Summation of Series and Gaussian Quadratures

GRADIMIR V. MILOVANOVIĆ

Dedicated to Walter Gautschi on the occasion of his 65*th birthday*

Abstract. In 1985, Gautschi and the author constructed Gaussian quadrature formulae on $(0,+\infty)$ involving Einstein and Fermi functions as weights and applied then to the summation of slowly convergent series which can be represented in terms of the derivative of a Laplace transform, or in terms of the Laplace transform itself. A problem that may arise in this procedure is the determination of the respective inverse Laplace transform. For the class of slowly convergent series $\sum_{k=1}^{+\infty}(\pm 1)^k a_k$ with $a_k = k^{\nu-1}R(k)$, where $0<\nu\le 1$ and $R(s)$ is a rational function, Gautschi recently solved this problem. In the present paper, using complex integration and constructing Gauss-Christoffel quadratures on $(0,+\infty)$ with respect to the weight functions $w_1(t)=1/\cosh^2 t$ and $w_2(t)=\sinh t/\cosh^2 t$, we reduce the series $\sum_{k=m}^{+\infty} f(k)$ and $\sum_{k=m}^{+\infty}(-1)^k f(k)$ to weighted integrals of f involving weights w_1 and w_2, respectively. We illustrate this method with a few numerical examples.

1. INTRODUCTION

We consider the summation of series of the type

$$T_m = \sum_{k=m}^{+\infty} a_k \tag{1.1}$$

and

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

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where $m \in \mathbb{Z}$.

Methods of summation can be found, for example, in the books of Henrici [11], Lindelöf [12], and Mitrinović and Kečkić [13].

In a joint paper with Gautschi [9] we considered the construction of Gaussian quadrature formulas on $(0, +\infty)$ with respect to the weight functions

$$w(t) = \varepsilon(t) = \frac{t}{e^t - 1} \qquad \text{(Einstein's function)}$$

and

$$w(t) = \varphi(t) = \frac{1}{e^t + 1} \qquad \text{(Fermi's function)}$$

and showed that these formulae can be applied to sum slowly convergent series of the form T_1 and S_1 whose general term is expressible in terms of the derivative of a Laplace transform, or in terms of the Laplace transform itself. Namely, if $a_k = F'(k)$, where

$$F(s) = \int_0^{+\infty} e^{-st} f(t)\, dt, \qquad \operatorname{Re} s \geq 1,$$

we have

$$T_1 = \sum_{k=1}^{+\infty} F'(k) = -\int_0^{+\infty} f(t)\varepsilon(t)\, dt$$

and

$$S_1 = \sum_{k=1}^{+\infty} (-1)^k F'(k) = \int_0^{+\infty} f(t) t \varphi(t)\, dt.$$

Also, for $a_k = F(k)$, we have

$$S_1 = \sum_{k=1}^{+\infty} (-1)^k F(k) = -\int_0^{+\infty} f(t)\varphi(t)\, dt.$$

If the series T_1 and S_1 are slowly convergent and the respective function f on the right of the equalities above is smooth, then low-order Gaussian quadrature[1]

$$\int_0^{+\infty} g(t) w(t)\, dt = \sum_{\nu=1}^{n} \lambda_\nu g(\tau_\nu) + R_n(g),$$

[1]The functions $t \mapsto \varepsilon(t)$ and $t \mapsto \varphi(t)$ arise in solid state physics. Integrals with respect to the measure $d\lambda(t) = \varepsilon(t)^r\, dt$, $r = 1$ and $r = 2$, are widely used in phonon statistics and lattice specific heats and occur also in the study of radiative recombination processes. Similarly, integrals with $\varphi(t)$ are encountered in the dynamics of electrons in metals.

with $w(t) = \varepsilon(t)$ and $w(t) = \varphi(t)$, applied to the integrals on the right, provides a possible summation procedure. Numerical examples show fast convergence of this procedure (see [9, §4]). In the sequel we refer to this procedure as the "Laplace transform method." A problem which arises with this procedure is the determination of the original function f for a given series. For some other applications see Gautschi [6] and [7].

In [6], Gautschi treated the case when $a_k = k^{\nu-1}R(k)$, where $0 < \nu \le 1$ and $R(\,\cdot\,)$ is a rational function $R(s) = P(s)/Q(s)$, with P, Q real polynomials of degrees $\deg P \le \deg Q$. By interpreting the terms in T_1 and S_1 again as Laplace transforms at integer values, Gautschi expressed the sum of the series as a weighted integral over $\mathbb{R}_+$ of certain special functions related to the incomplete gamma function. The weighting involves the product of a fractional power and either Einstein's function $\varepsilon(t)$ (for T_1) or Fermi's function $\varphi(t)$ (for S_1). The case $\nu = 1$ of purely rational series complements some traditional techniques of summations via quadratures (cf. [11, §7.2II]).

In particular, Gautschi [6] analyzed examples with $a_k = k^{-1/2}/(k+a)^m$, where $\operatorname{Re} a \ge 0$ and $m \ge 1$. The series T_1 with $a = m = 1$ appeared in a study of spirals given by Davis [1] (see also Gautschi [8]).

In this paper we give an alternative summation/integration procedure for the series (1.1) and (1.2) when $a_k = f(k)$, where $z \mapsto f(z)$ is an analytic function in the region

$$\{z \in \mathbb{C} \mid \operatorname{Re} z \ge \alpha,\ m-1 < \alpha < m\}. \tag{1.3}$$

Our method requires the indefinite integral F of f chosen so as to satisfy certain decay properties ((C1) – (C3) below). Using contour integration over a rectangle in the complex plane we are able to reduce T_m and S_m to a problem of quadrature on $(0, +\infty)$ with respect to the weight functions

$$w_1(t) = \frac{1}{\cosh^2 t} \qquad \text{and} \qquad w_2(t) = \frac{\sinh t}{\cosh^2 t}, \tag{1.4}$$

respectively.

The contour integration is discussed in §2. The generation of the recursion coefficients in the three-term recurrence relation for the (monic) orthogonal polynomials $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; w_p)$, $k = 0, 1, \dots$, with respect to the weight function $w_p(t)$, $p = 1, 2$, is discussed in §3. Numerical examples are presented in §4.

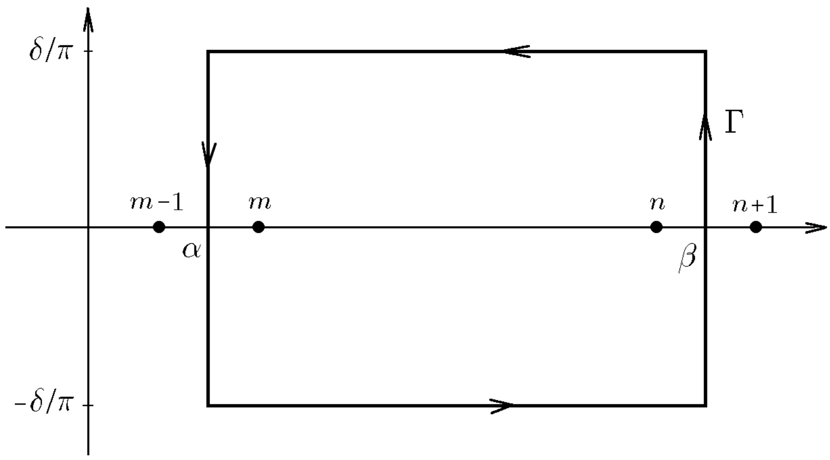

FIGURE 2.1
The contour of integration

2. PRELIMINARIES

Assume that f and g are analytic functions in a certain domain D of the complex plane with singularities $a_1, a_2, \dots$ and $b_1, b_2, \dots$, respectively, in a region $G = \operatorname{int}\Gamma\,(\subset D)$, where Γ is a closed contour. Then by Cauchy's residual theorem, we have

$$\frac{1}{2\pi i}\oint_\Gamma f(z)g(z)\,dz = \sum_\nu \operatorname*{Res}_{z=a_\nu}\Bigl(f(z)g(z)\Bigr) + \sum_\nu \operatorname*{Res}_{z=b_\nu}\Bigl(f(z)g(z)\Bigr). \tag{2.1}$$

Let

$$G = \Bigl\{z \in \mathbb{C} \mid \alpha \le \operatorname{Re} z \le \beta,\ |\operatorname{Im} z| \le \frac{\delta}{\pi}\Bigr\},$$

where $m-1 < \alpha < m$, $n < \beta < n+1$ $(m, n \in \mathbb{Z}, m \le n)$, $\Gamma = \partial G$ (see Figure 2.1), and $g(z) = \pi/\tan \pi z$. Then from (2.1) it immediately follows that (cf. [13, p. 212])

$$T_{m,n} = \sum_{\nu=m}^{n} f(\nu) = \frac{1}{2\pi i}\oint_\Gamma f(z)\frac{\pi}{\tan \pi z}\,dz - \sum_\nu \operatorname*{Res}_{z=a_\nu}\Bigl(f(z)\frac{\pi}{\tan \pi z}\Bigr).$$

Similarly, for $g(z) = \pi/\sin \pi z$ we have

$$S_{m,n} = \sum_{\nu=m}^{n} (-1)^\nu f(\nu) = \frac{1}{2\pi i}\oint_\Gamma f(z)\frac{\pi}{\sin \pi z}\,dz - \sum_\nu \operatorname*{Res}_{z=a_\nu}\Bigl(f(z)\frac{\pi}{\sin \pi z}\Bigr).$$

For a holomorphic function $z \mapsto f(z)$ in G, the last formulas become

$$T_{m,n} = \frac{1}{2\pi i} \oint_\Gamma f(z) \frac{\pi}{\tan \pi z}\, dz \quad \text{and} \quad S_{m,n} = \frac{1}{2\pi i} \oint_\Gamma f(z) \frac{\pi}{\sin \pi z}\, dz. \tag{2.2}$$

After integration by parts, formulas (2.2) reduce to

$$T_{m,n} = \frac{1}{2\pi i} \oint_\Gamma \Big(\frac{\pi}{\sin \pi z}\Big)^2 F(z)\, dz \tag{2.3}$$

and

$$S_{m,n} = \frac{1}{2\pi i} \oint_\Gamma \Big(\frac{\pi}{\sin \pi z}\Big)^2 \cos \pi z\, F(z)\, dz, \tag{2.4}$$

where $z \mapsto F(z)$ is an integral of $z \mapsto f(z)$.

Assume now the following conditions for the function $z \mapsto F(z)$ (cf. [12, p. 57]):

(C1) *F is a holomorphic function in the region* (1.3);

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

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

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

Set $\alpha = m - 1/2$ and $\beta = n + 1/2$.

On the lines $z = x \pm i(\delta/\pi)$, we have that

$$\Big|\frac{\pi}{\sin \pi z}\Big| = \Big|\frac{2i\pi}{e^{i\pi z} - e^{-i\pi z}}\Big| = \frac{2\pi e^{-\delta}}{|1 - e^{-2\delta} e^{\pm i2\pi x}|} \leq \frac{2\pi e^{-\delta}}{1 - e^{-2\delta}}$$

and also

$$|\cos \pi z| = \frac{1}{2}\, e^{\delta} |1 + e^{-2\delta} e^{\pm i2\pi x}| \leq \frac{1}{2}\, e^{\delta}(1 + e^{-2\delta}).$$

Therefore, under condition (C2), the integrals on the lines $z = x \pm i(\delta/\pi)$, $\alpha \leq x \leq \beta$,

$$\frac{1}{2\pi i} \int_{\alpha\pm i(\delta/\pi)}^{\beta\pm i(\delta/\pi)} \Big(\frac{\pi}{\sin \pi z}\Big)^2 F(z)\, dz, \qquad \frac{1}{2\pi i} \int_{\alpha\pm i(\delta/\pi)}^{\beta\pm i(\delta/\pi)} \Big(\frac{\pi}{\sin \pi z}\Big)^2 \cos \pi z\, F(z)\, dz,$$

tend to zero when $\delta \to +\infty$.

For $z = \beta + iy$ we have

$$\sin \pi z = (-1)^n \cosh \pi y, \qquad \cos \pi z = i(-1)^{n+1} \sinh \pi y,$$

$$\Big|\frac{\pi}{\sin\pi z}\Big|^2 = \frac{\pi^2}{\cosh^2\pi y} = \frac{4\pi^2}{(e^{\pi y}+e^{-\pi y})^2} \le 4\pi^2 e^{-2\pi|y|},$$

and

$$\Big|\frac{\pi}{\sin\pi z}\Big|^2 \,|\cos\pi z| \le 2\pi^2 e^{-\pi|y|},$$

so that

$$\left|\frac{1}{2\pi i}\int_{\beta-i(\delta/\pi)}^{\beta+i(\delta/\pi)}\Big(\frac{\pi}{\sin\pi z}\Big)^2 F(z)\,dz\right| \le 2\int_{-\delta}^{\delta} e^{-2|t|}\,|F(\beta+it/\pi)|\,dt$$

and

$$\left|\frac{1}{2\pi i}\int_{\beta-i(\delta/\pi)}^{\beta+i(\delta/\pi)}\Big(\frac{\pi}{\sin\pi z}\Big)^2 \cos\pi z\,F(z)\,dz\right| \le \int_{-\delta}^{\delta} e^{-|t|}\,|F(\beta+it/\pi)|\,dt.$$

When $\delta\to+\infty$ and $n\to+\infty$ (i.e., $\beta\to+\infty$), because of (C3), the previous integrals tend to zero.

Thus, when $\delta\to+\infty$ and $n\to+\infty$, the integrals in (2.3) and (2.4) over Γ reduce to integrals along the line $z=\alpha+iy$ $(-\infty<y<+\infty)$, so that

$$T_m = T_{m,\infty} = -\frac{1}{2\pi i}\int_{\alpha-i\infty}^{\alpha+i\infty}\Big(\frac{\pi}{\sin\pi z}\Big)^2 F(z)\,dz \tag{2.5}$$

and

$$S_m = S_{m,\infty} = -\frac{1}{2\pi i}\int_{\alpha-i\infty}^{\alpha+i\infty}\Big(\frac{\pi}{\sin\pi z}\Big)^2 \cos\pi z\,F(z)\,dz. \tag{2.6}$$

Equality (2.5) can be reduced to

$$T_m = -\frac{1}{2}\int_{-\infty}^{+\infty}\frac{1}{\cosh^2 t}F(\alpha+it/\pi)\,dt,$$

i.e.,

$$T_m = \int_0^{+\infty}\Phi(\alpha,t/\pi)\,w_1(t)\,dt, \tag{2.7}$$

where w_1 is defined in (1.4) and

$$\Phi(x,y) = -\frac{1}{2}\left[F(x+iy)+F(x-iy)\right]. \tag{2.8}$$

Similarly, (2.7) reduces to

$$S_m = \int_0^{+\infty}\Psi(\alpha,t/\pi)\,w_2(t)\,dt, \tag{2.9}$$

where w_2 is also defined in (1.4) and

$$\Psi(x,y) = \frac{(-1)^m}{2i}\left[F(x+iy) - F(x-iy)\right]. \tag{2.10}$$

Formulas (2.7) and (2.9) suggest to apply Gaussian quadrature to the integrals on the right, using the weight functions w_1 and w_2, respectively. The required orthogonal polynomials can be computed using the discretized Stieltjes procedure (see Gautschi [3, §2.2], [4–5]).

Instead of reducing integration to the positive half-line, one might keep integration over the full real line and note that

$$T_m = \int_{-\infty}^{+\infty} \Phi\left(\alpha, t/(2\pi)\right) \frac{e^{-t}}{(1+e^{-t})^2}\, dt \tag{2.11}$$

and

$$S_m = \int_{-\infty}^{+\infty} \Psi\left(\alpha, t/(2\pi)\right) \sinh(t/2) \frac{e^{-t}}{(1+e^{-t})^2}\, dt. \tag{2.12}$$

Here, the weight function is $t \mapsto w(t) = e^{-t}/(1+e^{-t})^2$, the logistic weight, for which the recursion coefficients for the respective orthogonal polynomials are explicitly known[2]:

$$\alpha_k = 0, \quad \beta_0 = 1, \quad \beta_k = \frac{k^4\pi^2}{4k^2-1}, \qquad k = 1, 2, \ldots\ .$$

Thus, no procedure is required to generate the recursion coefficients. Some comments on the convergence of the corresponding Gaussian quadrature will be given in §4.

3. GENERATION OF THE RECURSION COEFFICIENTS

Let $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; w_p)$, $k = 0, 1, \ldots$, be the (monic) polynomials orthogonal with respect to the weight function $t \mapsto w_p(t)$, $p = 1, 2$, on $(0, +\infty)$, where

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

[2]The referee pointed out this fact.

They satisfy the three-term recurrence relation

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

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

where

$$\alpha_k = \alpha_k(w_p), \quad \beta_k = \beta_k(w_p) \qquad \Big(\beta_0(w_p) = \int_0^{+\infty} w_p(t)\, dt\Big).$$

Knowing the first n of these coefficients α_k, β_k, $k = 0, 1, \ldots, n-1$, one can easily obtain the k-point Gaussian quadrature formula

$$\int_0^{+\infty} g(t) w_p(t)\, dt = \sum_{\nu=1}^{k} \lambda_\nu g(\tau_\nu) + R_{k,p}(g), \qquad R_{k,p}(\mathcal{P}_{2k-1}) \equiv 0, \qquad (3.2)$$

for any k with $1 \le k \le n$. The nodes $\tau_\nu = \tau_{\nu,p}^{(k)}$, indeed, are the eigenvalues of the symmetric tridiagonal Jacobi matrix

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

while the weights $\lambda_\nu = \lambda_{\nu,p}^{(k)}$ are given by $\lambda_\nu = \beta_0 v_{\nu,1}^2$ in terms of the first components $v_{\nu,1}$ of the corresponding normalized eigenvectors (cf. Gautschi [2, §5.1] and Golub and Welsch [10]).

In order to construct the recursion coefficients we use the discretized Stieltjes procedure as in [9], with the discretization based on the Gauss-Laguerre quadrature rule,

$$\begin{aligned} \int_0^{+\infty} p(t) w_1(t)\, dt &= \int_0^{+\infty} p(t/2)\, \frac{2}{(1+e^{-t})^2}\, e^{-t}\, dt \\ &\cong \sum_{k=1}^{N} \lambda_k^L p(\tau_k^L/2)\, \frac{2}{\left(1+e^{-\tau_k^L}\right)^2} \end{aligned}$$

and

$$\begin{aligned}\int_0^{+\infty} p(t)w_2(t)\,dt &= \int_0^{+\infty} p(t)\,\frac{2(1-e^{-2t})}{(1+e^{-2t})^2}\,e^{-t}\,dt\\ &\cong \sum_{k=1}^{N} \lambda_k^L p(\tau_k^L)\,\frac{2(1-e^{-2\tau_k^L})}{(1+e^{-2\tau_k^L})^2},\end{aligned}$$

where $p \in \mathcal{P}$. Here, τ_k^L and λ_k^L are the parameters of the N-point Gauss-Laguerre quadrature formula.

The first 40 recursion coefficients ($n = 40$) can be obtained accurately to 30 decimal digits with $N = 520$ for w_1 and $N = 720$ for w_2. We used the MICROVAX 3400 in Q-arithmetic (machine precision $\approx 1.93 \times 10^{-34}$). The same results were obtained also by a discretization procedure based on the composite Fejér quadrature rule, decomposing the interval of integration into four subintervals, $[0, +\infty] = [0, 10] \cup [10, 100] \cup [100, 500] \cup [500, +\infty]$ and using $N = 280$ points on each subinterval in both cases. We tabulate the results to 29 decimals in Table 1 and 2 of the Appendix.

Using (2.7)–(2.10) and (3.2) we can state the following results:

Theorem 3.1. *Let F be an integral of f such that the conditions* (C1), (C2), (C3) *are satisfied with $c = 2$. If $\lambda_\nu = \lambda_{\nu,1}^{(n)}$ and $\tau_\nu = \tau_{\nu,1}^{(n)}$ are the parameters of the n-point Gaussian quadrature* (3.2) *with weight function w_1, then*

$$T_m = \sum_{k=m}^{+\infty} f(k) = \sum_{\nu=1}^{n} \lambda_{\nu,1}^{(n)} \Phi(m - \tfrac{1}{2}, \tfrac{1}{\pi}\tau_{\nu,1}^{(n)}) + R_{n,1}(\Phi),$$

where Φ is defined by (2.8).

Theorem 2. *Let F be an integral of f such that the conditions* (C1), (C2), (C3) *are satisfied with $c = 1$. If $\lambda_\nu = \lambda_{\nu,2}^{(n)}$ and $\tau_\nu = \tau_{\nu,2}^{(n)}$ are the parameters of the n-point Gaussian quadrature* (3.2) *with weight function w_2, then*

$$S_m = \sum_{k=m}^{+\infty} (-1)^k f(k) = \sum_{\nu=1}^{n} \lambda_{\nu,2}^{(n)} \Psi(m - \tfrac{1}{2}, \tfrac{1}{\pi}\tau_{\nu,2}^{(n)}) + R_{n,2}(\Psi),$$

where Ψ is defined by (2.10).

Remark 3.1. If $\lambda_\nu = \lambda_\nu^{(n)}$ and $\tau_\nu = \tau_\nu^{(n)}$ are the parameters of the n-point Gaussian quadrature with respect to the logistic weight w, then according to (2.11) and (2.12),

$$T_m = \sum_{k=m}^{+\infty} f(k) \approx \sum_{\nu=1}^{n} \lambda_\nu \Phi(m - \tfrac{1}{2}, \tfrac{1}{2\pi}\tau_\nu) \tag{3.3}$$

and

$$S_m = \sum_{k=m}^{+\infty} (-1)^k f(k) = \sum_{\nu=1}^{n} \lambda_\nu \Psi(m - \tfrac{1}{2}, \tfrac{1}{2\pi}\tau_\nu) \sinh(\tau_\nu/2), \tag{3.4}$$

where Φ and Ψ are defined by (2.8) and (2.10), respectively. In Example 4.1 below, we will also consider these formulas.

4. NUMERICAL EXAMPLES

In this section we illustrate our method using a few examples from [9] and [6]. All computations were done in Q-arithmetic on the MICROVAX 3400 computer.

Example 4.1. Consider

$$T_1 = \sum_{k=1}^{+\infty} \frac{1}{(k+1)^2} = \frac{\pi^2}{6} - 1 \qquad \text{and} \qquad S_1 = \sum_{k=1}^{+\infty} \frac{(-1)^k}{(k+1)^2} = \frac{\pi^2}{12} - 1.$$

Here, $f(z) = (z+1)^{-2}$, and $F(z) = -(z+1)^{-1}$, the integration constant being zero on account of the condition (C3). Thus,

$$\Phi(x,y) = \mathrm{Re}\, \frac{1}{z+1} = \frac{x+1}{(x+1)^2 + y^2}$$

and

$$\Psi(x,y) = \mathrm{Im}\, \frac{1}{z+1} = \frac{-y}{(x+1)^2 + y^2}\,.$$

Table 4.1 shows the n-point approximations $T_1(n)$ and $S_1(n)$ to T_1 and S_1, respectively, together with the relative errors $r_n(T_1)$ and $r_n(S_1)$, for $n = 5(5)40$. In each entry the first digit in error is underlined. (Numbers in parentheses indicate decimal exponents.)

The corresponding relative errors in the "Laplace transform method" [9] applied to T_1 are given in Table 4.4. The recursion coefficients α_k, β_k for orthogonal polynomials $\pi_k(\,\cdot\,;\varepsilon)$ were calculated also with 30 correct decimal digits.

As we can see, for smaller values of n (≤ 15) we obtained better results than in the "Laplace transform method". Furthermore, these results can be significantly improved if we apply this method to sum the series T_m, $m > 1$. That is, we use

$$T_1 = \sum_{k=1}^{m-1} \frac{1}{(k+1)^2} + T_m, \qquad T_m = \sum_{k=m}^{+\infty} \frac{1}{(k+1)^2}\,. \tag{4.1}$$

Then, for $m = 2(1)5$ we obtain results whose relative errors are presented in Table 4.2. Also, in Table 4.3 we present the corresponding results for the sum S_1 expressed in a similar way.

Table 4.1
Gaussian approximation of the sums T_1 and S_1 and relative errors

n	$T_1(n)$	$r_n(T_1)$	$S_1(n)$	$r_n(S_1)$
5	$.644934\underline{1}49$	1.3(−7)	$-.1775\underline{5}20$	1.1(−4)
10	$.644934066\underline{7}76$	1.1(−10)	$-.17753\underline{3}03$	3.5(−7)
15	$.644934066848\underline{1}58$	1.1(−13)	$-.17753296\underline{5}69$	5.0(−9)
20	$.64493406684822\underline{7}33$	1.4(−15)	$-.1775329665\underline{9}17$	8.9(−11)
25	$.6449340668482264\underline{4}05$	6.2(−18)	$-.177532966575\underline{2}86$	3.4(−12)
30	$.644934066848226436\underline{3}07$	2.6(−19)	$-.177532966575\underline{9}29$	2.4(−13)
35	$.6449340668482264364 7\underline{6}04$	5.6(−21)	$-.17753296657588\underline{3}2$	2.0(−14)
40	$.644934066848226436472\underline{3}3$	1.3(−22)	$-.17753296657588\underline{7}0$	1.5(−15)

Table 4.2
Relative errors in Gaussian approximation of the sum T_1 expressed in the form (4.1) for $m = 2(1)5$

n	$m = 2$	$m = 3$	$m = 4$	$m = 5$
5	5.4(−9)	1.9(−10)	8.6(−12)	3.7(−13)
10	1.1(−13)	1.7(−16)	7.9(−18)	2.0(−19)
15	3.8(−17)	3.7(−20)	1.1(−22)	3.8(−25)
20	4.0(−20)	1.2(−24)	1.9(−27)	2.3(−29)
25	1.1(−22)	2.0(−27)	2.6(−30)	2.5(−33)
30	1.4(−25)	1.1(−31)	2.2(−33)	
35	3.2(−27)	2.4(−32)		
40	3.6(−30)			

The rapidly increasing of convergence of the summation process as m increases in due to the poles $\pm i(m + \frac{1}{2})\pi$ of $\Phi(m - \frac{1}{2}, \frac{t}{\pi})$ moving away from the real line.

TABLE 4.3
Relative errors in Gaussian approximation of the sum
$S_1 = \sum_{k=1}^{m-1} (-1)^k (k+1)^{-1} + S_m$ *for* $m = 2(1)5$

n	$m=2$	$m=3$	$m=4$	$m=5$
5	1.9(−6)	2.2(−7)	1.5(−8)	4.5(−10)
10	1.9(−9)	2.3(−12)	1.0(−12)	1.1(−14)
15	8.1(−13)	1.9(−15)	3.2(−16)	9.2(−18)
20	6.6(−14)	1.1(−16)	6.2(−19)	7.6(−21)
25	6.2(−16)	6.8(−19)	2.5(−21)	1.3(−23)
30	2.4(−18)	9.7(−21)	1.2(−24)	1.3(−26)
35	1.1(−19)	4.3(−23)	1.3(−25)	2.1(−28)
40	5.6(−21)	1.3(−24)	1.1(−27)	9.8(−31)

TABLE 4.4
Relative errors in Gaussian approximation of the sum T_1
using the "Laplace transform method" for $m = 1(1)3$

n	$m=1$	$m=2$	$m=3$
5	3.0(−4)	8.4(−3)	3.0(−2)
10	1.1(−8)	1.8(−5)	3.8(−4)
15	3.2(−13)	2.8(−8)	3.7(−6)
20	8.0(−18)	3.9(−11)	3.1(−8)
25	1.8(−22)	5.1(−14)	2.5(−10)
30	3.9(−27)	6.3(−17)	1.9(−12)
35	8.7(−32)	7.6(−20)	1.4(−14)
40	4.6(−33)	8.8(−23)	1.0(−16)

It is interesting to note that a similar approach with the "Laplace transform method" does not lead to acceleration of convergence. For example, in the case of (4.1), we have that

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

Then, applying Gaussian quadrature to the integral on the right, using $w(t) = \varepsilon(t)$ as a weight function on $(0, +\infty)$, we can obtain approximations for the sum T_1 for different values of n and m. The corresponding relative errors for $n = 5(5)40$ and $m = 1(1)3$ are presented in Table 4.4. As we can see, the convergence of the process (as m increases) slows down considerably. 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 in Table 4.4 when $m = 1$.

TABLE 4.5

Relative errors in Gaussian approximation of the sum T_1 and S_1 with respect to the logistic weight for $m = 1(1)5$

n		$m = 1$	$m = 2$	$m = 3$	$m = 4$	$m = 5$
5	T_1	4.7(−5)	5.2(−7)	1.9(−8)	1.5(−9)	1.8(−10)
	S_1	1.1(−3)	1.1(−3)	8.2(−4)	6.3(−4)	4.8(−4)
10	T_1	1.1(−6)	1.2(−9)	6.2(−12)	8.0(−14)	2.0(−15)
	S_1	4.1(−6)	1.3(−7)	1.3(−7)	1.1(−7)	1.0(−7)
15	T_1	1.1(−7)	2.8(−11)	3.4(−14)	1.2(−16)	8.9(−19)
	S_1	4.0(−7)	1.2(−10)	1.7(−11)	1.6(−11)	1.5(−11)
20	T_1	2.1(−8)	1.8(−12)	7.5(−16)	9.4(−19)	2.7(−21)
	S_1	7.5(−8)	6.5(−12)	5.1(−15)	2.2(−15)	2.1(−15)
25	T_1	5.5(−9)	2.1(−13)	3.7(−17)	2.0(−20)	2.6(−23)
	S_1	2.0(−8)	7.5(−13)	1.4(−16)	3.8(−19)	2.9(−19)
30	T_1	1.9(−9)	3.5(−14)	3.1(−18)	8.6(−22)	5.6(−25)
	S_1	7.0(−9)	1.3(−13)	1.1(−17)	3.1(−21)	4.3(−23)
35	T_1	7.7(−10)	7.7(−15)	3.8(−19)	5.8(−23)	2.1(−26)
	S_1	2.8(−9)	2.8(−14)	1.4(−18)	2.1(−22)	7.1(−26)
40	T_1	3.5(−10)	2.1(−15)	6.1(−20)	5.5(−24)	1.2(−27)
	S_1	1.3(−9)	7.5(−15)	2.2(−19)	2.0(−23)	4.4(−27)

It is interesting to mention that Gaussian quadrature over the full real line with respect to the logistic function (cf. (3.3) and (3.4)) converges considerably more slowly than shown in Tables 4.1 – 4.3 for one-sided integration, even though the poles of the integrand have a distance twice as large from the real line. The reason, probably, is that these poles are now centered over the integral of integration, whereas in (2.7) and (2.9) they are located over the left endpoint of the interval. Numerical results for $n = 5(5)40$ and $m = 1(1)5$ are given in Table 4.5.

Example 4.2. The application of the "Laplace transform method" to the series

$$\sum_{k=1}^{+\infty}(k-1)k^{-3}\exp(-1/k) = .34291894384460978096183767790 2 \qquad (4.2)$$

leads to an itegration of the Bessel function $t \mapsto J_0(2\sqrt{t})$. However, we work here with the exponential function $F(z) = -e^{-1/z}/z$, i.e.,

$$\Phi(x,y) = \frac{1}{r^2}e^{-x/r^2}\Big(x\cos\frac{y}{r^2} + y\sin\frac{y}{r^2}\Big), \qquad r^2 = x^2 + y^2.$$

As to accuracy, a similar situation prevails as in the previous example. Table 4.6 shows the relative errors in Gaussian approximations for $n = 2(4)18$ and $m = 1(1)3$.

TABLE 4.6

Relative errors in Gaussian approximation of the sum (4.2)

n	$m=1$	$m=2$	$m=3$
2	2.9(−3)	1.2(−5)	2.1(−8)
6	1.3(−4)	3.7(−8)	1.2(−10)
10	1.8(−5)	3.7(−11)	9.9(−14)
14	1.2(−6)	1.2(−12)	1.2(−16)
18	1.3(−7)	8.5(−15)	6.6(−19)

Example 4.3. Consider now

$$T_1(a) = \sum_{k=1}^{+\infty}\frac{1}{\sqrt{k}(k+a)}\,. \qquad (4.3)$$

This series with $a = 1$ appeared in a study of spirals (see Davis [1]) and defines the "Theodorus constant." Gautschi [8, p. 69] mentioned that the first 1 000 000 terms of the series $T_1(1)$ gives the result $1.8580\ldots$, i.e., $T_1(1) \approx 1.86$ (only 3-digit accuracy). Using the "method of Laplace transform," Gautschi (see [6, Example 5.1] and [8]) calculated (4.3) for $a = .5$, 1., 2., 4., 8., 16., and 32. As a increases, the convergence of the Gauss quadrature formula slows down considerably. For example, when $a = 8.$ we have results with relative errors presented in Table 4.7.

In order to achieve better accuracy, when a is large, Gautschi [6] used "stratified" summation by letting $k = \lambda + \kappa a_0$ and summing over all $\kappa \geq 0$ for

$\lambda = 1, 2, \ldots, a_0$, where $a_0 = \lfloor a \rfloor$ denotes the largest integer $\leq a$ ($a = a_0 + a_1$, $a_0 \geq 1$, $0 \leq a_1 < 1$).

TABLE 4.7
Relative errors in the "method of Laplace transform" for the series (4.3) *with* $a = 8$.

$n = 5$	$n = 10$	$n = 15$	$n = 20$	$n = 25$	$n = 30$	$n = 35$	$n = 40$
1.4(−1)	2.3(−2)	1.5(−3)	1.9(−4)	2.5(−5)	2.1(−6)	2.5(−7)	2.6(−8)

Here, we can apply directly our method to (4.3) with

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

where the integration constant is taken so that $F(\infty) = 0$. For computing the arctan function in the complex plane ($z^2 \neq -1$) we use the formula

$$\arctan z = \frac{1}{2} \arg(u + iv) + \frac{i}{4} \log \frac{x^2 + (y+1)^2}{x^2 + (y-1)^2},$$

where $z = x + iy$, $u = 1 - x^2 - y^2$, $v = 2x$.

TABLE 4.8
Relative errors in Gaussian approximation of the sum (4.4) *for* $m = 4$

n	$a = .5$	$a = 1.$	$a = 2.$	$a = 4.$
5	1.4(−11)	8.4(−12)	4.5(−12)	2.6(−12)
10	6.8(−18)	4.4(−18)	2.2(−18)	1.2(−18)
15	5.4(−22)	2.7(−22)	1.6(−22)	1.0(−22)
20	1.2(−25)	5.9(−26)	3.3(−26)	2.0(−26)
25	1.0(−28)	5.2(−29)	3.0(−29)	1.9(−29)
30	1.1(−31)	5.7(−32)	3.3(−32)	2.0(−32)
n	$a = 8.$	$a = 16.$	$a = 32.$	$a = 64.$
5	1.7(−12)	1.1(−12)	7.6(−13)	5.2(−13)
10	7.7(−19)	5.1(−19)	3.4(−19)	2.4(−19)
15	6.7(−23)	4.5(−23)	3.0(−23)	2.1(−23)
20	1.3(−26)	8.7(−27)	5.9(−27)	4.1(−27)
25	1.2(−29)	8.1(−30)	5.5(−30)	3.8(−30)
30	1.3(−32)	9.0(−33)	6.2(−33)	3.6(−33)

As before, we can represent (4.3) in the form

$$T_1(a) = \sum_{k=1}^{m-1} \frac{1}{\sqrt{k}(k+a)} + T_m(a), \qquad T_m(a) = \sum_{k=m}^{+\infty} \frac{1}{\sqrt{k}(k+a)}, \tag{4.4}$$

and then use Gaussian quadrature formula to calculate $T_m(a)$. Relative errors in approximations for $T_1(a)$, when $m = 4$ and $a = p_s$, $s = 0(1)7$, where $p_0 = .5$ and $p_{s+1} = 2p_s$, are displayed in Table 4.8.

As we can see from Table 4.8, the method presented is very efficient. Moreover, its convergence is slightly faster if the parameter a is larger. The exact sums $T_1(a)$ (to 30 significant digits), as determined by Gaussian quadrature, are, respectively,

$$\begin{aligned}
T_1(.5) &= 2.13441664298623726110148952804,\\
T_1(1) &= 1.86002507922119030718069591572,\\
T_1(2) &= 1.53968051235330201287501841998,\\
T_1(4) &= 1.21827401466989084582915976291,\\
T_1(8) &= 0.931372934003103871685751389665,\\
T_1(16) &= 0.694931714641045590163046071669,\\
T_1(32) &= 0.509926517027211348036131967602,\\
T_1(64) &= 0.369931698249671132209942364907.
\end{aligned}$$

Remark 4.1. The hyperbolic sine can be included as a factor in the integrand of S_m so that we use only the first weight function w_1. Some further investigations including a such approach will be given elsewhere.

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APPENDIX

Recursion coefficients α_k, β_k for the (monic) polynomials $\pi_k(\,\cdot\,; w_1)$ and $\pi_k(\,\cdot\,; w_2)$ orthogonal on $[0, +\infty]$ with respect to the weight functions $w_1(t) = 1/\cosh^2 t$ and $w_2(t) = \sinh t/\cosh^2 t$.

TABLE 1

Recursion coefficients for the polynomials $\{\pi_k(\,\cdot\,; w_1)\}$

k	alpha(k)	beta(k)
0	6.9314718055994530941723212146D-01	1.0000000000000000000000000000D+00
1	1.5939617276162479667832968293D+00	3.4201401950591179356910505700D-01
2	2.5704790635153506023229623757D+00	1.0982490302711024757750615776D+00
3	3.5593114896246001274923935698D+00	2.3594667503510884842534739092D+00
4	4.5521493508450628251971332577D+00	4.1206409259734225312996126403D+00
5	5.5470312425421284751577289507D+00	6.3814456471249773626945182034D+00
6	6.5431525681679808686029097276D+00	9.1416968963426452858867320270D+00
7	7.5400892325620730871114672774D+00	1.2401381399063813475148435922D+01
8	8.5375932538428070942983060280D+00	1.6160548266582688987382097742D+01
9	9.5355097763213333094562689617D+00	2.0419257322046748675142843925D+01
10	1.0533736923204318781615154727D+01	2.5177563621944731971785459237D+01
11	1.1532204728042289304076302587D+01	3.0435514377967418893654074886D+01
12	1.2530863397285539709205379979D+01	3.6193149336866216766280298026D+01
13	1.3529676424709201161977948095D+01	4.2450501914096420694349014313D+01
14	1.4528616366238649759936923691D+01	4.9207600334152388529884708177D+01
15	1.5527662144549085001093840486D+01	5.6464468600539404421339117817D+01
16	1.6526797270963617088725743755D+01	6.4221127279508584288069879207D+01
17	1.7526008637918384115438928070D+01	7.2477594123026429127768796077D+01
18	1.8525285677873595322626240259D+01	8.1233884562576556315784371707D+01
19	1.9524619764282356143811287725D+01	9.0490012101807598077869428931D+01
20	2.0524003776469000808420287625D+01	1.0024598863057796230602500654D+02
21	2.1523431777972483795565020695D+01	1.1050182467790393695842356506D+02
22	2.2522898774997739104475221939D+01	1.2125752961722091282304977559D+02
23	2.3522400532434740169895471727D+01	1.3251311183419835936824676638D+02
24	2.4521933431914333844086960942D+01	1.4426857886494552420053970101D+02
25	2.5521494361008953916301117690D+01	1.5652393751063399744666521992D+02
26	2.6521080625816019321035035488D+01	1.6927919393319937224868498934D+02
27	2.7520689881310473079490224088D+01	1.8253435373575359768739746871D+02
28	2.8520320075351817558103962351D+01	1.9628942203055681831758711401D+02
29	2.9519969403292101885517710969D+01	2.1054440349679927174793684049D+02
30	3.0519636270892725508068645610D+01	2.2529930242998360956857484232D+02
31	3.1519319263811160102194446841D+01	2.4055412278434155283089849728D+02
32	3.2519017122325364860097489319D+01	2.5630886820944080908989180435D+02
33	3.3518728720265847977149048624D+01	2.7256354208191992660956976966D+02
34	3.4518453047352129107974392492D+01	2.8931814753311628056421932118D+02
35	3.5518189194302192384745772760D+01	3.0657268747321520934747766482D+02
36	3.6517936340214859483708742306D+01	3.2432716461243855083544879391D+02
37	3.7517693741826232595406177242D+01	3.4258158147970247439504427768D+02
38	3.8517460724319973131421574908D+01	3.6133594043910298476082499375D+02
39	3.9517236673432689751095699863D+01	3.8059024370452926742931339305D+02

TABLE 2

Recursion coefficients for the polynomials $\{\pi_k(\,\cdot\,; w_2)\}$

k	alpha(k)	beta(k)
0	1.5707963267948966192313216916D+00	1.0000000000000000000000000000D+00
1	3.3371537318859924271186691475D+00	1.1964612764365364055097913098D+00
2	5.2620526190569131940940182735D+00	4.3671477023239855599943524385D+00
3	7.2219253825195963241917294956D+00	9.4920030157217803141931237018D+00
4	9.1955961335463704468573492230D+00	1.6599821474981044395118009643D+01
5	1.1176787153959861421766477155D+01	2.5695925696948527548388764699D+01
6	1.3162545671480695161080532645D+01	3.6782876995537958236321971782D+01
7	1.5151280183457372636272981837D+01	4.9862797030082115498885468165D+01
8	1.7142074910355614719206187525D+01	6.4937217691157557639041385008D+01
9	1.9134367428880868802960977055D+01	8.2007184973877795823095758742D+01
10	2.1127790670570973020159149723D+01	1.0107343286446229617992854696D+02
11	2.3122092802305852725111608578D+01	1.2213650371804518096526015893D+02
12	2.5117094183073749853776676037D+01	1.4519681646446703916664836504D+02
13	2.7112662673152088266615190672D+01	1.7025470480128094752412337012D+02
14	2.9108698612086965724633219820D+01	1.9731044019102761578748694484D+02
15	3.1105125237247274403041559211D+01	2.2636424699020615288701984186D+02
16	3.3101882342887042357068459953D+01	2.5741631307631730571242796003D+02
17	3.5098921957678223189144970437D+01	2.9046679760473857817906878653D+02
18	3.7096205324045538864657425358D+01	3.2551583679630579995868145078D+02
19	3.9093700741028742066090000630D+01	3.6256354832163887272429990003D+02
20	4.1091381993825721133124054539D+01	4.0161003466701202740268160150D+02
21	4.3089227190472453205414608922D+01	4.4265538575229310787279024438D+02
22	4.5087217886538866344915524963D+01	4.8569968099341757939040819938D+02
23	4.7085338417168533273674616542D+01	5.3074299094721482202656092833D+02
24	4.9083575380786676535285072721D+01	5.7778537863805553910813201974D+02
25	5.1081917235375518997646639470D+01	6.2682690063889639352450194411D+02
26	5.3080353979410943839777149039D+01	6.7786760796037296068125701887D+02
27	5.5078876897247722033269544524D+01	7.3090754678815650675485255235D+02
28	5.7077478354113316331839369353D+01	7.8594675909912964021774835024D+02
29	5.9076151629678729094404765489D+01	8.4298528317988766942549950784D+02
30	6.1074890781911762948790067278D+01	9.0202315406585390658662356570D+02
31	6.3073690534909888422271725032D+01	9.6306040391537984246753922954D+02
32	6.5072546185876460896065556424D+01	1.0260970623302243321695955116D+03
33	6.7071453527495507374353683412D+01	1.0911331566315193667444829680D+03
34	6.9070408782780794385036513587D+01	1.1581687120985568583801970567D+03
35	7.1069408550097444925803391953D+01	1.2272037521763441123907032577D+03
36	7.3068449756530880218659125979D+01	1.2982382986567826423869436105D+03
37	7.5067529618145579567604035523D+01	1.3712723718374572499127807181D+03
38	7.7066645605962108797192785006D+01	1.4463059906613287130107636415D+03
39	7.9065795416704862652340841220D+01	1.5233391728400654792796299133D+03

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Faculty of Electronic Engineering, Department of Mathematics, University of Niš, P. O. Box 73, 18000 Niš, Yugoslavia