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Biorthogonal Polynomials and Numerical Integration Formulas for Infinite Intervals

Avram Sidi[1]

Computer Science Department,
Technion – Israel Institute of Technology,
Haifa 32000, Israel

Doron S. Lubinsky[2]

School of Mathematics,
Georgia Institute of Technology,
Atlanta, GA 30332-0160, USA

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Abstract: In this work, we consider a class of numerical quadrature formulas for the infinite-range integrals $\int_0^\infty w(x)f(x)\,dx$, where $w(x) = x^\alpha e^{-x}$ and $w(x) = x^\alpha E_p(x)$, $E_p(x)$ being the Exponential Integral. These formulas are obtained by applying the Levin $\mathcal{L}$ and Sidi $\mathcal{S}$ transformations, two effective convergence acceleration methods, to the asymptotic expansions of $\int_0^\infty w(x)/(z-x)\,dx$ as $z \to \infty$, and they turn out to be interpolatory. In addition, their abscissas turn out to have some interesting properties: For example, if x_{ni}, $i = 1,\ldots,n$, are the abscissas of the appropriate n-point formula, then the polynomial $\prod_{i=1}^n (z - x_{ni})$ is orthogonal to some set of n real exponential functions, $e^{-\sigma_{nk}x}$, $k = 1,\ldots,n$, where σ_{nk}^{-1} are the zeros of some known polynomials. We provide some tables and numerical examples that show the effectiveness of our numerical quadrature formulas.

Keywords: Biorthogonal polynomials; Orthogonal polynomials; Convergence acceleration; Numerical integration; Rational approximation

Mathematics Subject Classification: 33C45, 33C47, 40A25, 41A20, 41A55, 65B10, 65D30, 65D32

1 Introduction

In two papers [10], [13], the first author introduced an approach that enables one to derive some new numerical quadrature formulas for integrals of the form

$$I[f] = \int_a^b w(x)f(x)\,dx, \tag{1.1}$$

[1] Corresponding author. E-mail: asidi@cs.technion.ac.il
[2] E-mail: lubinsky@math.gatech.edu

where (a,b) can be a finite or infinite interval and $w(x)$ is a nonnegative weight function all of whose moments exist. The cases that were considered in particular were those for which

(i) $(a,b) = (0,1)$ and $w(x) = x^{\alpha}(1-x)^{\beta}(\log x^{-1})^{\nu}$, where $\alpha > -1$, $\beta + \nu > -1$,

(ii) $(a,b) = (0,\infty)$ and $w(x) = x^{\alpha}e^{-x}$ and $w(x) = x^{\alpha}E_p(x)$, where $E_p(x) = \int_1^{\infty} e^{-xt}t^{-p}\,dt$ is the Exponential Integral, and $\alpha > -1$, $\alpha + p > 0$ (integrals $I[f]$ involving this $w(x)$ arise in radiation theory with $p = 1,2$), and

(iii) $(a,b) = (-\infty,\infty)$ and $w(x) = |x|^{\beta}e^{-x^2}$, $\beta > -1$.

The quadrature formulas are of the form

$$I_n[f] = \sum_{i=1}^{n} w_{ni} f(x_{ni}) \tag{1.2}$$

and they are ultimately obtained as follows: Let $u(x;z) = 1/(z-x)$, z being a fixed parameter, and approximate the integral

$$H(z) = \int_a^b \frac{w(x)}{z-x}\,dx = I[u(\cdot\,;z)], \tag{1.3}$$

by the quadrature formula $I_n[u(\cdot\,;z)] = H_n(z)$, that is,

$$H_n(z) = \sum_{i=1}^{n} \frac{w_{ni}}{z - x_{ni}}. \tag{1.4}$$

Here z is a complex variable, and we would like $H_n(z)$ to be a good approximation to $H(z)$ for $z \notin (a,b)$, in the sense that we want the sequence $\{H_n(z)\}$ to converge to $H(z)$ uniformly in compact subsets of the complex plane cut along the line segment (a,b). Now, $H_n(z)$ is a rational function, with degree of numerator at most $n-1$ and degree of denominator exactly n. Therefore, we need to construct rational approximations (with degree of numerator at most $n-1$ and degree of denominator exactly n) that approximate $H(z)$ with high accuracy in the complex plane. Clearly, the abscissas x_{ni} and weights w_{ni} of $I_n[f]$ are the poles and corresponding residues of the rational function $H_n(z)$.

Now, the function $H(z)$ has an asymptotic expansion in negative powers of z given as in

$$H(z) \sim \sum_{i=1}^{\infty} \frac{\mu_i}{z^i} \quad \text{as } z \to \infty, \quad z \notin (a,b), \tag{1.5}$$

where

$$\mu_i = \int_a^b w(x)x^{i-1}\,dx, \quad i = 1,2,\ldots\ . \tag{1.6}$$

Note that, in case (a,b) is a finite interval, the series $\sum_{i=1}^{\infty} \mu_i/z^i$ converges to $H(z)$ for all complex z such that $|z| > \max(|a|,|b|)$. That is, equality holds in (1.5) for $|z| > \max(|a|,|b|)$. When (a,b) is an infinite interval, however, this series is strongly divergent for all $z \neq 0$. Thus, it represents $H(z)$ only asymptotically as $z \to \infty$.

Whether the series $\sum_{i=1}^{\infty} \mu_i/z^i$ converges or diverges, one very effective way of constructing good rational approximations to $H(z)$ is by applying a nonlinear convergence acceleration method to the sequence $\{S_m(z)\}$ of the partial sums of $\sum_{i=1}^{\infty} \mu_i/z^i$, where

$$S_0(z) = 0 \quad \text{and} \quad S_m(z) = \sum_{i=1}^{m} \frac{\mu_i}{z^i}, \quad m = 1, 2, \ldots \,. \tag{1.7}$$

When the Shanks [9] transformation is used to accelerate the convergence of $\{S_m(z)\}$, the resulting $H_n(z)$ are Padé approximants and the resulting numerical quadrature formulas $I_n[f]$ in (1.2) are the Gaussian formulas for the integral $I[f]$ in (1.1). For Padé approximants, see Baker [2] and Baker and Graves-Morris [3], and [15, Chapter 17]. For the Shanks transformation, see [15, Chapter 16], and for application of Padé approximants as just described, see also [15, Section 25.5].

Now, for the weight functions mentioned in the first paragraph of this section, it turns out that the Levin [6] $\mathcal{L}$ transformation (in particular, the t-transformation, a special case of $\mathcal{L}$ transformation) can be used to accelerate the convergence of $\{S_m(z)\}$, and this results in different rational approximations and numerical quadrature formulas of high accuracy. By applying an appropriately modified version of the t-transformation, in [10] and [13], the first author obtained quadrature formulas that use the *same* set of abscissas when (i) $(a, b) = (0, 1)$ and $w(x) = x^\alpha(1-x)^\beta(\log x^{-1})^\nu$, such that ν is a small nonnegative integer and β is arbitrary, and (ii) when $(a, b) = (0, \infty)$ and $w(x) = x^\alpha e^{-x}$ and $w(x) = x^\alpha E_p(x)$, p being arbitrary. See also Sidi [15, pp. 430–433]. These formulas were observed to have accuracies comparable to those of the corresponding Gaussian formulas. (The Gaussian formulas for the weight function $w(x) = x^\alpha e^{-x}$ are quite standard and can be obtained from open literature, Abramowitz and Stegun [1], for example. Those for $w(x) = x^\alpha E_p(x)$ are not standard; for limited tables, see Danloy [4]. They can be computed by using Gautschi's ORTHPOL package [5], however.)

The polynomials $\phi_n(z) = \prod_{i=1}^{n}(z - x_{ni})$, where x_{ni} are the abscissas of $I_n[f]$ obtained as the poles of the rational approximations of the preceding paragraph, turn out to have some interesting biorthogonality and asymptotic properties, which are discussed in Sidi and Lubinsky [16], Sidi [14], and Lubinsky and Sidi [7]. For a summary of these, see [15, Chapter 19, p. 368]. For most recent results concerning zero distributions and asymptotics of the $\phi_n(z)$, see Lubinsky and Sidi [8].

In the present work, we return to the development of the formulas $I_n[f]$ for the cases $(a, b) = (0, \infty)$ and $w(x) = x^\alpha e^{-x}$ and $w(x) = x^\alpha E_p(x)$. As mentioned above, these cases were originally treated in [13] by applying the Levin t-transformation directly to the asymptotic expansion of $H(z)$ in (1.5) when $w(x) = x^\alpha e^{-x}$ and by applying a modification of it to the asymptotic expansion of $H(z)$ when $w(x) = x^\alpha E_p(x)$. Following a summary of the previous work, in the present work, we first extend the treatment of numerical quadrature formulas proposed in the previous papers that employed the $\mathcal{L}$ transformation by allowing integrand derivative information in these formulas. Simultaneously, we present a treatment using the Sidi [15, Chapter 19] $\mathcal{S}$ transformation (and a modification of it). The $\mathcal{S}$ transformation has been observed to produce more accurate approximations than the $\mathcal{L}$ transformation when applied to strongly divergent series; see also Weniger [17]. Because the moment series in (1.5) that are relevant to us here are strongly divergent, we expect the numerical quadrature formulas obtained by employing the $\mathcal{S}$ transformation to produce better accuracy than those obtained by employing the $\mathcal{L}$ transformation.

In the next section, we give a brief description of the $\mathcal{L}$ and $\mathcal{S}$ transformations. Following that, in Section 3, we consider the development of the numerical quadrature formulas for the infinite-range integrals $I[f]$ mentioned in the preceding paragraph via the the $\mathcal{L}$ and $\mathcal{S}$ transformations, and discuss some of their properties. In particular, we show that they are interpolatory in nature. In Section 4, we study the properties of the abscissas x_{ni} of the resulting numerical quadrature formulas and show that the polynomials $\phi_n(z) = \prod_{i=1}^{n}(z - x_{ni})$ enjoy an interesting biorthogonality property. In Section 5, we provide tables of abscissas and weights for the rules obtained from the $\mathcal{S}$ transformation for the weight function $w(x) = e^{-x}$, and we also provide some numerical examples with this weight function. Finally, in Section 6, we provide the treatment of the case $(a, b) = (-\infty, \infty)$, $w(x) = |x|^\beta e^{-x^2}$.

2 Summary of $\mathcal{L}$ and $\mathcal{S}$ Transformations

We start by summarizing the essential points concerning the $\mathcal{L}$ and $\mathcal{S}$ transformations. Let the sequence $\{A_m\}$ be such that

$$A_{m-1} = A + \omega_m h(m), \tag{2.1}$$

such that A is either $\lim_{m\to\infty} A_m$ when the latter exists or the antilimit of $\{A_m\}$ when $\{A_m\}$ diverges, and $h(m)$ is a function having an asymptotic expansion of the form

$$h(m) \sim \sum_{i=0}^{\infty} \frac{\beta_i}{m^i} \quad \text{as } m \to \infty. \tag{2.2}$$

[The antilimit of $\{A_m\}$ in this paper—with $A_m = S_m(z)$—is the Borel sum of the series $\sum_{i=1}^{\infty} \mu_i/z^i$.] Substituting (2.2) in (2.1), we have

$$A_{m-1} \sim A + \omega_m \sum_{i=0}^{\infty} \frac{\beta_i}{m^i} \quad \text{as } m \to \infty. \tag{2.3}$$

With A_m and ω_m available, the Levin $\mathcal{L}$ transformation [based on the asymptotic expansion in (2.3)] is defined via the linear systems of equations

$$A_{m-1} = A_n^{(j)} + \omega_m \sum_{i=0}^{n-1} \frac{\bar{\beta}_i}{m^i}, \quad m = j+1, j+2, \ldots, j+n+1. \tag{2.4}$$

Here $j = 0, 1, \ldots,$ and $n = 1, 2, \ldots,$ and $A_n^{(j)}$ is the approximation to A, while $\bar{\beta}_i$ are additional (auxiliary) unknowns of no interest to us. The solution of (2.4) for $A_n^{(j)}$ can be expressed in closed form as in

$$A_n^{(j)} = \frac{\sum_{i=0}^{n}(-1)^{n-i}\binom{n}{i}(j+i+1)^{n-1}A_{j+i}/\omega_{j+i+1}}{\sum_{i=0}^{n}(-1)^{n-i}\binom{n}{i}(j+i+1)^{n-1}/\omega_{j+i+1}}. \tag{2.5}$$

Note that the linear system in (2.4) has been obtained from (2.3) by replacing A by $A_n^{(j)}$, β_i by $\bar{\beta}_i$, and the asymptotic equality sign $\sim$ by $=$, and by truncating the infinite series $\sum_{i=0}^{\infty} \beta_i/m^i$ at the $i = n-1$ term, and finally by collocating the equality obtained at the $n+1$ points $m = j+1, j+2, \ldots, j+n+1$, thus obtaining $n+1$ equations to accommodate the $n+1$ unknowns $A_n^{(j)}$ and $\bar{\beta}_0, \bar{\beta}_1, \ldots, \bar{\beta}_{n-1}$.

In Levin's work [6], $\omega_m = m^\sigma(A_m - A_{m-1})$, where σ is some integer at most 1. When $\sigma = 0$, the $\mathcal{L}$ transformation is called the t-transformation, and when $\sigma = 1$, it is called the u-transformation. In developing our numerical quadrature formulas, however, we do not use Levin's ω_m; our ω_m are designed such that the asymptotic expansion in (2.3) is valid (with different β_i though) and the resulting quadrature formulas enjoy a great amount of flexibility and elegance. We will come to this point later.

We now turn to the $\mathcal{S}$ transformation. We start by observing that the asymptotic expansion of $h(m)$ in (2.2) can also be written in the form

$$h(m) \sim \sum_{i=0}^{\infty} \frac{\beta_i'}{(c+m)_i} \quad \text{as } m \to \infty. \tag{2.6}$$

Here c is some constant at our disposal and $(u)_i$ is the Pochhamer symbol defined by $(u)_0 = 1$ and $(u)_i = \prod_{k=1}^{i}(u+k-1)$ for $i = 1, 2, \ldots$. [In fact, the β_i' in (2.6) are determined uniquely by the β_i

of (2.2), and vice versa, via $\beta_0' = \beta_0$, $\beta_1' = \beta_1$, $-\beta_1' c + \beta_2' = \beta_2$, $\beta_1' c^2 - \beta_2'(2c+1) + \beta_3' = \beta_3$, etc.] Hence

$$A_{m-1} \sim A + \omega_m \sum_{i=0}^{\infty} \frac{\beta_i'}{(c+m)_i} \quad \text{as } m \to \infty. \tag{2.7}$$

Analogously to the $\mathcal{L}$ transformation, the $\mathcal{S}$ transformation [based on the new asymptotic expansion in (2.7)] is defined via the linear systems of equations

$$A_{m-1} = A_n^{(j)} + \omega_m \sum_{i=0}^{n-1} \frac{\widetilde{\beta}_i}{(c+m)_i}, \quad m = j+1, j+2, \ldots, j+n+1. \tag{2.8}$$

Here also $j = 0, 1, \ldots,$ and $n = 1, 2, \ldots,$ and $A_n^{(j)}$ is the approximation to A, and $\widetilde{\beta}_i$ are additional (auxiliary) unknowns of no interest to us. The solution for $A_n^{(j)}$ in this case also can be expressed in closed form (see Sidi[11]) as in

$$A_n^{(j)} = \frac{\sum_{i=0}^{n} (-1)^{n-i} \binom{n}{i} (c+j+i+1)_{n-1} A_{j+i}/\omega_{j+i+1}}{\sum_{i=0}^{n} (-1)^{n-i} \binom{n}{i} (c+j+i+1)_{n-1}/\omega_{j+i+1}}. \tag{2.9}$$

Numerical experience suggests that the "diagonal" sequences $\{A_n^{(j)}\}_{n=1}^{\infty}$ with j fixed have the best convergence properties, and these are the ones that are of relevance to us in the present work. For details and convergence and stability results on the $\mathcal{L}$ and $\mathcal{S}$ transformations, we refer the reader to [15, Chapter 19]. See also Weniger [17].

3 Development of Numerical Quadrature Formulas Via the $\mathcal{L}$ and $\mathcal{S}$ Transformations

Let $H(z)$, μ_i, and $S_m(z)$ be as in Section 1.

When $w(x) = x^{\alpha} e^{-x}$, we have

$$\mu_i = \int_0^{\infty} e^{-x} x^{\alpha+i-1}\, dx = \Gamma(\alpha+i), \quad i = 1, 2, \ldots, \tag{3.1}$$

where $\Gamma(z)$ is the Gamma function. Thus, the asymptotic expansion of $H(z)$ as $z \to \infty$ diverges factorially. It has been shown in Sidi [12] that $A_m = S_m(z)$ satisfies (2.1)–(2.3) for all $z \notin [0, \infty)$ with

$$\omega_m = \frac{\Gamma(\alpha+m)}{m z^m}, \quad \beta_i = z e^{-z} \frac{\partial^i}{\partial \xi^i} [e^{(1-\alpha)\xi} \exp(z e^{\xi})]\big|_{\xi=0}. \tag{3.2}$$

When $w(x) = x^{\alpha} E_p(x)$, where we recall that $E_p(x) = \int_1^{\infty} e^{-xt} t^{-p}\, dt$, we have

$$\mu_i = \int_0^{\infty} E_p(x) x^{\alpha+i-1}\, dx = \frac{\Gamma(\alpha+i)}{p+\alpha+i-1}, \quad i = 1, 2, \ldots . \tag{3.3}$$

The asymptotic expansion of $H(z)$ as $z \to \infty$ diverges factorially in this case too. It has been shown in [12] that $A_m = S_m(z)$, in this case too, satisfies (2.1)–(2.3) for all $z \notin [0, \infty)$ with

$$\omega_m = \frac{\Gamma(\alpha+m)}{m z^m}, \quad \beta_i = z \frac{\partial^i}{\partial \xi^i} \left[e^{(1-\alpha)\xi} \exp(z e^{\xi}) \int_0^{\xi} e^{(1-p)\sigma} \exp(-z e^{\sigma})\, d\sigma \right]\Bigg|_{\xi=0}. \tag{3.4}$$

Since the partial sums $S_m(z)$ of the moment series of $H(z)$, for both weight functions $w(x) = x^\alpha e^{-x}$ and $w(x) = x^\alpha E_p(x)$, satisfy (2.1)–(2.3) for all $z \notin [0,\infty)$, the functions $H(z)$ can be approximated with high accuracy by applying to the sequences $\{S_m(z)\}$ the $\mathcal{L}$ and $\mathcal{S}$ transformations. Because ω_m in (3.2) and (3.4) are the *same* for both of these weight functions, the asymptotic expansions of the corresponding $H(z)$ have the *same* form shown in (2.1)–(2.3). This enables us to treat these two weight functions simultaneously with the $\mathcal{L}$ and $\mathcal{S}$ transformations. This is what we do next.

3.1 Application of the $\mathcal{L}$ Transformation

Let us apply the (modified) $\mathcal{L}$ transformation to the sequence $\{S_m(z)\}$. Letting $A_m = S_m(z)$ and $\omega_m = \frac{\Gamma(\alpha+m)}{mz^m}$ [as in (3.2) and (3.4)] in (2.5), and writing $A_n^{(j)}(z)$ instead of $A_n^{(j)}$ (because $A_n^{(j)}$ is a function of z now), we obtain

$$A_n^{(j)}(z) = \frac{\displaystyle\sum_{i=0}^{n}(-1)^{n-i}\binom{n}{i}(j+i+1)^n \frac{z^{j+i}S_{j+i}(z)}{\Gamma(\alpha+j+i+1)}}{\displaystyle\sum_{i=0}^{n}(-1)^{n-i}\binom{n}{i}(j+i+1)^n \frac{z^{j+i}}{\Gamma(\alpha+j+i+1)}}. \tag{3.5}$$

Clearly, $A_n^{(j)}(z)$ is a rational function, and since

$$z^m S_m(z) = \mu_m + \mu_{m-1}z + \cdots + \mu_1 z^{m-1}, \tag{3.6}$$

the numerator $N_n^{(j)}(z)$ of $A_n^{(j)}(z)$ has degree $j+n-1$, while its denominator $D_n^{(j)}(z)$ has degree $j+n$ and has a zero of order j at $z=0$ and is of the form

$$\begin{aligned} D_n^{(j)}(z) &= \sum_{i=0}^{n}(-1)^{n-i}\binom{n}{i}\frac{(j+i+1)^n}{\Gamma(\alpha+j+i+1)}z^{j+i} \\ &= \sum_{i=0}^{n}(-1)^{n-i}\binom{n}{i}\frac{1}{\Gamma(\alpha+j+i+1)}\frac{1}{z}\left(z\frac{d}{dz}\right)^n z^{j+i+1} \\ &= (-1)^n\frac{n!}{\Gamma(\alpha+j+n+1)}\frac{1}{z}\left(z\frac{d}{dz}\right)^n\left[z^{j+1}L_n^{(\alpha+j)}(z)\right], \end{aligned} \tag{3.7}$$

where $L_n^{(\gamma)}(z)$ is the Laguerre polynomial of degree n given by

$$L_n^{(\gamma)}(z) = \frac{1}{n!}\sum_{i=0}^{n}(-1)^i\binom{n}{i}\frac{\Gamma(\gamma+n+1)}{\Gamma(\gamma+i+1)}z^i. \tag{3.8}$$

Using Rolle's theorem and the fact that $L_n^{(\gamma)}(z)$ has n simple zeros in $(0,\infty)$, it was shown in [13] that $D_n^{(j)}(z)$ has n simple zeros in $(0,\infty)$, in addition to the zero of order j at $z=0$. If the numerical quadrature formulas are to employ only function values but no derivative values, then we should take either (i) $j=0$, giving us an n-point rule, or (ii) $j=1$, giving us an $(n+1)$-point rule, $x=0$ being an abscissa of this rule. For $j \geq 2$, we need to supply the first $j-1$ derivatives of $f(x)$ at $x=0$.

3.2 Application of the $\mathcal{S}$ Transformation

Let us now apply the $\mathcal{S}$ transformation to the sequence $\{S_m(z)\}$. Letting $A_m = S_m(z)$ and $\omega_m = \frac{\Gamma(\alpha+m)}{mz^m}$ [as in (3.2) and (3.4)] in (2.9), and writing $A_n^{(j)}(z)$ instead of $A_n^{(j)}$ (because $A_n^{(j)}$ is a function of z now), we obtain

$$A_n^{(j)}(z) = \frac{\displaystyle\sum_{i=0}^{n}(-1)^{n-i}\binom{n}{i}(j+i+1)(c+j+i+1)_{n-1}\frac{z^{j+i}S_{j+i}(z)}{\Gamma(\alpha+j+i+1)}}{\displaystyle\sum_{i=0}^{n}(-1)^{n-i}\binom{n}{i}(j+i+1)(c+j+i+1)_{n-1}\frac{z^{j+i}}{\Gamma(\alpha+j+i+1)}}. \tag{3.9}$$

Let us now choose $c = 1$. Then, $A_n^{(j)}(z)$ assumes the elegant form [cf. (3.5)]

$$A_n^{(j)}(z) = \frac{\displaystyle\sum_{i=0}^{n}(-1)^{n-i}\binom{n}{i}(j+i+1)_n\frac{z^{j+i}S_{j+i}(z)}{\Gamma(\alpha+j+i+1)}}{\displaystyle\sum_{i=0}^{n}(-1)^{n-i}\binom{n}{i}(j+i+1)_n\frac{z^{j+i}}{\Gamma(\alpha+j+i+1)}}. \tag{3.10}$$

Clearly, this $A_n^{(j)}(z)$ is also a rational function, and its numerator $N_n^{(j)}(z)$ has degree $j+n-1$, while its denominator $D_n^{(j)}(z)$ has degree $j+n$ and has a zero of order j at $z = 0$, and

$$\begin{aligned} D_n^{(j)}(z) &= \sum_{i=0}^{n}(-1)^{n-i}\binom{n}{i}\frac{(j+i+1)_n}{\Gamma(\alpha+j+i+1)}z^{j+i} \\ &= \sum_{i=0}^{n}(-1)^{n-i}\binom{n}{i}\frac{1}{\Gamma(\alpha+j+i+1)}\frac{d^n}{dz^n}z^{j+i+n} \\ &= (-1)^n\frac{n!}{\Gamma(\alpha+j+n+1)}\frac{d^n}{dz^n}\left[z^{j+n}L_n^{(\alpha+j)}(z)\right], \end{aligned} \tag{3.11}$$

$L_n^{(\gamma)}(z)$ being the Laguerre polynomial given in (3.8). Again, using Rolle's theorem and the fact that $L_n^{(\gamma)}(z)$ has n simple zeros in $(0,\infty)$, it can be shown in this case as well that $D_n^{(j)}(z)$ has n simple zeros in $(0,\infty)$, in addition to the zero of order j at $z = 0$. Again, if the numerical quadrature formulas are to employ only function values but no derivative values, then we should take either (i) $j = 0$, giving us an n-point rule, or (ii) $j = 1$, giving us an $(n+1)$-point rule, $x = 0$ being an abscissa of this rule. For $j \geq 2$, we need to supply the first $j-1$ derivatives of $f(x)$ at $x = 0$.

3.3 Derivation of Numerical Quadrature Formulas

Let us write $A_n^{(j)}(z)$ in (3.5) and (3.10) in the unified form

$$A_n^{(j)}(z) = \frac{N_n^{(j)}(z)}{D_n^{(j)}(z)} = \frac{\sum_{i=0}^{n}\lambda_i z^{j+i}S_{j+i}(z)}{\sum_{i=0}^{n}\lambda_i z^{j+i}}, \tag{3.12}$$

where

$$\lambda_i = \begin{cases} (-1)^{n-i}\binom{n}{i}\dfrac{(j+i+1)^n}{\Gamma(\alpha+j+i+1)} & \text{for } \mathcal{L} \text{ transformation} \\ (-1)^{n-i}\binom{n}{i}\dfrac{(j+i+1)_n}{\Gamma(\alpha+j+i+1)} & \text{for } \mathcal{S} \text{ transformation} \end{cases}. \tag{3.13}$$

(i) When $j = 0$, $A_n^{(0)}(z)$ produces an n-point quadrature formula

$$I_n[f] = \sum_{i=1}^{n} w_{ni} f(x_{ni}), \tag{3.14}$$

where x_{ni} are the zeros of the polynomial $\sum_{i=0}^{n} \lambda_i z^i$ and

$$w_{ni} = \operatorname{Res} A_n^{(0)}(z)\big|_{z=x_{ni}} = \left.\frac{\sum_{i=0}^{n} \lambda_i z^i S_i(z)}{\sum_{i=0}^{n} i\lambda_i z^{i-1}}\right|_{z=x_{ni}}. \tag{3.15}$$

(ii) When $j = 1$, $A_n^{(1)}(z)$ produces a Radau-like $(n+1)$-point quadrature formula

$$\widehat{I}_n[f] = \sum_{i=0}^{n} w_{ni} f(x_{ni}), \tag{3.16}$$

where x_{ni} are the zeros of the polynomial $\sum_{i=0}^{n} \lambda_i z^{i+1}$ (we set $x_{n0} = 0$) and

$$w_{ni} = \operatorname{Res} A_n^{(1)}(z)\big|_{z=x_{ni}} = \left.\frac{\sum_{i=0}^{n} \lambda_i z^{i+1} S_{i+1}(z)}{\sum_{i=0}^{n} (i+1)\lambda_i z^{i}}\right|_{z=x_{ni}}. \tag{3.17}$$

(iii) When $j \geq 2$, $A_n^{(j)}(z)$ produces an $(n+j)$-point quadrature formula

$$I_n^{(j)}[f] = \sum_{i=0}^{j-1} \widehat{w}_{ni} \frac{f^{(i)}(0)}{i!} + \sum_{i=1}^{n} w_{ni} f(x_{ni}), \tag{3.18}$$

where x_{ni} are the positive zeros of the polynomial $\sum_{i=0}^{n} \lambda_i z^{j+i}$ and $\widehat{w}_{ni}$ and w_{ni} are defined via the partial fraction expansion

$$A_n^{(j)}(z) = \sum_{i=0}^{j-1} \frac{\widehat{w}_{ni}}{z^{i+1}} + \sum_{i=1}^{n} \frac{w_{ni}}{z - x_{ni}}. \tag{3.19}$$

Of course, $I_n[f]$ (with $j = 0$) and $\widehat{I}_n[f]$ (with $j = 1$) are special cases of $I_n^{(j)}[f]$.

Remarks.

1. If we order the positive zeros of $D_n^{(j)}(z)$, namely, $x_{n1}, \ldots, x_{nn}$, and the zeros $y_{n1}, \ldots, y_{nn}$ of $L_n^{(\alpha+j)}(x)$ in increasing order, we have by Rolle's theorem that $x_{ni} < y_{ni}$, $i = 1, \ldots, n$.

2. Since the abscissas of the quadrature rules are the zeros of $D_n^{(j)}(z)$, and $D_n^{(j)}(z)$ is *independent of* p, the sets of abscissas $\{x_{ni}\}$ are independent of p. Thus, one set of abscissas can be used for computing the integrals $I[f] = \int_0^\infty x^\alpha E_p(x) f(x)\,dx$ with every p, as well as $I[f] = \int_0^\infty x^\alpha e^{-x} f(x)\,dx$. This fact makes the quadrature formulas of this work, as well as of [10] and [13], flexible.

We end this section with two results concerning $I_n^{(j)}[f]$.

Theorem 3.1 *With $I_n^{(j)}[f]$ as in* (3.18), *there holds*

$$I_n^{(j)}[f] = I[f] \quad \text{for every } f \in \pi_{n+j-1}.$$

That is, the rule $I_n^{(j)}[f]$ is interpolatory.

Proof. By (2.4), (1.5), and the fact that $\lambda_n \neq 0$, it follows that

$$\begin{aligned} H(z) - A_n^{(j)}(z) &= \frac{\sum_{i=0}^{n} \lambda_i z^{j+i} [H(z) - S_{j+i}(z)]}{\sum_{i=0}^{n} \lambda_i z^{j+i}}, \\ &= \frac{\sum_{i=0}^{n} \lambda_i z^{j+i} O(z^{-j-i-1})}{\sum_{i=0}^{n} \lambda_i z^{j+i}} \quad \text{as } z \to \infty, \\ &= O\big(z^{-j-n-1}\big) \quad \text{as } z \to \infty. \end{aligned} \tag{3.20}$$

This also implies that

$$A_n^{(j)}(z) = S_{j+n}(z) + O\big(z^{-j-n-1}\big) \quad \text{as } z \to \infty. \tag{3.21}$$

Expanding the partial fraction expansion of $A_n^{(j)}(z)$ given in (3.19) in negative powers of z, we obtain

$$A_n^{(j)}(z) \sim \sum_{k=1}^{j} \frac{\widehat{w}_{n,k-1}}{z^k} + \sum_{k=1}^{\infty} \frac{1}{z^k} \left(\sum_{i=0}^{n} w_{ni} x_{ni}^{k-1} \right) \quad \text{as } z \to \infty. \tag{3.22}$$

By (3.22) and (3.21), we therefore have

$$\begin{aligned} \widehat{w}_{n,k-1} + \sum_{i=0}^{n} w_{ni} x_{ni}^{k-1} &= \mu_k, \quad k = 1, \ldots, j, \\ \sum_{i=0}^{n} w_{ni} x_{ni}^{k-1} &= \mu_k, \quad k = j+1, \ldots, j+n. \end{aligned}$$

By (3.18), these equalities are nothing but

$$I_n^{(j)}[x^{k-1}] = I[x^{k-1}], \quad k = 1, \ldots, j+n,$$

which is what we had to prove. ∎

Theorem 3.2 *Let $f(x) = 1/(z-x)$, where z is an arbitrary (complex) scalar not in the real interval $[0, \infty)$. Then*

$$I_n^{(j)}[f] = A_n^{(j)}(z). \tag{3.23}$$

Proof. We have $f(x_{ni}) = 1/(z - x_{ni})$ and $f^{(i)}(x) = i!/(z-x)^{i+1}$ so that $f^{(i)}(0) = i!/z^{i+1}$. Substituting these in the expression given for $I_n^{(j)}[f]$ in (3.18), and comparing with the partial fraction expansion of $A_n^{(j)}(z)$ given in (3.19), the result follows. ∎

Remark. As the computation of $A_n^{(j)}(z)$ via (3.12) is straightforward and can be achieved with high accuracy, the result of Theorem 3.2 can serve as a tool for checking the accuracy of the tables of the abscissas and weights for $I_n^{(j)}[f]$.

Finally, from the way the numerical quadrature formulas above have been obtained, it is clear that, by applying the $\mathcal{L}$ and $\mathcal{S}$ transformations with *any* weight function $w(x)$, we end up with approximations $A_n^{(j)}(z)$ that are precisely of the form given in (3.12) (with appropriate λ_i, of course). This implies that everything mentioned in this subsection, namely, (3.14)–(3.19) and Theorems 3.1 and 3.2, applies to *arbitrary* weight functions $w(x)$.

4 Biorthogonality Properties of $D_n^{(j)}(z)$

The polynomials $D_n^{(j)}(z)$ constructed in the preceding section enjoy some interesting biorthogonality properties as the next theorems show. The first theorem was already mentioned without proof in [14]. The second is new. We provide the proof of the second theorem, that of the first being similar.

Theorem 4.1 *The polynomial $D_n^{(j)}(x)$ in (3.7) is orthogonal to all functions of the form $\sum_{k=1}^{n} d_k e^{-\sigma_{nk}x}$, in the sense that*

$$\int_0^\infty x^\alpha D_n^{(j)}(x) e^{-\sigma_{nk}x}\,dx = 0, \quad k = 1, \ldots, n, \tag{4.1}$$

where σ_{nk} are distinct and positive and σ_{nk}^{-1} are the n positive roots of the polynomial

$$\psi_n(z) = \sum_{i=0}^{n} (-1)^{n-i} \binom{n}{i} (j+i+1)^n z^i = (-1)^n z^{-j-1} \left(z\frac{d}{dz}\right)^n [z^{j+1}(1-z)^n]. \tag{4.2}$$

The polynomials $\psi_n(z)$ of (4.2) were introduced in [10] and analyzed in [16] and [7].

Theorem 4.2 *The polynomial $D_n^{(j)}(x)$ in (3.11) is orthogonal to all functions of the form $\sum_{k=1}^{n} d_k e^{-\sigma_{nk}x}$, in the sense that*

$$\int_0^\infty x^\alpha D_n^{(j)}(x) e^{-\sigma_{nk}x}\,dx = 0, \quad k = 1, \ldots, n, \tag{4.3}$$

where σ_{nk} are distinct and positive and σ_{nk}^{-1} are the n positive roots of the polynomial

$$\psi_n(z) = \sum_{i=0}^{n} (-1)^{n-i} \binom{n}{i} (j+i+1)_n z^i = (-1)^n z^{-j} \frac{d^n}{dz^n} [z^{j+n}(1-z)^n]. \tag{4.4}$$

Proof. By the fact that

$$\int_0^\infty e^{-\sigma x} x^\beta\,dx = \frac{\Gamma(\beta+1)}{\sigma^{\beta+1}}, \quad \Re\sigma > 0, \quad \Re\beta > -1,$$

we have

$$\begin{aligned}\int_0^\infty x^\alpha D_n^{(j)}(x) e^{-\sigma x}\,dx &= \sum_{i=0}^{n} (-1)^{n-i} \binom{n}{i} \frac{(j+i+1)_n}{\Gamma(\alpha+j+i+1)} \int_0^\infty e^{-\sigma x} x^{\alpha+j+i}\,dx \\ &= \sum_{i=0}^{n} (-1)^{n-i} \binom{n}{i} \frac{(j+i+1)_n}{\sigma^{\alpha+j+i+1}} \\ &= z^{\alpha+j+1} \psi_n(z)\big|_{z=\sigma^{-1}},\end{aligned}$$

from which the result follows. ∎

Remarks.

1. Using the Rodrigues formula for Jacobi polynomials $P_n^{(\alpha,\beta)}(z)$ (see [1, p. 785]), we conclude that $\psi_n(z)$ in Theorem 4.2 is a constant multiple of $P_n^{(0,j)}(2z-1)$, that is, of $P_n^{(0,j)}$ shifted to the interval $[0,1]$ (from $[-1,1]$). Thus, when $j = 0$, $\psi_n(z)$ is a constant multiple of the Legendre polynomial $P_n = P_n^{(0,0)}$ shifted to the interval $[0,1]$.

2. Note that each of the polynomials $D_n^{(j)}(x)$, $n = 1, 2, \ldots,$ we have considered is orthogonal to a different set of exponential functions.

3. The results of Theorems 4.1 and 4.2 have been used in [8] in the study of zero distributions and asymptotics of the polynomials $D_n^{(j)}(z)$ in the z-plane.

Finally, the next result follows from Theorems 3.1 and 4.1 and 4.2.

Theorem 4.3 *With* $w(x) = x^\alpha e^{-x}$ *or* $w(x) = x^\alpha E_p(x)$ *in* (1.1)*, and for every* $j = 0, 1, \ldots,$ *the rules* $I_n^{(j)}[f]$ *in* (3.18) *are exact for functions* $f(x)$ *of the form*

$$f(x) = \sum_{i=0}^{j+n-1} c_i x^i + D_n^{(j)}(x) \sum_{k=1}^{n} d_k v(x) e^{-\sigma_{nk} x}; \quad v(x) = x^\alpha / w(x), \tag{4.5}$$

and where $D_n^{(j)}(x)$ *and* σ_{nk} *are as in Theorem 4.1 or as in Theorem 4.2. That is, for such* $f(x)$*, there holds*

$$I_n^{(j)}[f] = I[f], \quad j = 0, 1, \ldots\ . \tag{4.6}$$

Proof. Let us write $f(x)$ in the form

$$f(x) = p(x) + u(x); \quad p(x) = \sum_{i=0}^{j+n-1} c_i x^i, \quad u(x) = D_n^{(j)}(x) \sum_{k=1}^{n} d_k v(x) e^{-\sigma_{nk} x}.$$

From Theorem 3.1, we already know that $I_n^{(j)}[p] = I[p]$. Now, by Theorem 4.1 or Theorem 4.2, we have that $I[u] = 0$. Since $D_n^{(j)}(x)$ has a zero of multiplicity j at $x = 0$, so does $u(x)$, hence $u^{(i)}(0) = 0$, $i = 0, 1, \ldots, j-1$. (This is immediate for $w(x) = x^\alpha e^{-x}$. It can be verified for $w(x) = x^\alpha E_p(x)$ by using the appropriate expansions of $E_p(x)$ for $x \to 0+$ in [1, p. 229].) In addition, $u(x_{ni}) = 0$, $i = 1, \ldots, n$. Therefore, $I_n^{(j)}[u] = 0$ as well. This completes the proof. ∎

Remark. As mentioned already in Section 1, if we apply the Shanks transformation to the series in (1.5), the resulting rational appoximations turn out to be Padé approximants to $H(z)$. The $[n-1/n]$ Padé approximant is the analogue of our $A_n^{(0)}(z)$, and its denominator $\phi_n(z)$ is the nth orthogonal polynomial in the sense $\int_a^b w(x)\phi_n(x)\big(\sum_{i=0}^{n-1} d_i x^i\big)dx = 0$, and its zeroes $x'_{n1}, \ldots, x'_{nn}$ [all real, simple, and in (a, b)] are the abscissas of the n-point Gaussian quadrature formula $G_n[f] = \sum_{i=1}^{n} w'_{ni} f(x'_{ni})$ for $I[f] = \int_a^b w(x) f(x)\, dx$. In addition, $G_n[f]$ is exact for polynomials of degree $2n-1$, that is, $G_n[f] = I[f]$ for all $f \in \pi_{2n-1}$. This last fact can also be expressed in the form

$$G_n[f] = I[f] \quad \text{for all } f(x) = \sum_{i=0}^{n-1} c_i x^i + \phi_n(x) \sum_{k=1}^{n} d_k x^{k-1}. \tag{4.7}$$

Thus, the result (4.6) of Theorem 4.3 (with *biorthogonal* polynomials) is the analogue of (4.7) for Gaussian quadrature (with *orthogonal* polynomials).

5 Tables for the New Quadrature Formulas with $w(x) = e^{-x}$ and Numerical Examples

In Table 1, we give a comparison of the approximations $A_n^{(0)}(z)$ obtained by applying the $\mathcal{S}$ and $\mathcal{L}$ transformations to the asymptotic expansion $\sum_{i=1}^{\infty} \mu_i / z^i$ of the function $H(z) = \int_0^\infty e^{-x}/(z - x)\, dx = -e^{-z} E_1(-z)$. Thus, $A_n^{(0)}(z)$ were computed via (3.9) and (3.5), respectively. Recalling from Theorem 3.2 that $A_n^{(0)}(z) = I_n[u(\cdot\,; z)]$, where $u(x; z) = 1/(z-x)$, this is also a comparison of the quadrature formulas $I_n[f]$ obtained via the two transformations. The results in Table 1 show clearly that the formulas from the $\mathcal{S}$ transformation have better accuracy than those from the $\mathcal{L}$ transformation, especially for large z. The computations for this table were done in quadruple-precision arithmetic.

We now consider the computation of the abscissas and the weights of our numerical quadrature formulas. Since the polynomials $D_n^{(j)}(z)$ are known explicitly, we can use any polynomial solver to determine their zeros. However, for large n, the computation of these zeros to machine accuracy becomes difficult, the apparent reason being that the coefficients λ_i of the polynomial $D_n^{(j)}(z)$ have widely differing orders of magnitude. This suggests that, for large n, the zeros of $D_n^{(j)}(z)$ can be determined with a desired level of accuracy by using variable-precision arithmetic. We have done our computations in quadruple-precision arithmetic.

In Table 2, we give the abscissas x_{ni} and weights w_{ni} for the n-point rules $I_n[f]$, with the weight function $w(x) = e^{-x}$, from the $\mathcal{S}$ transformation [see (3.14) and (3.15)], for $2 \leq n \leq 12$, with 25-digit accuracy. Note that, once the abscissas x_{ni} have been computed, the corresponding weights w_{ni} can be computed with no problem via (3.15). (Tables of abscissas and weights for the n-point rules $I_n[f]$, with the same weight function, from the $\mathcal{L}$ transformation are already in [13].) In view of Table 2 and the tables in [13], it seems reasonable to conjecture that the weights w_{ni} are positive for every n.

In Table 3, we provide the numerical results obtained by applying the quadrature rules $I_n[f]$ in (3.14) from the $\mathcal{S}$ and $\mathcal{L}$ transformations to the integrals $\int_0^\infty e^{-x} f_i(x)\,dx$, $i = 1, 2, 3$, with $f_1(x) = e^{-x}$, $I[f_1] = 1/2$; $f_2(x) = 1/(e^x + a)$, $I[f_2] = [a - \log(a+1)]/a^2$; and $f_3(x) = (x+a+1)/(x+a)^2$, $I[f_3] = 1/a$. From this table, we realize that the results obtained with the quadrature rules from the $\mathcal{S}$ transformation seem to be better. Note that the computations for these examples were done in quadruple-precision arithmetic as well.

6 Treatment of the Integrals $\int_{-\infty}^{\infty} |t|^\beta e^{-t^2} f(t)\,dt$

The treatment of the preceding sections can easily be extended to the integrals

$$J[f] = \int_{-\infty}^{\infty} |t|^\beta e^{-t^2} f(t)\,dt. \tag{6.1}$$

Making use of the fact that the weight function is an even function of t, we can express this integral in the form

$$J[f] = \frac{1}{2}\int_0^\infty t^\beta e^{-t^2} [f(t) + f(-t)]\,dt.$$

Making the change of variables $x = t^2$, this integral can be expressed as in

$$J[f] = \frac{1}{4}\int_0^\infty x^{(\beta-1)/2} e^{-x} [f(\sqrt{x}) + f(-\sqrt{x})]\,dx. \tag{6.2}$$

Clearly,

$$\begin{aligned} &J[f] = I[g] = \int_0^\infty x^\alpha e^{-x} g(x)\,dx; \\ &\alpha = \frac{\beta-1}{2}, \quad g(x) = \frac{f(\sqrt{x}) + f(-\sqrt{x})}{4}. \end{aligned} \tag{6.3}$$

Thus, we can apply the numerical quadrature formulas of the preceding sections with $\alpha = (\beta-1)/2$. In the notation of Section 3, we then have

$$I_n[g] = \frac{1}{4}\sum_{i=1}^{n} w_{ni}\,[f(\sqrt{x_{ni}}) + f(-\sqrt{x_{ni}})], \tag{6.4}$$

$$\widehat{I}_n[g] = \frac{1}{4}\left\{2w_{n0}f(0) + \sum_{i=1}^{n} w_{ni}\,[f(\sqrt{x_{ni}}) + f(-\sqrt{x_{ni}})]\right\}, \tag{6.5}$$

$$I_n^{(2)}[g] = \frac{1}{4}\left\{2\widehat{w}_{n0}f(0) + \widehat{w}_{n1}f''(0) + \sum_{i=1}^{n} w_{ni}\,[f(\sqrt{x_{ni}}) + f(-\sqrt{x_{ni}})]\right\}, \tag{6.6}$$

and, in general,

$$I_n^{(j)}[g] = \frac{1}{4}\left\{2\sum_{i=0}^{j-1}\widehat{w}_{ni}\frac{f^{(2i)}(0)}{(2i)!} + \sum_{i=1}^{n} w_{ni}\,[f(\sqrt{x_{ni}}) + f(-\sqrt{x_{ni}})]\right\}. \tag{6.7}$$

We leave the details to the reader.

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Table 1: $\Delta_n(\mathcal{S};z)$ and $\Delta_n(\mathcal{L};z)$ stand for the relative errors $|A_n^{(0)}(z)-H(z)|/|H(z)|$, where $A_n^{(0)}(z)$ are obtained by applying the $\mathcal{S}$ and $\mathcal{L}$ transformations to the asymptotic expansion $\sum_{i=1}^{\infty}\mu_i/z^i$ of $H(z)=\int_0^{\infty}e^{-x}/(z-x)\,dx=-e^{-z}E_1(-z)$.

n	$\Delta_n(\mathcal{S};-1)$	$\Delta_n(\mathcal{L};-1)$	$\Delta_n(\mathcal{S};-2)$	$\Delta_n(\mathcal{L};-2)$	$\Delta_n(\mathcal{S};-3)$	$\Delta_n(\mathcal{L};-3)$	$\Delta_n(\mathcal{S};-4)$	$\Delta_n(\mathcal{L};-4)$	$\Delta_n(\mathcal{S};-5)$	$\Delta_n(\mathcal{L};-5)$
1	1.179D − 01	1.179D − 01	1.070D − 01	1.070D − 01	9.016D − 02	9.016D − 02	7.694D − 02	7.694D − 02	6.687D − 02	6.687D − 02
2	6.125D − 03	6.296D − 03	3.677D − 03	1.158D − 02	4.633D − 03	9.698D − 03	4.198D − 03	7.675D − 03	3.584D − 03	6.109D − 03
3	1.011D − 03	1.947D − 03	3.725D − 04	8.681D − 04	1.058D − 05	1.008D − 03	1.193D − 04	8.165D − 04	1.378D − 04	6.269D − 04
4	2.371D − 04	6.153D − 04	1.847D − 05	3.801D − 05	1.605D − 05	8.000D − 05	4.588D − 06	8.216D − 05	1.011D − 06	6.557D − 05
5	1.373D − 05	2.815D − 05	4.733D − 06	2.866D − 05	5.845D − 10	5.741D − 07	4.805D − 07	6.602D − 06	2.687D − 07	6.429D − 06
6	4.857D − 06	2.810D − 05	1.189D − 07	4.895D − 06	1.207D − 07	1.399D − 06	1.978D − 08	1.780D − 07	8.536D − 09	5.156D − 07
7	1.730D − 06	6.732D − 06	6.901D − 08	5.023D − 08	5.376D − 09	3.055D − 07	2.759D − 09	7.201D − 08	1.082D − 09	1.891D − 08
8	2.599D − 07	7.625D − 07	1.146D − 08	1.785D − 07	1.110D − 09	2.816D − 08	2.292D − 10	1.825D − 08	4.211D − 11	3.846D − 09
9	9.385D − 09	6.198D − 07	8.180D − 11	3.881D − 08	1.688D − 10	3.002D − 09	1.664D − 11	2.254D − 09	7.967D − 12	1.102D − 09
10	1.813D − 08	3.385D − 08	3.044D − 10	5.483D − 10	1.717D − 12	1.556D − 09	3.512D − 12	3.109D − 11	1.118D − 13	1.541D − 10
11	5.948D − 09	4.757D − 08	6.226D − 11	2.084D − 09	3.431D − 12	2.222D − 10	3.158D − 14	5.417D − 11	7.916D − 14	8.794D − 12
12	1.037D − 09	9.451D − 09	2.859D − 12	3.748D − 10	4.203D − 13	1.345D − 11	4.914D − 14	1.248D − 11	2.906D − 15	1.749D − 12
13	1.960D − 11	3.280D − 09	1.699D − 12	5.001D − 11	1.942D − 14	1.204D − 11	5.311D − 15	9.394D − 13	7.771D − 16	5.960D − 13
14	9.047D − 11	1.319D − 09	5.452D − 13	3.233D − 11	1.421D − 14	1.891D − 12	3.148D − 16	2.265D − 13	9.719D − 17	7.921D − 14
15	3.865D − 11	1.911D − 10	7.041D − 14	2.607D − 12	1.975D − 15	1.801D − 13	1.455D − 16	8.235D − 14	3.348D − 18	6.014D − 16
16	9.874D − 12	1.602D − 10	6.025D − 15	1.737D − 12	6.023D − 17	1.301D − 13	1.270D − 17	8.644D − 15	1.915D − 18	2.614D − 15
17	1.134D − 12	5.873D − 12	5.376D − 15	4.829D − 13	7.789D − 17	1.651D − 14	1.585D − 18	1.547D − 15	1.436D − 19	5.388D − 16
18	4.030D − 13	1.876D − 11	1.359D − 15	4.769D − 14	1.483D − 17	3.865D − 15	5.733D − 19	6.939D − 16	2.021D − 20	2.325D − 17
19	3.220D − 13	8.194D − 13	1.392D − 16	4.475D − 14	4.760D − 19	1.687D − 15	5.357D − 20	7.395D − 17	5.521D − 21	1.494D − 17
20	1.266D − 13	2.205D − 12	3.380D − 17	3.267D − 15	4.763D − 19	9.192D − 17	7.005D − 21	1.744D − 17	3.015D − 22	4.063D − 18
21	3.288D − 14	2.485D − 13	2.064D − 17	3.169D − 15	1.407D − 19	8.652D − 17	2.973D − 21	7.163D − 18	8.638D − 23	2.532D − 19
22	3.725D − 15	2.651D − 13	5.326D − 18	7.467D − 16	1.615D − 20	2.178D − 17	3.665D − 22	5.545D − 19	2.084D − 23	1.179D − 19
23	1.773D − 15	4.651D − 14	6.020D − 19	1.682D − 16	2.078D − 21	1.751D − 18	2.478D − 23	2.672D − 19	1.115D − 24	3.564D − 20
24	1.479D − 15	3.300D − 14	1.433D − 19	9.023D − 17	1.375D − 21	1.789D − 18	1.856D − 23	8.287D − 20	3.881D − 25	2.031D − 21
25	6.500D − 16	7.668D − 15	1.014D − 19	3.234D − 18	3.017D − 22	1.903D − 19	3.303D − 24	1.094D − 21	1.025D − 25	1.256D − 21
26	2.001D − 16	4.292D − 15	3.066D − 20	8.904D − 18	1.986D − 23	9.593D − 20	5.622D − 26	4.601D − 21	7.415D − 27	3.549D − 22
27	3.640D − 17	1.207D − 15	4.911D − 21	8.159D − 19	1.020D − 23	3.019D − 20	1.210D − 25	9.408D − 22	1.824D − 27	8.972D − 24
28	4.499D − 18	5.867D − 16	3.743D − 22	7.759D − 19	4.429D − 24	2.268D − 21	3.318D − 26	1.059D − 22	6.237D − 28	1.650D − 23
29	7.903D − 18	1.868D − 16	5.748D − 22	1.737D − 19	8.784D − 25	2.707D − 21	3.381D − 27	7.900D − 23	7.256D − 29	3.762D − 24
30	4.435D − 18	8.454D − 17	2.258D − 22	5.970D − 20	3.262D − 26	2.507D − 22	5.994D − 28	7.633D − 24	2.932D − 30	1.565D − 25

Table 2: Abscissas and weights for $I_n[f] = \sum_{i=1}^{n} w_{ni} f(x_{ni})$, where $I_n[f] \approx I[f] = \int_0^\infty e^{-x} f(x)\,dx$, obtained via the $\mathcal{S}$ transformation.

x_{ni}	w_{ni}
$n=2$	
$1.835034190722739672675719 8D-01$	$5.000000000000000000000000D-01$
$1.816496580927726032732428 0D+00$	$5.000000000000000000000000D-01$
$n=3$	
$9.419117735168029671418681 0D-02$	$2.804002175407203843340256 3D-01$
$9.114803269804037400629226 8D-01$	$5.966007876981607833608211 0D-01$
$3.494328495667915963222890 5D+00$	$1.229989947611188323051532 7D-01$
$n=4$	
$5.712687944466079937569671 6D-02$	$1.764527464218091618078915 1D-01$
$5.502619602796629332373422 6D-01$	$5.129919876781330387716849 5D-01$
$2.036267093527512516019379 0D+00$	$2.878852011958154331993734 8D-01$
$5.356344066748163751367582 0D+00$	$2.267006470424236622105007 0D-02$
$n=5$	
$3.829267158605846201093834 1D-02$	$1.205198706039195376653653 1D-01$
$3.683192405385639533042915 6D-01$	$4.109501786320576154328903 0D-01$
$1.350017063393234806816051 6D+00$	$3.726454786588215148701921 2D-01$
$3.410636154987553350215738 9D+00$	$9.233552715353686664900888 1D-02$
$7.332734869494589427652979 7D+00$	$3.548944951664465382543386 6D-03$
$n=6$	
$2.743772375433513657019518 0D-02$	$8.729625421704901207581222 9D-02$
$2.637636148052547830698305 5D-01$	$3.264400667735891895337150 4D-01$
$9.633621689598973286185823 0D-01$	$3.890113872866718854053163 7D-01$
$2.402861471299641467746182 5D+00$	$1.735194366175315578213505 3D-01$
$4.954568951162404659505985 0D+00$	$2.323353870565620507880268 4D-02$
$9.388006070018466624489224 5D+00$	$4.993163995021500850031381 7D-04$
$n=7$	
$2.061876664425497141091842 4D-02$	$6.604914510259901141932635 3D-02$
$1.981615909005662243723836 5D-01$	$2.617729753019917764837199 8D-01$
$7.226216610460073178670409 6D-01$	$3.702111729600461648920448 1D-01$
$1.792806210639615203652833 1D+00$	$2.357139949183184194297575 8D-01$
$3.642978840314446859202856 9D+00$	$6.122391326439698207895788 0D-02$
$6.621367683528006093620955 0D+00$	$4.963691295202968155702533 3D-03$
$1.150144524692710332987301 2D+01$	$6.510715744467754049087740 4D-05$
$n=8$	
$1.605788798159580654916409 5D-02$	$5.167392352085883499681763 1D-02$
$1.543083448623057430547531 0D-01$	$2.129374449102237733868582 9D-01$
$5.622626483866922047830049 5D-01$	$3.377003496775111853222192 7D-01$
$1.391358059081365073482375 7D+00$	$2.718840083858553711733757 7D-01$
$2.808634271429715607473149 6D+00$	$1.070514504799564282139584 3D-01$
$5.025957011218085669080855 1D+00$	$1.780327938603431448732499 3D-02$
$8.381603663973248002382522 4D+00$	$9.415268865044662344222376 7D-04$
$1.365981811306699189319417 5D+01$	$8.016753055626185023376621 5D-06$

x_{ni}	w_{ni}
$n = 9$	
$1.28581410905411260169424 82D-02$	$4.15096986263356229047865 33D-02$
$1.2355161763290833595829754D-01$	$1.7580053959074465813625752D-01$
$4.4999921251964414995519046D-01$	$3.0216152723507489674727595D-01$
$1.1120127858244298990863809D+00$	$2.8653253172327544978570934D-01$
$2.2371000900708226359110782D+00$	$1.4982046658590328757905407D-01$
$3.9735419902720843625758251D+00$	$3.9528470845865785459181816D-02$
$6.5212944423061143462966124D+00$	$4.4827618245140329916882832D-03$
$1.0215534746614497378046362D+01$	$1.6305983346267691436126078D-04$
$1.5854106973668957766153311D+01$	$9.4373482358948168523152187D-07$
$n = 10$	
$1.0527350521001250063597765D-02$	$3.4064497636886100828224905D-02$
$1.0115125516083048507086064D-01$	$1.4717805068332423461168624D-01$
$3.6832035040497974532586604D-01$	$2.6824980335883854567763375D-01$
$9.0944537610600356414862872D-01$	$2.8650126299591818766895300D-01$
$1.8260659320474794160430286D+00$	$1.8365089583322467823823875D-01$
$3.2304197664554339435517087D+00$	$6.6852766969592079372708566D-02$
$5.2596039433138381480405436D+00$	$1.2467268895511358166682917D-02$
$8.1073493186694312391452287D+00$	$1.0090732690684859556394458D-03$
$1.2109251786600370653165987D+01$	$2.6273224776469946688254427D-05$
$1.8077864920720631555444551D+01$	$1.0713285985953354417391605D-07$
$n = 11$	
$8.7772066283589749586457203D-03$	$2.8451085986469357437336293D-02$
$8.4332960561633210555549853D-02$	$1.2478307734627654933813946D-01$
$3.0703277315250711249819021D-01$	$2.3768444051021843239590554D-01$
$7.5774587995002976540708723D-01$	$2.7754719804220903012372265D-01$
$1.5197073822521857629028412D+00$	$2.0707914842392199634940932D-01$
$2.6820955491946508978381755D+00$	$9.5451366787107123638446105D-02$
$4.3473419240011058600460983D+00$	$2.5321425795284570793053869D-02$
$6.6458247818266615806040303D+00$	$3.4706786603506863411311313D-03$
$9.7682664881815595872642955D+00$	$2.0757536762555770961437043D-04$
$1.4052567196843263068044925D+01$	$3.9912790481137645247583362D-06$
$2.0326307857408044179880161D+01$	$1.1801488582108716503871778D-08$
$n = 12$	
$7.4297435924029256529648498D-03$	$2.4115776612618605813014418D-02$
$7.1385111658405118868727049D-02$	$1.0699854483925163552287846D-01$
$2.5986745967585343476467054D-01$	$2.1085213234780900034459360D-01$
$6.4114332646178703341982909D-01$	$2.6371874468429376582141324D-01$
$1.2849097444352827893916832D+00$	$2.2105203512056177663637987D-01$
$2.2643627056903895776294943D+00$	$1.2190077287971340277472858D-01$
$3.6602954723670298677498132D+00$	$4.2043581225155077758339713D-02$
$5.5687758007772380719608233D+00$	$8.4054751293468075361056366D-03$
$8.1161745895066048699408481D+00$	$8.7271358194703334442743790D-04$
$1.1492096094674710643202306D+01$	$3.9645014364439177086902283D-05$
$1.6037781713477291846204535D+01$	$5.7729746652434071266964803D-07$
$2.2595778237683003821214305D+01$	$1.2674719309303194709186953D-09$

Table 3: $\Delta_n[f_i]$ stands for the absolute error $|I_n[f_i]-I[f_i]|$ in the quadrature formula $I_n[f]$ in (3.14) obtained from the $\mathcal{S}$ and $\mathcal{L}$ transformations. Also, $f_1(x)=e^{-x}$, $I[f_1]=1/2$; $f_2(x)=1/(e^x+a)$, $I[f_2]=[a-\log(a+1)]/a^2$, and $f_3(x)=(x+a+1)/(x+a)^2$, $I[f_3]=1/a$. For each n, the first and second numbers in each column are those obtained from the $\mathcal{S}$ and $\mathcal{L}$ transformations, respectively.

n	method	$\Delta_n[f_1]$	$\Delta_n[f_2;a=1]$	$\Delta_n[f_2;a=0.1]$	$\Delta_n[f_3;a=1]$	$\Delta_n[f_3;a=10]$
1	$\mathcal{S}$	$1.065D-01$	$7.069D-02$	$1.029D-01$	$1.111D-01$	$4.308D-03$
1	$\mathcal{L}$	$1.065D-01$	$7.069D-02$	$1.029D-01$	$1.111D-01$	$4.308D-03$
2	$\mathcal{S}$	$2.528D-03$	$9.799D-03$	$4.790D-03$	$2.000D-02$	$1.849D-04$
2	$\mathcal{L}$	$1.665D-02$	$1.509D-02$	$1.765D-02$	$5.487D-03$	$2.805D-04$
3	$\mathcal{S}$	$1.279D-03$	$1.418D-03$	$8.258D-04$	$6.790D-04$	$7.954D-06$
3	$\mathcal{L}$	$2.053D-03$	$3.500D-03$	$2.758D-03$	$6.033D-03$	$2.250D-05$
4	$\mathcal{S}$	$2.285D-04$	$1.494D-04$	$2.442D-04$	$6.561D-04$	$3.097D-07$
4	$\mathcal{L}$	$1.466D-04$	$9.156D-04$	$3.924D-04$	$1.060D-03$	$2.036D-06$
5	$\mathcal{S}$	$1.870D-05$	$2.015D-05$	$3.507D-05$	$1.027D-04$	$9.213D-09$
5	$\mathcal{L}$	$1.728D-05$	$2.676D-04$	$4.489D-05$	$1.397D-04$	$1.980D-07$
6	$\mathcal{S}$	$1.596D-07$	$1.884D-05$	$1.868D-06$	$3.304D-06$	$9.741D-11$
6	$\mathcal{L}$	$1.066D-05$	$8.529D-05$	$7.672D-07$	$1.003D-04$	$1.996D-08$
7	$\mathcal{S}$	$1.778D-07$	$5.920D-06$	$4.818D-07$	$5.842D-06$	$8.885D-12$
7	$\mathcal{L}$	$3.084D-06$	$2.861D-05$	$2.107D-06$	$8.840D-06$	$2.029D-09$
8	$\mathcal{S}$	$2.666D-08$	$6.159D-07$	$1.270D-07$	$1.589D-06$	$5.053D-13$
8	$\mathcal{L}$	$7.119D-07$	$9.689D-06$	$1.053D-06$	$6.464D-06$	$2.020D-10$
9	$\mathcal{S}$	$1.893D-09$	$3.151D-07$	$3.925D-09$	$1.738D-07$	$4.248D-15$
9	$\mathcal{L}$	$1.449D-07$	$3.144D-06$	$3.736D-07$	$1.859D-06$	$1.898D-11$
10	$\mathcal{S}$	$7.400D-12$	$1.522D-07$	$3.646D-09$	$4.306D-08$	$1.527D-15$
10	$\mathcal{L}$	$2.694D-08$	$9.021D-07$	$1.103D-07$	$2.914D-07$	$1.579D-12$
11	$\mathcal{S}$	$1.994D-11$	$9.125D-09$	$5.060D-10$	$2.902D-08$	$1.808D-17$
11	$\mathcal{L}$	$4.632D-09$	$1.843D-07$	$2.716D-08$	$2.217D-07$	$9.823D-14$
12	$\mathcal{S}$	$2.662D-12$	$1.418D-08$	$1.072D-10$	$8.459D-09$	$5.662D-18$
12	$\mathcal{L}$	$7.368D-10$	$8.714D-09$	$5.054D-09$	$1.814D-09$	$6.301D-16$
13	$\mathcal{S}$	$1.680D-13$	$4.069D-09$	$3.047D-11$	$1.223D-09$	$1.345D-19$
13	$\mathcal{L}$	$1.071D-10$	$3.760D-08$	$3.651D-10$	$2.295D-08$	$1.119D-15$
14	$\mathcal{S}$	$3.088D-15$	$9.393D-10$	$3.373D-12$	$1.923D-10$	$2.828D-20$
14	$\mathcal{L}$	$1.374D-11$	$2.652D-08$	$2.254D-10$	$2.991D-09$	$2.311D-16$
15	$\mathcal{S}$	$2.050D-15$	$6.634D-10$	$1.682D-12$	$2.023D-10$	$6.942D-22$
15	$\mathcal{L}$	$1.400D-12$	$1.296D-08$	$1.377D-10$	$2.244D-09$	$2.999D-17$
16	$\mathcal{S}$	$2.482D-16$	$3.261D-11$	$1.411D-13$	$7.913D-11$	$1.853D-22$
16	$\mathcal{L}$	$6.102D-14$	$4.691D-09$	$4.619D-11$	$5.826D-10$	$2.430D-18$