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On summation/integration methods for slowly convergent series

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Dedicated to Professor Gheorghe Coman on the occasion of his 80th anniversary

Abstract. A survey on summation/integration methods for computation of slowly convergent series is presented. Methods are based on some transformations of series to integrals, with respect to certain nonclassical weight functions over $\mathbb{R}_+$, and an application of suitable quadratures of Gaussian type for numerical calculating of such integrals with a high accuracy. In particular, applications to some series with irrational terms are considered. Several numerical examples are included in order to illustrate the efficiency of these methods.

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1. Introduction

In this paper we give an account on the so-called *summation/integration* methods for fast summation of slowly convergent series and present their application, including series with irrational terms. We consider convergent series of the form

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

with a given function $z \mapsto f(z)$, with certain properties with respect to the variable z. Here, the function f can depend on several other parameters, e.g., $f(z; x, y, \ldots)$, so that these summation processes can be applied also to some classes of functional series, not only to numerical series. Regarding the properties of the function f is often appropriate to extract a finite number of first terms in (1.1), e.g.,

$$\sum_{k=1}^{+\infty}(\pm 1)^k f(k) = \sum_{k=1}^{m-1}(\pm 1)^k f(k) + \sum_{k=m}^{+\infty}(\pm 1)^k f(k), \tag{1.2}$$

and then apply the procedure to the series starting with the index $k = m$.

The basic idea of these methods is to transform the second series in (1.2) (or directly the series (1.1) if $m = 1$) to an integral with respect to certain weight function w on $\mathbb{R}_+$, and then to approximate this weighted integral by a quadrature sum,

$$\sum_{k=m}^{+\infty} (\pm 1)^k f(k) = \int_0^{+\infty} g(t)w(t)\,\mathrm{d}t \approx \sum_{\nu=1}^{N} A_\nu g(\tau_\nu), \tag{1.3}$$

where the function g is connected with the original function f in some way.

Thus, such summation/integration methods need two steps: (1) transformation "sum to integral"; (2) construction of the quadrature rules

$$\int_0^{+\infty} g(t)w(t)\,\mathrm{d}t = \sum_{\nu=1}^{N} A_\nu g(\tau_\nu) + R_N(g; w), \tag{1.4}$$

with respect to the weight function w.

In our approach in (1.4) we take the Gaussian quadrature formulas, where the nodes $\tau_\nu \equiv \tau_\nu^{(n)}$ and the weight coefficients (Christoffel numbers) $A_\nu \equiv A_\nu^{(n)}$, $\nu = 1, \ldots, N$, can be determined by the well-known Golub-Welsch algorithm [6] if we know the coefficients in the three-term recurrence relation of the corresponding polynomials orthogonal with respect to the weight function w. Usually the weight function w is *strong non-classical* and those recursive coefficients must 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 (cf. [2]). The problem is very sensitive with respect to small perturbations in the data. The basic references are [2], [4], [8], and [10].

For the construction of Gaussian quadrature rules (1.4) with respect to the strong non-classical weight functions w on $\mathbb{R}_+$ today we use a recent progress in symbolic computation and variable-precision arithmetic, as well as our MATHEMATICA package `OrthogonalPolynomials` (see [1], [12]). The package is downloadable from Web Site: `http://www.mi.sanu.ac.rs/ gvm/`. 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 weight function w (cf. [2], [4], [8], [10]). In this construction we need only a procedure for the symbolic calculation of moments or their calculation in variable-precision arithmetic.

In the sequel, we mention only two methods for such kind of transformations: *Laplace transform method* and *Contour integration over a rectangle*, including a similar procedure for series with irrational terms. Several numerical examples are given in order to illustrate the efficiency of these methods.

2. Laplace transform method

In this section we present the basic idea of the *Laplace transform method* and give some considerations about applicability of this method. For details and several examples see [5], [8, pp. 398–401] and [11].

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

Consider only the case when

$$f(s) = \mathcal{L}[g(t)] = \int_0^{+\infty} \mathrm{e}^{-st} g(t)\,\mathrm{d}t, \quad \operatorname{Re} s \geq 1.$$

Then

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

i.e.,

$$\sum_{k=1}^{+\infty} (\pm 1)^k f(k) = \int_0^{+\infty} \frac{\pm \mathrm{e}^{-t}}{1 \mp \mathrm{e}^{-t}}\, g(t)\,\mathrm{d}t = \pm \int_0^{+\infty} \frac{1}{\mathrm{e}^t \mp 1}\, g(t)\,\mathrm{d}t.$$

In this way, the *summation of series* (1.1) is transformed to *integration problems*

$$T = \sum_{k=1}^{+\infty} f(k) = \int_0^{+\infty} \mathrm{e}^{-t} \frac{g(t)}{1 - \mathrm{e}^{-t}}\,\mathrm{d}t = \int_0^{+\infty} \frac{t}{\mathrm{e}^t - 1} \frac{g(t)}{t}\,\mathrm{d}t \tag{2.1}$$

and

$$S = \sum_{k=1}^{+\infty} (-1)^k f(k) = \int_0^{+\infty} \frac{1}{\mathrm{e}^t + 1} (-g(t))\,\mathrm{d}t. \tag{2.2}$$

The first integral representation (2.1) for the series T suggests an application of the Gauss-Laguerre quadrature rule (with respect to the exponential weight $w(t) = \mathrm{e}^{-t}$) to the function

$$\frac{g(t)}{1 - \mathrm{e}^{-t}} = \frac{t}{1 - \mathrm{e}^{-t}} \frac{g(t)}{t},$$

supposing that $g(t)/t$ is a smooth function. However, the convergence of these Gauss-Laguerre rules can be very slow, according to the presence of poles on the imaginary axis at the points $2k\pi\mathrm{i}$ ($k = \pm 1, \pm 2, \ldots$).

Therefore, a better choice is the second integral representation in (2.1), with the Bose-Einstein weight function $\varepsilon(t) = t/(\mathrm{e}^t - 1)$ on $\mathbb{R}^+$. Supposing again that $t \mapsto g(t)/t$ is a smooth function, the corresponding Gauss-Bose-Einstein quadrature formula converges rapidly.

In the case of "alternating" series, the obtained integral representation (2.2) needs a construction of Gaussian quadrature rule with respect to the Fermi-Dirac weight function $\varphi(t) = 1/(\mathrm{e}^t + 1)$ on $\mathbb{R}^+$.

Thus, for computing series T and S we need the Gauss-Bose-Einstein quadrature rule

$$\int_0^{+\infty} \varepsilon(t) u(t)\,\mathrm{d}t = \sum_{k=1}^{N} A_k u(\xi_k) + R_N(u; \varepsilon) \tag{2.3}$$

and the Gauss-Fermi-Dirac quadrature rule

$$\int_0^{+\infty} \varphi(t)u(t)\,\mathrm{d}t = \sum_{k=1}^{N} B_k u(\eta_k) + R_N(u;\varphi), \tag{2.4}$$

respectively, whose parameters, nodes (ξ_k and η_k) and weight coefficients (A_k and B_k), for each $N \le n$, can be calculated by the MATHEMATICA package `OrthogonalPolynomials`, starting from the corresponding moments of the weight functions, $\mu_k(\varepsilon) = \int_0^{+\infty} x^k\varepsilon(t)\,\mathrm{d}t$ and $\mu_k(\varphi) = \int_0^{+\infty} x^k\varphi(t)\,\mathrm{d}t$, $k = 0, 1, \ldots, 2n-1$. The convergence of the quadrature formulas (2.3) and (2.4) is fast for smooth functions $t \mapsto u(t)$ ($u(t) = g(t)/t$ and $g(t)$), so that low-order Gaussian rules provide one possible summation procedure.

However, if g is no longer smooth function, for example, if its behaviour as $t \to 0$ is such that $g(t) = t^\gamma h(t)$, where $0 < \gamma < 1$ and $h(0)$ is a constant, then the previous formulas for series T and S should be reduced to the following forms

$$T = \int_0^{+\infty} \frac{t^\gamma}{\mathrm{e}^t - 1}\, h(t)\,\mathrm{d}t \tag{2.5}$$

and

$$S = \int_0^{+\infty} \frac{t^\gamma}{\mathrm{e}^t + 1}(-h(t))\,\mathrm{d}t, \tag{2.6}$$

respectively.

Introducing the weight functions from (2.5) and (2.6) as $\varepsilon_\gamma(t)$ and $\varphi_\gamma(t)$, respectively, then their moments are

$$\mu_k(\varepsilon_\gamma) = \zeta(k+\gamma+1)\Gamma(k+\gamma+1), \quad k \ge 0, \tag{2.7}$$

and

$$\begin{aligned} \mu_k(\varphi_\gamma) &= \left(1 - 2^{-k-\gamma}\right)\zeta(k+\gamma+1)\Gamma(k+\gamma+1) \\ &= \left(1 - 2^{-k-\gamma}\right)\mu_k(\varepsilon_\gamma), \quad k \ge 0, \end{aligned} \tag{2.8}$$

where $\Gamma(z)$ is gamma function and $\zeta(z)$ is the Riemann zeta function.

Evidently, the moments for the Bose-Einstein weight are

$$\mu_k(\varepsilon) = \mu_k(\varepsilon_1) = (k+1)!\zeta(k+2), \quad k \ge 0,$$

while for the Fermi-Dirac weight these moments are $\mu_k(\varphi) = \mu_k(\varphi_0)$, except $k = 0$, i.e.,

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

Example 2.1. For the series

$$\sum_{k=1}^{+\infty} \frac{(\pm 1)^k}{k\sqrt{k+1}}$$

we put

$$f(s) = \frac{1}{s\sqrt{s+1}} = \int_0^{+\infty} \mathrm{e}^{-st}\operatorname{erf}(\sqrt{t})\,\mathrm{d}t, \quad \operatorname{Re} s > 0,$$

i.e., $g(t) = \mathrm{erf}(\sqrt{t})$, where $\mathrm{erf}(z)$ is the error function (the integral of the Gaussian distribution), given by

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \mathrm{e}^{-t^2}\,\mathrm{d}t.$$

According to the first integral representation in (2.1), we can apply the Gauss-Laguerre quadrature rule

$$T = \sum_{k=1}^{+\infty} \frac{1}{k\sqrt{k+1}} = \int_0^{+\infty} \mathrm{e}^{-t}\Psi(t)\,\mathrm{d}t = \sum_{\nu=1}^{N} A_\nu^L \Psi(\tau_\nu^L) + R_N^L(\Psi), \tag{2.9}$$

where

$$\Psi(t) = \frac{\mathrm{erf}(\sqrt{t})}{1-\mathrm{e}^{-t}} = \frac{1}{\sqrt{\pi t}}\left(2 + \frac{1}{3}t + \frac{1}{30}t^2 - \frac{1}{315}t^3\right) + O\big(t^{7/2}\big). \tag{2.10}$$

Otherwise, the exact value of T is

$$T = 2.184009470267851952894734157852949070443908406263229420200\ldots$$

(see Example 3.1).

Here we have an example in which the function g is no longer smooth, having a square root singularity at $t = 0$. Relative errors in the Gauss-Laguerre approximations

$$Q_N^{\mathrm{Lag}} = \sum_{\nu=1}^{N} A_\nu^L \Psi(\tau_\nu^L)$$

are given in Table 1. Numbers in parentheses indicate decimal exponents, e.g. 5.01(−3) means 5.03×10^{-3}.

TABLE 1. Relative errors in different quadrature sums in Example 2.1

N	Q_N^{Lag}	Q_N^{BE}	Q_N^{genBE}
10	1.40(−1)	1.57(−1)	6.58(−11)
20	9.98(−2)	1.09(−1)	1.65(−20)
30	8.17(−2)	8.76(−2)	4.46(−30)
40	7.09(−2)	7.53(−2)	1.23(−39)
50	6.34(−2)	6.70(−2)	3.45(−49)

Another way for calculating the value of T is to apply the Gauss-Bose-Einstein quadrature rule (2.3) to the last integral in (2.1), where $u(t) = \mathrm{erf}(\sqrt{t})/t$. The corresponding relative errors in the Bose-Einstein approximations Q_N^{BE} are presented in the same table.

As we can see, these two quadrature sums are quite inefficient. In order to get a quadrature sequence with a fast convergence, we note first that

$$\mathrm{erf}(\sqrt{t}) = \sqrt{\frac{t}{\pi}}\left(2 - \frac{2}{3}t + \frac{1}{5}t^2 - \frac{1}{21}t^3\right) + O\big(t^{9/2}\big).$$

This means that we should take the integral (2.1) in the form

$$T = \sum_{k=1}^{+\infty} \frac{1}{k\sqrt{k+1}} = \int_0^{+\infty} \frac{\sqrt{t}}{\mathrm{e}^t - 1} \frac{\mathrm{erf}(\sqrt{t})}{\sqrt{t}}\,\mathrm{d}t,$$

and then apply the Gaussian rule with respect to the generalized Bose-Einstein weight $t^{-1/2}\varepsilon(t) = \sqrt{t}/(\mathrm{e}^t - 1)$ (see [5] and [3]). In the last column of Table 1 we give the corresponding quadrature approximations Q_N^{genBE}. The fast convergence of Q_N^{genBE} is evident!

3. Method of contour integration over a rectangle

As we have seen in the previous section, the function g in (1.3) is connected with the original function f over its Laplace transform, while the weight functions are $\varepsilon(t) = t/(\mathrm{e}^t - 1)$ and $\varphi(t) = 1/(\mathrm{e}^t + 1)$ (or their generalized forms).

In 1994 we developed a method based on a contour integration over a rectangle Γ in the complex plane [9], in which the weight w in (1.3) is one of the hyperbolic functions

$$w_1(t) = \frac{1}{\cosh^2 t} \quad \text{and} \quad w_2(t) = \frac{\sinh t}{\cosh^2 t}, \tag{3.1}$$

and the function g can be expressed in terms of the indefinite integral F of f chosen so as to satisfy the following decay properties: (see [7], [9], [8]):

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

$$\{z \in \mathbb{C} \mid \mathrm{Re}\, z \geq \alpha,\ m - 1 < \alpha < m\}, \tag{3.2}$$

where $m, n \in \mathbb{Z}$ $(m < n \leq +\infty)$;

(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* $c = 1$ *for "alternating" series*).

Taking $\Gamma = \partial G$ and $G = \{z \in \mathbb{C} : \alpha \leq \mathrm{Re}\, z \leq \beta, |\mathrm{Im}\, z| \leq \delta/\pi\}$ with $m - 1 < \alpha < m$, $n < \beta < n + 1$, and $\delta > 0$, we proved in [9] (see also [8]) that

$$T_{m,n} = \sum_{k=m}^{n} f(k) = \frac{1}{2\pi i} \oint_\Gamma \left(\frac{\pi}{\sin \pi z}\right)^2 F(z)\,\mathrm{d}z \tag{3.3}$$

and

$$S_{m,n} = \sum_{k=m}^{n} (-1)^k f(k) = \frac{1}{2\pi i} \oint_\Gamma \left(\frac{\pi}{\sin \pi z}\right)^2 \cos \pi z\, F(z)\,\mathrm{d}z, \tag{3.4}$$

where F is an integral of f.

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 $(0, +\infty)$,

$$\sum_{k=m}^{+\infty} f(k) = \int_0^{+\infty} w_1(t)\Phi\left(m - \frac{1}{2}, \frac{t}{\pi}\right) \mathrm{d}t \tag{3.5}$$

and

$$\sum_{k=m}^{+\infty}(-1)^k f(k) = (-1)^m \int_0^{+\infty} w_2(t)\Psi\left(m-\frac{1}{2},\frac{t}{\pi}\right)\mathrm{d}t, \tag{3.6}$$

where the weight functions w_1 and w_2 are given by (3.1), and Φ and Ψ by

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

and

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

The integrals (3.5) and (3.6) can be calculated by using the N-point Gaussian quadratures with respect to the hyperbolic weights w_1 and w_2,

$$\int_0^{+\infty} g(t)w_s(t)\,\mathrm{d}t = \sum_{\nu=1}^{N} A_{\nu,s}^N g(\tau_{\nu,s}^N) + R_{N,s}(g) \quad (s=1,2), \tag{3.7}$$

with weights $A_{\nu,s}^N$ and nodes $\tau_{\nu,s}^N$, $\nu=1,\ldots,N$ $(s=1,2)$. Such quadratures are exact for all polynomials of degree at most $2N-1$ ($g\in\mathcal{P}_{2N-1}$) and their numerical construction is given in [9] and [11]. For example, for constructing Gaussian quadratures for $s=1$ and $N\le 50$, we use the first $2N=100$ moments (in symbolic form) and then we construct the recursion coefficients in the three-term recurrence relation for orthogonal polynomials with respect to the hyperbolic weight function w_1 on $(0,+\infty)$. The following procedure in the MATHEMATICA package `OrthogonalPolynomials` provides Gaussian quadratures (with `Precision->60`) for each $N=5(5)50$ (i.e., `{n,5,50,5}`):

```
 <<orthogonalPolynomials`
  f[s_]:=1/(s(s+1)^(1/2));
  F[z_]:=Log[(Sqrt[1+z]-1)/(1+Sqrt[1+z])];
  Phi[x_,y_]:=-Re[F[x+I y]]; w1[x_]:=1/Cosh[x]^2;
  mom=Join[{1,Log[2]},Table[(2^(k-1)-1)k!/4^(k-1)Zeta[k],
      {k,2,99}]];
  {al,be}=aChebyshevAlgorithm[mom,WorkingPrecision->100];
(* {al1,be1}=aChebyshevAlgorithm[mom,WorkingPrecision->130];
   N[Max[Abs[al/al1-1],Abs[be/be1-1]],3] *)
  pq[n_]:=aGaussianNodesWeights[n,al,be,WorkingPrecision->65,
      Precision->60];
  nw=Table[pq[n],{n,5,50,5}];
```

The part between the comment signs (`(*` and `*)`) is used only to determine the maximal relative error in the recursive coefficients, which is, in our case, 4.16×10^{-63}. Therefore, the precision of Gaussian parameters (nodes and weights) is at least 60 decimal digits!

Example 3.1. We again consider the series from Example 2.1.

Here, $f(z)=1/(z\sqrt{1+z})$, and $F(z)=\log\left(\frac{\sqrt{z+1}-1}{\sqrt{z+1}+1}\right)$, the integration constant being zero on account of the condition (C3).

Thus, using the Gaussian quadrature (3.7) (for $s = 1$), we approximate the series T by

$$T = \sum_{k=1}^{+\infty} \frac{1}{k\sqrt{k+1}} \approx Q_{N,m} = \sum_{k=1}^{m-1} \frac{1}{k\sqrt{k+1}} + \sum_{\nu=1}^{N} A_{\nu,1}^{N} \Phi\left(m - \frac{1}{2}, \frac{\tau_{\nu,1}^{N}}{\pi}\right).$$

For $m = 1$ the first sum on the right side is empty. The corresponding code in MATHEMATICA is:

```
Q[m_]:=If[m==1,0,Sum[f[j],{j,1,m-1}]] +
     Table[nw[[k]][[2]].Phi[m-1/2,nw[[k]][[1]]/Pi],{k,1,10}];
```

The quadrature sums $Q_{N,1}$ and $Q_{N,3}$ are presented in Table 2, and $Q_{N,15}$ in Table 3. Digits in error are underlined.

TABLE 2. Quadrature sums $Q_{N,m}$ for $m = 1$ and $m = 3$

N	$Q_{N,1}$	$Q_{N,3}$
5	$2.18\underline{399979}$	$2.184009\underline{469}$
10	$2.184009\underline{183}$	$2.184009470267\underline{8658}$
15	$2.18400947\underline{764}$	$2.1840094702678519\underline{550}$
20	$2.18400946\underline{996}$	$2.18400947026785195289\underline{639}$
25	$2.184009470\underline{281}$	$2.18400947026785195289473\underline{9799}$
30	$2.18400947026\underline{793}$	$2.184009470267851952894734\underline{17553}$
35	$2.18400947026\underline{770}$	$2.1840094702678519528947341\underline{57762}$
40	$2.18400947026\underline{78697}$	$2.18400947026785195289473415785\underline{2089}$

TABLE 3. Quadrature sums $Q_{N,15}$

N	$Q_{N,15}$
5	$2.1840094702678519\underline{8767}$
10	$2.1840094702678519528947341\underline{581999}$
15	$2.1840094702678519528947341578529490\underline{706127}$
20	$2.18400947026785195289473415785294907044390\underline{84170}$
25	$2.18400947026785195289473415785294907044390840626\underline{3233}$
30	$2.184009470267851952894734157852949070443908406263229420\underline{199}$

As we can see, the sequence of quadrature sums $\{Q_{N,m}\}_N$ converges faster for larger m. This rapidly increasing of convergence of the summation process as m increases in due to the logarithmic singularities $\pm \mathrm{i}\pi\left(m - \frac{1}{2}\right)$ of the function

$$z \mapsto \Phi\left(m - \frac{1}{2}, \frac{z}{\pi}\right), \; z = t + \mathrm{i}s,$$

moving away from the real line. In Figure 1 we present the function

$$(t, s) \mapsto \left|\Phi\left(m - \frac{1}{2}, \frac{1}{\pi}(t + \mathrm{i}s)\right)\right|,$$

when $m = 1$ and $m = 5$.

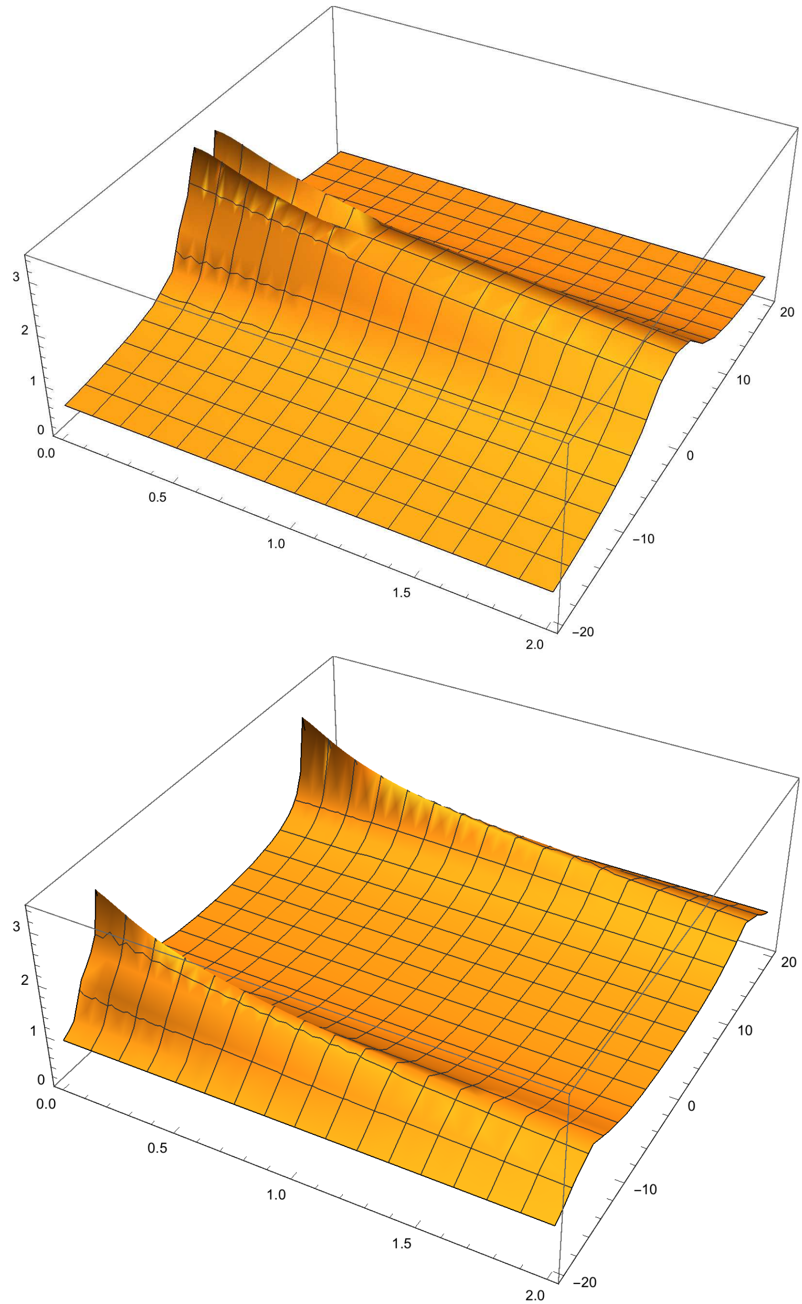

Figure 1. The function $(t,s) \mapsto \left|\Phi\left(m-\frac{1}{2}, \frac{1}{\pi}(t+\mathrm{i}s)\right)\right|$ for $m=1$ (top) and $m=5$ (bottom)

For example, for $m = 15$ we obtained the same values of $Q_{N,15}$ for $N = 40(5)50$ and it can be taken as an exact value of the sum,

$$T = 2.1840094702678519528947341578529490704439084062632294202000251.$$

for calculating the relative errors,

$$\mathrm{err}_{N,m} = \left|\frac{Q_{N,m} - T}{T}\right|,$$

in other quadrature sums $Q_{N,m}$ for smaller $m < 15$. These relative errors for some selected m are presented in Table 4.

TABLE 4. Relative errors $\mathrm{err}_{N,m}$ in the quadrature sums $Q_{N,m}$

N	$m = 1$	$m = 2$	$m = 3$	$m = 5$	$m = 10$
5	4.43(−6)	3.59(−9)	4.65(−10)	8.05(−13)	8.28(−16)
10	1.31(−7)	5.02(−12)	6.34(−15)	6.25(−19)	8.30(−25)
15	3.38(−9)	6.19(−15)	9.81(−19)	6.88(−24)	2.77(−32)
20	1.39(−10)	1.31(−17)	7.59(−22)	1.14(−28)	2.84(−38)
25	6.15(−12)	2.57(−19)	2.58(−24)	1.15(−31)	6.01(−44)
30	3.73(−14)	4.17(−21)	8.10(−27)	6.13(−35)	1.09(−48)

4. Series with irrational terms

In this section we consider some important series of the form

$$U_{\pm}(a,\nu) = \sum_{k=1}^{+\infty} \frac{(\pm 1)^{k-1}}{(k^2 + a^2)^{\nu+1/2}}\,.$$

In 1916 Kapteyn (see [14, p. 386]) proved the formula

$$U_{+}(a,\nu) = \sum_{k=1}^{+\infty} \frac{1}{(k^2 + a^2)^{\nu+1/2}} = \frac{\sqrt{\pi}}{(2a)^{\nu}\Gamma(\nu+1/2)} \int_0^{+\infty} \frac{t^{\nu}}{\mathrm{e}^t - 1}\, J_{\nu}(at)\,\mathrm{d}t$$

which is valid when $\mathrm{Re}\,\nu > 0$ and $|\,\mathrm{Im}\,a| < 1$. Here, J_ν is the Bessel function of the order ν, defined by

$$J_{\nu}(t) = \sum_{k=0}^{+\infty} \frac{(-1)^k}{k!\Gamma(k+\nu+1)} \left(\frac{t}{2}\right)^{2k+\nu}. \tag{4.1}$$

Since for $F(p) = 1/(p^2 + a^2)^{\nu+1/2}$ $\big(\mathrm{Re}\,\nu > -1/2,\ \mathrm{Re}\,p > |\,\mathrm{Im}\,a|\big)$, using the method of Laplace transform, we find the original function

$$f(t) = \frac{\sqrt{\pi}}{(2a)^{\nu}\Gamma(\nu+1/2)}\, t^{\nu} J_{\nu}(at),$$

as well as

$$U_-(a,\nu) = \sum_{k=1}^{+\infty} \frac{(-1)^{k-1}}{(k^2+a^2)^{\nu+1/2}} = \frac{\sqrt{\pi}}{(2a)^\nu \Gamma(\nu+1/2)} \int_0^{+\infty} \frac{t^\nu}{\mathrm{e}^t+1} J_\nu(at)\,\mathrm{d}t.$$

Thus, this method leads to an integration of the Bessel function $t \mapsto J_\nu(at)$ with Einstein's weight $\varepsilon(t)$ or Fermi's weight $\varphi(t)$. For some special values of ν, we can use also quadratures with respect to the weights $t^{\pm 1/2}\varepsilon(t)$ and $t^{\pm 1/2}\varphi(t)$ (see [5] and [3]).

In the following example we show how to compute $U_\pm(a,\nu)$, $0<\nu<1$, with a high accuracy.

Example 4.1. According to the expansion of the Bessel function (4.1), we can consider $U_\pm(a,\nu)$ in the form (as the corresponding series in Example 2.1)

$$U_\pm(a,\nu) = \sum_{k=1}^{+\infty} \frac{(\pm 1)^{k-1}}{(k^2+a^2)^{\nu+1/2}} = \frac{\sqrt{\pi}}{2^\nu \Gamma(\nu+1/2)} \int_0^{+\infty} \frac{t^{2\nu}}{\mathrm{e}^t \mp 1} \frac{J_\nu(at)}{(at)^\nu}\,\mathrm{d}t,$$

and then construct Gaussian quadratures with respect to the (generalized) Einstein and Fermi weights $\varepsilon_{2\nu}(t)$ and $\varphi_{2\nu}(t)$ on $(0,+\infty)$, respectively. Their moments are given by (2.7) and (2.8), respectively, where $\gamma = 2\nu$.

These series are slowly convergent for small ν. For example, for the remainder $R_n(a,\nu)$ of the series $U_+(a,\nu)$, we have

$$R_n(a,\nu) = \sum_{k=n+1}^{+\infty} \frac{1}{(k^2+a^2)^{\nu+1/2}} < \int_n^{+\infty} \frac{\mathrm{d}x}{(x^2+a^2)^{\nu+1/2}}.$$

For $n \gg a$ the right hand side in the previous inequality can be simplified as

$$\int_n^{+\infty} \frac{\mathrm{d}x}{x^{2\nu+1}} = \frac{1}{2\nu n^{2\nu}},$$

so that we can roughly conclude that for a small ε, the remainder $R_n(a,\nu) < \varepsilon$ if $n > n_\varepsilon = \left[(2\nu\varepsilon)^{-1/(2\nu)}\right]$. The values of n_ε for $\varepsilon = 10^{-3}$ and some given values of ν are presented in Table 5.

TABLE 5. The values of n_ε for $\varepsilon = 10^{-3}$ and some values of ν

ν	5×10^{-1}	10^{-1}	10^{-2}	10^{-3}	10^{-4}
n_ε	10^3	3×10^{18}	9×10^{234}	3×10^{2849}	7×10^{33494}

Using the MATHEMATICA package `OrthogonalPolynomials` and e.g. the first 100 moments $\mu_k(\varepsilon_{2\nu})$, $k=0,1,\ldots,99$, in the symbolic form (2.7), we can construct for a given $\nu = 10^{-4}$ the first 50 recursive coefficients in the three-term recurrence relation with the maximal relative errors of about 6.09×10^{-53} if we use the `WorkingPrecision -> 95` in the Chebyshev method of moments, implemented in this package by the command

```
<<orthogonalPolynomials`
  moments=Table[Gamma[1+k+2v]Zeta[1+k+2v], {k,0,99}];
  mv=moments/.{v -> 1/10000};
  {alfaE,betaE}=aChebyshevAlgorithm[mv,WorkingPrecision->95];
```

These coefficients enables us to construct the corresponding Gaussian rules for any $N \le 50$,

$$\int_0^{+\infty} \frac{t^{2\nu}}{\mathrm{e}^t \mp 1} u(t)\,\mathrm{d}t \approx Q_N(u;\varepsilon_{2\nu}) = \sum_{k=1}^{N} A_k u(\xi_k), \tag{4.2}$$

where ξ_k and A_k, $k = 1,\ldots,N$, are nodes and weight coefficients. Corresponding Gaussian approximations $Q_N(u;\varepsilon_{2\nu})$, for

$$u(t) = u(t;a,\nu) = \frac{\sqrt{\pi}}{2^\nu \Gamma(\nu+1/2)} \cdot \frac{J_\nu(at)}{(at)^\nu}, \tag{4.3}$$

$a = 1/4$ and $\nu = 10^{-4}$, are presented in Table 6. Digits in error are underlined. In the same table we give also the relative errors $\mathrm{err}_N(a,\nu)$ in these approximations, taking $Q_{50}(u;\varepsilon_{2\nu})$ as the exact value of the sum.

TABLE 6. Gaussian approximations $Q_N(u;\varepsilon_{2\nu})$ and relative errors $\mathrm{err}_N(a,\nu)$ for $u(t)$ given by (4.3)

N	$Q_N(u;\varepsilon_{2\nu})$	$\mathrm{err}_N(a,\nu)$
5	$5000.541106014\underline{918}$	8.29(−14)
10	$5000.5411060145037123\underline{3515}$	1.53(−22)
15	$5000.541106014503712334387545429\underline{320}$	1.29(−31)
20	$5000.5411060145037123343875454299674624970\underline{83}$	3.71(−41)
25	$5000.541106014503712334387545429967462497268917455\underline{9}$	1.11(−49)

The relative errors $\mathrm{err}_N(a,\nu)$ for $0 < a < 1$ and $\nu = 10^{-4}$ in log-scale are displayed in Figure 2 for $N = 5(5)15$ nodes in the quadrature formula (4.2).

Remark 4.2. When $a \to 0$ the function $u(t)$, defined by (4.3), tends to the constant $2^{-v}/\Gamma(v+1)$. Then the quadrature sums in (4.2) give the same value for each N,

$$U_+(0,10^{-4}) = 5000.57723022787681959380316665535223274218008470820,$$

which is, in fact, an approximative value of the well-known ζ function at the point $2\nu + 1 = 1.0002$.

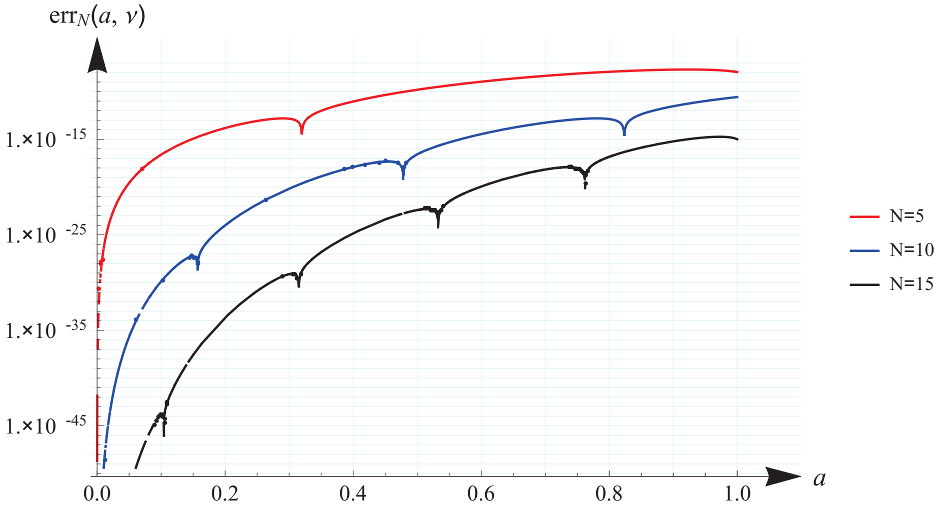

Figure 2. Relative errors in quadrature sums $Q_N(u;\varepsilon_{2\nu})$ for $N=5$ (red line), $N=10$ (blue line), and $N=15$ nodes (black line), when $\nu=10^{-4}$

Finally, we consider an alternative method for the series of the form

$$\sum_{k=-\infty}^{+\infty} f(k,\sqrt{k^2+a^2}) \quad \text{and} \quad \sum_{k=-\infty}^{+\infty} (-1)^k f(k,\sqrt{k^2+a^2}) \quad (a>0),$$

where f is a rational function. Such series can be reduced to some appropriate integrals, by integrating the corresponding function $z\mapsto F(z)=f(z,\sqrt{z^2+a^2})g(z)$, with $g(z)=\pi/\tan\pi z$ and $g(z)=\pi/\sin\pi z$, respectively, over certain circle C_n with the cuts.

In the sequel we illustrate this alternative method in the simplest case when $f(z,w)=1/w$, i.e., to summation of the series

$$U_-(a,0)=\sum_{k=1}^{+\infty}\frac{(-1)^{k-1}}{\sqrt{k^2+a^2}}, \quad a>0. \tag{4.4}$$

Thus, we integrate the function $z\mapsto F(z)=g(z)/\sqrt{z^2+a^2}$, with $g(z)=\pi/\sin\pi z$, over the circle

$$C_n=\left\{z\in\mathbb{C}\;\middle|\;|z|=n+\frac{1}{2}\right\}, \qquad n>a,$$

with cuts along the imaginary axis, so that the critical singularities ia and $-$ia are eliminated (cf. [13, p. 217]). Precisely, the contour of integration Γ is given by $\Gamma = C_n^1\cup l_1\cup\gamma_1\cup l_2\cup C_n^2\cup l_3\cup\gamma_2\cup l_4$, where C_n^1 and C_n^2 are parts of the circle C_n, γ_1 and γ_2 are small circular parts of radius ε and centres at $\pm$ia, and l_k $(k=1,2,3,4)$ are the corresponding line segments (see Figure 3).

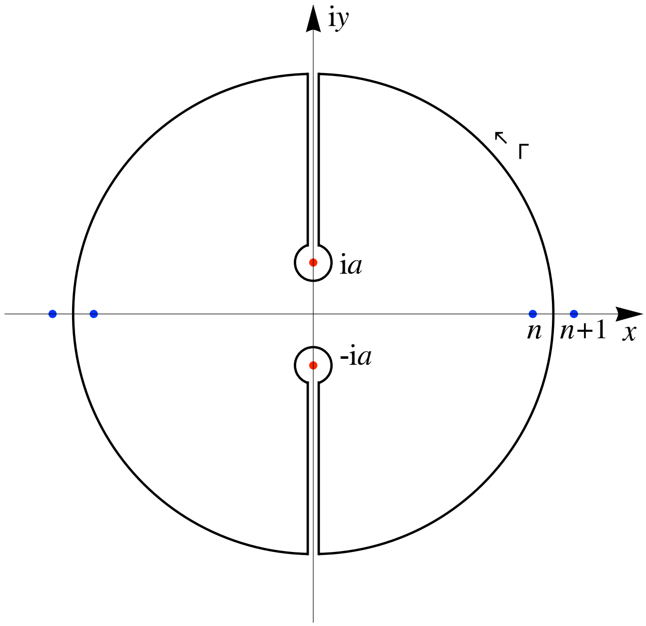

Figure 3. The contour of integration Γ

Let $F^*(z)$ be the branch of $F(z)$ which corresponds to the value of the square root which is positive for $z = 1$. Since

$$\oint_\Gamma F^*(z)\,\mathrm{d}z = 2\pi\mathrm{i} \sum_{k=-n}^{n} \frac{(-1)^k}{\sqrt{k^2+a^2}},$$

and $\int_{\gamma_1} \to 0$, $\int_{\gamma_2} \to 0$, when $\varepsilon \to +0$, and $\int_{C_n^1 \cup C_n^2} \to 0$, when $n \to +\infty$, we obtain

$$\sum_{k=1}^{+\infty} \frac{(-1)^k}{\sqrt{k^2+a^2}} = -\frac{1}{2a} + \int_a^{+\infty} \frac{\mathrm{d}u}{\sinh \pi u \sqrt{u^2-a^2}},$$

i.e.,

$$\sum_{k=1}^{+\infty} \frac{(-1)^{k-1}}{\sqrt{k^2+a^2}} = \frac{1}{2a} - \frac{1}{2} \int_{-1}^{+1} \left(t \sinh \frac{\pi a}{t} \right)^{-1} \frac{\mathrm{d}t}{\sqrt{1-t^2}}.$$

Thus, we have reduced $U_-(a,0)$ to a problem of Gauss-Chebyshev quadrature. Since $t \mapsto \big(t \sinh(\pi a/t)\big)^{-1}$ is an even function we can apply the $(2n)$-point Gauss-Chebyshev approximations with only n functional evaluations, so that we have

$$U_-(a,0) \approx GC(N;a) = \frac{1}{2a} - \frac{\pi}{2N} \sum_{k=1}^{N} \left(\tau_k \sinh \frac{\pi a}{\tau_k} \right)^{-1}, \tag{4.5}$$

where $\tau_k = \cos\big((2k-1)\pi/(4N)\big)$, $k = 1, \ldots, N$.

Example 4.3. We consider now the series

$$U_-(a,0)=\sum_{k=1}^{+\infty}\frac{(-1)^{k-1}}{\sqrt{k^2+a^2}}$$

for two different values of a, $a=1/4$ and $a=10$, whose exact values are

$$U_-\Big(\frac{1}{4},0\Big)=0.66632618906466580605283262942098890800417625596202\ldots$$

and

$$U_-(10,0)=0.04999999999998988303868784011212623150952067574918\ldots,$$

respectively.

For calculating the sum $U_-(a,0)$ we apply the Gauss-Chebyshev quadrature approximation (4.5), the Gauss-Fermi-Dirac rule (2.4), as well as the quadrature rule (3.7) for $s=2$.

The relative errors in the Gauss-Chebyshev quadrature sums $GC(N;a)$ for small value $a=1/4$ are given in Table 7, and for $a=10$ in Table 8. In these tables we also present the corresponding relative errors for the Gauss-Fermi-Dirac quadrature sums

$$GFD(N;a)=\sum_{k=1}^{N}B_k u(\eta_k),$$

obtained by (2.4), where $u(t)=J_0(at)$.

TABLE 7. Relative errors in the quadrature sums $GC(N;a)$, $GFD(N;a)$ and $Q_{N,m}(a)$ for $a=1/4$

N	$GC(N;a)$	$GFD(N;a)$	$Q_{N,1}(a)$	$Q_{N,5}(a)$	$Q_{N,10}(a)$
10	7.15(−4)	8.78(−19)	2.68(−5)	5.77(−14)	4.72(−20)
20	2.28(−5)	2.64(−37)	2.59(−7)	3.15(−23)	1.69(−28)
30	8.99(−8)	1.85(−55)	1.82(−8)	4.46(−25)	2.22(−35)
40	3.54(−7)		7.46(−10)	4.00(−29)	2.65(−41)
50	4.40(−8)		4.93(−11)	5.11(−33)	6.60(−47)

Finally, we apply the quadrature rule (3.7) for $s=2$ to compute the weighted integral (3.6). The construction of this quadrature we need the moments (cf. [11])

$$\mu_k^{(2)}=\int_0^{+\infty}t^k w_2(t)\,\mathrm{d}t=\begin{cases}1, & k=0,\\[4pt] k\Big(\dfrac{\pi}{2}\Big)^k|E_{k-1}|, & k\,(\text{odd})\ge 1,\\[4pt] \dfrac{2k}{4^k}\left[\psi^{(k-1)}(\tfrac14)-\psi^{(k-1)}(\tfrac34)\right], & k\,(\text{even})\ge 2,\end{cases}$$

where $\zeta(k)$ is the Riemann zeta function, E_k are Euler's numbers, and $\psi(z)$ is the logarithmic derivative of the gamma function, i.e., $\psi(z)=\Gamma'(z)/\Gamma(z)$.

TABLE 8. Relative errors in the quadrature sums $GC(N;a)$, $GFD(N;a)$ and $Q_{N,m}(a)$ for $a = 10$

N	$GC(N;a)$	$GFD(N;a)$	$Q_{N,1}(a)$	$Q_{N,5}(a)$	$Q_{N,10}(a)$
10	1.86(−22)	2.26	4.86(−14)	8.68(−17)	6.60(−20)
20	3.38(−31)	1.98	2.70(−14)	7.06(−21)	7.69(−28)
30	4.83(−38)	1.05	3.38(−15)	1.00(−23)	3.77(−33)
40	5.38(−45)	4.94(−2)	4.65(−15)	7.95(−26)	1.50(−37)
50	3.70(−49)	4.42(−1)	1.05(−15)	1.02(−27)	2.15(−41)

As in Example 3.1 we consider quadrature sums in the form

$$Q_{N,m}(a) = \sum_{k=1}^{m-1} \frac{(-1)^{k-1}}{\sqrt{k^2+a^2}} + (-1)^{m-1} \sum_{\nu=1}^{N} A_{\nu,2}^{N} \Psi\left(m - \frac{1}{2}, \frac{\tau_{\nu,2}^{N}}{\pi}\right),$$

where $\Psi(x,y) = \operatorname{Im} F(x+\mathrm{i}y)$ and $F(z) = \log(z+\sqrt{z^2+a^2})$. Although condition (C3), in this case, is not satisfied the sequence of quadrature sums $Q_{N,m}(a)$ converges. This means that this requirement can be weakened, but it will be studied elsewhere.

As we can see, the convergence of Gauss-Chebyshev approximations $GC(N;a)$ is faster if the parameter a is larger. However, the Laplace transform method ($GFD(N;a)$) is very efficient for a small parameter a, but, when a increases, the integrand $J_0(at)$ becomes a highly oscillatory function and the convergence of the quadrature process slows down considerably.

Also, we can see a rapidly increasing of convergence of the summation process $Q_{N,m}(a)$ as m increases.

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