta\Big(k + \frac{3}{2}\Big), \quad k = 0, 1, \ldots,$$

where the gamma function and the Riemann zeta function are computable by variable-precision calculation.

Using the Chebyshev algorithm with sufficiently high precision, Gautschi [14] has obtained Gaussian quadratures and applied them to the summation of this series for $N = 5(10)75$.

N	$Q_{10}^{(N)}(1)$
5	$1.86002507922119\boxed{16\ldots}$
15	$1.86002507922119030718069591571 71\boxed{74\ldots}$
25	$1.8600250792211903071806959157171433246665241\boxed{43\ldots}$
35	$1.860025079221190307180695915717143324666524121523451\boxed{53\ldots}$
45	$1.86002507922119030718069591571714332466652412152345149304919 9\boxed{21\ldots}$
55	$1.8600250792211903071806959157171433246665241215234514930491995035983\boxed{80\ldots}$

Table 4: Gaussian approximation of the sum $T_1(1)$.

Now, we directly apply the *method of contour integration* to $T_m(a)$, where

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

Then we use the Gaussian quadrature formula with respect to the weight function $w_1(t) = 1/\cosh^2 t$ on $\mathbb{R}_+$ to calculate $T_m(a)$.

In order to construct Gaussian rules for $N \le 100$, we need the recursion coefficients α_k and β_k for $k \le N-1 = 99$, i.e., the moments for $k \le 2N-1 = 199$. Taking the `WorkingPrecision` to be 160, we obtain the first hundred recursion coefficients α_k and β_k, with relative errors less than 1.86×10^{-78}.

For this series we have

$$f(z) = \frac{1}{\sqrt{z}(z+a)} \quad \text{and} \quad F(z) = \frac{2}{\sqrt{a}}\left(\arctan\sqrt{\frac{z}{a}} - \frac{\pi}{2}\right),$$

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

$$T_1(a) \approx Q_m^{(N)}(a) = \sum_{k=1}^{m-1} \frac{1}{\sqrt{k}(k+a)} + \sum_{\nu=1}^{N} A_{\nu,1}^N \Phi\Big(m - \frac{1}{2}, \frac{\tau_{\nu,1}^N}{\pi}\Big),$$

where $\Phi(x,y)$ is defined in Theorem 5.1. The Gaussian approximation $Q_m^{(N)}(a)$ for $a = 1$, $m = 10$, and $N = 5(10)55$ are presented in Table 4. Boxed digits are in error.As we can see the method is very efficient.

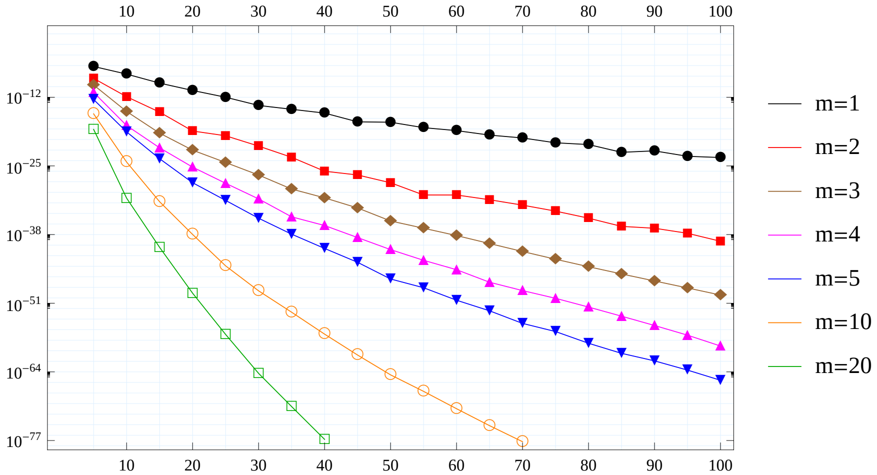

Figure 4: Relative errors in the Gaussian approximation $T_1(1) \approx Q_m^{(N)}(1)$ for $N = 5(5)100$ and some selected values of m.

Relative errors of $Q_m^{(N)}(1)$ for $N = 5(5)100$ and different values of m (≤ 20) are presented in Figure 4 in a log-scale.

Numerical results also show that the convergence is slightly faster if the parameter a is larger. For example, if $a = 1000$, then taking $m = 20$ and $N = 5(5)25$, the corresponding relative errors in the Gaussian approximations are $2.32(-20)$, $1.06(-33)$, $6.01(-43)$, $1.18(-51)$, $1.89(-59)$, respectively.

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Gradimir V. Milovanović,
Mathematical Institute,
Serbian Academy of Sciences and Arts,
Kneza Mihaila 36,
11000 Beograd, Serbia.
gvm@mi.sanu.ac.rs