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Quadrature rules with multiple nodes for evaluating integrals with strong singularities☆

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Abstract

We present a method based on the Chakalov–Popoviciu quadrature formula of Lobatto type, a rather general case of quadrature with multiple nodes, for approximating integrals defined by Cauchy principal values or by Hadamard finite parts. As a starting point we use the results obtained by L. Gori and E. Santi (cf. On the evaluation of Hilbert transforms by means of a particular class of Turán quadrature rules, Numer. Algorithms 10 (1995), 27–39; Quadrature rules based on s-orthogonal polynomials for evaluating integrals with strong singularities, Oberwolfach Proceedings: Applications and Computation of Orthogonal Polynomials, ISNM 131, Birkhäuser, Basel, 1999, pp. 109–119). We generalize their results by using some of our numerical procedures for stable calculation of the quadrature formula with multiple nodes of Gaussian type and proposed methods for estimating the remainder term in such type of quadrature formulae. Numerical examples, illustrations and comparisons are also shown.

MSC: primary 41A55; secondary 65D30; 65D32

Keywords: Quadratures with multiple nodes; σ-orthogonal polynomials; Finite part integral in sense of Hadamard; Cauchy principal value; Remainder term for analytic functions; Contour integral representation; Error estimate

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1. Introduction

Recently, we have considered some numerical procedures for stable calculating quadrature formulae with multiple nodes of Gaussian type. Also we have proposed some methods for estimating the remainder term in such type of quadrature formulae. For more details on the quadrature formulae with multiple nodes and their construction see [6,14,15,20].

Let $n \in \mathbb{N}$ and let $\sigma_{-1,n,1} = (p, s_1, s_2, \ldots, s_n, q)$ be a sequence of nonnegative integers. Here, we consider a rather general case of the quadrature formulas with multiple nodes of Gaussian type, i.e.,

$$\int_{-1}^{1} f(x)w(x)\,\mathrm{d}x = G_{\sigma_{-1,n,1}}(f) + R_{\sigma_{-1,n,1}}[f], \tag{1.1}$$

where

$$G_{\sigma_{-1,n,1}}(f) = \sum_{i=0}^{p-1} A_{i,0} f^{(i)}(-1) + \sum_{v=1}^{n}\sum_{i=0}^{2s_v} A_{i,v} f^{(i)}(\tau_v) + \sum_{i=0}^{q-1} A_{i,n+1} f^{(i)}(1).$$

We called the quadrature formula (1.1) (see for example [23,24]) the Chakalov–Popoviciu quadrature formula of Lobatto type (ChPL formula). The integrand f is a differentiable function, and w is a weight function on the interval $[-1, 1]$. The fixed nodes $-1, 1$ in (1.1) have multiplicities p, q, respectively. The arbitrary nodes τ_v $(v = 1, 2, \ldots, n)$, for which is important to assume that are ordered, say

$$\tau_1 < \tau_2 < \cdots < \tau_n, \quad \tau_v \in (-1, 1), \tag{1.2}$$

have odd multiplicities $2s_1 + 1, 2s_2 + 1, \ldots, 2s_n + 1$, respectively. The quadrature formula (1.1) has the maximum degree of exactness $N - 1$, where

$$N = 2\left(\sum_{v=1}^{n} s_v + n\right) + p + q, \tag{1.3}$$

and the corresponding orthogonality conditions

$$\int_{-1}^{1} (1+x)^p (1-x)^q \prod_{v=1}^{n} (x-\tau_v)^{2s_v+1} x^k w(x)\,\mathrm{d}x = 0, \quad k = 0, 1, \ldots, n-1, \tag{1.4}$$

are satisfied.

If $p = q = 0$, i.e., the first and last sum in $G_{\sigma_{-1,n,1}}(f)$ are equal to zero, then the ChPL quadrature formula reduces to the Chakalov–Popoviciu quadrature; in particular to the Gauss–Turán quadrature formula when $s_1 = s_2 = \cdots = s_n = s$, $s \in \mathbb{N}$. Finally, if $s = 0$ we have the standard Gauss quadrature formula.

For some $m \in \mathbb{N}_0$, $t \in (-1, 1)$, let $f \in C^m[-1, 1]$, with $f^{(m)}$ Hölder continuous. Denote by

$$I_m(wf; t) := \fint_{-1}^{1} \frac{f(x)}{(x-t)^{m+1}}\, w(x)\,\mathrm{d}x \tag{1.5}$$

the finite part integral in sense of Hadamard. In the sequel, we shall use the following definition (see [9]):

$$I_m(wf;t) = \int_{-1}^{1} \frac{f(x) - \sum_{k=0}^{m} \frac{f^{(k)}(t)}{k!}(x-t)^k}{(x-t)^{m+1}}\, w(x)\,\mathrm{d}x + \sum_{k=0}^{m} \frac{f^{(k)}(t)}{k!} I_{m-k}(w;t). \tag{1.6}$$

When $m=0$ (1.5) reduces to the Hilbert transform with the Cauchy principal value integral (see [8]).

Integrals with strong singularities are involved in several singular boundary integral equations. Such integrals are defined in the Cauchy principal value sense or as the Hadamard finite part, and their numerical evaluation is of interest in many problems of applied mathematics. Some quadrature methods are given for both these types of integrals (see for instance [9] and the very recent paper [10], as well as the references therein). A method based on the Gauss–Turán quadrature formulae for the particular class of weight functions (see [7]),

$$w_{n,\mu}(x) = |U_{n-1}(x)/n|^{2\mu+1}(1-x^2)^{\mu}, \tag{1.7}$$

where $\mu > -1$ is a parameter and U_j, $j \in \mathbb{N}$, are the Chebyshev polynomials of the second kind, for approximating the previous kinds of singular or hypersingular integrals has been presented recently by Gori and Santi [8,9].

In this paper we generalize the results from [8,9] by using the ChPL quadrature formulae (a rather general case of Gaussian quadratures with multiple nodes which includes the Gauss–Turán quadratures) for approximating integrals with strong singularities, as well as using more general classes of weight functions. An application of quadrature formulae to integrals with strong singularities can produce the undesirable effect that one of nodes in the corresponding quadrature formula being too close (or coinciding with) the singularity, giving rise to severe numerical cancellations. Gori and Santi [8,9] proposed how to avoid this problem by using the Gauss–Turán quadrature formulae for the Gori–Michelli weight functions (1.7). Besides this kind of weights, in this paper, we consider more general weight functions. In Section 2 we propose a method for numerical calculation of the corresponding integrals with strong singularities by using ChPL quadrature formulae and analyze numerically the cancellation problem (see Example 2.1). As we will see a plenty of ChPL quadrature formulas, for instance, with the same number of nodes and degree of exactness, enable us to avoid the numerical cancellation and to use those ChPL quadratures, which have their nodes "far" to the singularity t, for numerically stable calculation of the corresponding integral. We also discuss some error estimates for our method in Section 3, in particular under analyticity assumptions on the integrand. As contours we consider circles and confocal ellipses. The advantage of the elliptical contours is that such choice needs the analyticity of f "almost" only on the interval $[-1, 1]$. We derive error bounds for singular integrals from our bounds for the regular integration problem (see [16–19]).

2. ChPL quadrature rules for finite part integrals

Applying the rule (1.1) to the ordinary integral in (1.6) yields the following quadrature rule with multiple nodes for a Hadamard finite part integral,

$$\begin{aligned} I_m(wf;t) &= \sum_{\nu=0}^{n+1} \sum_{k=0}^{2s_\nu} B_{k,\nu}^{(m)}(t) f^{(k)}(\tau_\nu) + \sum_{k=0}^{m} C_{m-k}(t) \frac{f^{(k)}(t)}{k!} + e_{\sigma-1,n,1}^{(m)}(f;t) \\ &=: Q_{\sigma-1,n,1}^{(m)}(f;t) + e_{\sigma-1,n,1}^{(m)}(f;t), \end{aligned} \tag{2.1}$$

where $s_0 = (p-1)/2$, $s_{n+1} = (q-1)/2$, $\tau_0 = -1$, $\tau_{n+1} = 1$, and the nodes $\{\tau_\nu\}_{\nu=1}^{n}$ are the zeros of the nth σ-orthogonal polynomial in $[-1, 1]$ with respect to the weight $w(x)(1+x)^p(1-x)^q$. The function f is assumed to have the required derivatives at least at the nodes $-1, 1, \tau_\nu$, $\nu = 1, 2, \ldots, n$; t is assumed to be different from any $-1, 1, \tau_1, \tau_2, \ldots, \tau_n$; and there results $e^{(m)}_{\sigma_{-1,n,1}}(f; t) = 0$ when $f \in \mathscr{P}_{N+m-1}$, N is given by (1.3). Furthermore, by using (1.1) we obtain

$$B^{(m)}_{k,\nu}(t) = \sum_{h=k}^{2s_\nu} (-1)^{h-k} \binom{h}{k} \frac{(m+h-k)!}{m!(\tau_\nu - t)^{m+1+h-k}} A_{h,\nu},$$

$$C_{m-k}(t) = I_{m-k}(w; t) - G_{\sigma_{-1,n,1}}[(x-t)^{k-m-1}], \tag{2.2}$$

where $\nu=0, 1, \ldots, n+1$. The knowledge of $I_0(w; t)$ is required, which then yields I_{m-k}, $k=0, 1, \ldots, m-1$. Namely, differentiating with respect to t, we have

$$\fint_{-1}^{1} \frac{w(x)\,\mathrm{d}x}{(x-t)^{m-k+1}} = \frac{1}{(m-k)!} \frac{d^{m-k}}{\mathrm{d}t^{m-k}} \left(\fint_{-1}^{1} \frac{w(x)\,\mathrm{d}x}{x-t} \right).$$

The evaluation of the Hilbert transform (as a Cauchy principal value integral)

$$\fint_{-1}^{1} \frac{w^{(\alpha,\beta)}(x)}{x-t}\,\mathrm{d}x, \quad |t| < 1,$$

of the Jacobi weight function $w^{(\alpha,\beta)}(x) = (1-x)^\alpha(1+x)^\beta$ by analytic and numerical means was analyzed by Gautschi and Wimp [5]. For the evaluation of $C_{m-k}(t)$, in some cases, we refer to [13,22].

For $p = q = s_1 = \cdots = s_n = 0$, (2.1) reduces to the Gaussian type of quadrature rule given in [12].

When one of the nodes, say τ_ν, coincides with t, and f is assumed to have derivatives up to the order $m + 2s_\nu + 1$ at τ_ν ($\nu = 1, 2, \ldots, n$), a formula similar to (2.1) can be derived in an analogous way as in [9], where

$$Q^{(m)}_{\sigma_{-1,n,1}}(f; t) = \sum_{\substack{\nu=0\\ \nu\neq j}}^{n+1} \sum_{k=0}^{2s_\nu} A_{k,\nu} \left[\frac{\partial^k g(x,t)}{\partial x^k} \right]_{x=\tau_\nu} + \sum_{k=0}^{2s_j} A_{k,j} \frac{k!\, f^{(m+k+1)}(t)}{(m+k+1)!}$$
$$+ \sum_{k=0}^{m} \frac{f^{(k)}(t)}{k!} I_{m-k}(w; t) \quad (\tau_j = t)$$

and

$$g(x,t) = \frac{f(x) - \sum_{k=0}^{m} f^{(k)}(t)(x-t)^k/k!}{(x-t)^{m+1}}.$$

Example 2.1. Let, for simplicity, $p = q = 0$, i.e., the first and last sum of $G_{\sigma_{-1,n,1}}(f)$ be equal to zero. Then, instead of $\sigma_{-1,n,1}$ we use the simpler notation σ_n, what means $\sigma_n = (s_1, s_2, \ldots, s_n)$. In [9] the following integral:

$$I_1(t) = \fint_{-1}^{1} \frac{\mathrm{e}^{3x}}{(x-t)^2} \frac{\mathrm{d}x}{\sqrt{1-x^2}}, \quad t \in (-1, 1),$$

was calculated by using the corresponding Gauss–Turán quadrature formula with 3 nodes, for $t = 0.25$ and 0.99 ($s = 0, 1, 2, 3$). It is interesting to see if we can use the same formula for calculating $I_1(10^{-7})$, whose the exact value is $I_1(10^{-7}) = 20.806061163824591791493186 94\ldots$. Because of a symmetry and odd number of nodes, this formula contains the node $\tau_2 = 0$ which is too closes to the singularity $t = 10^{-7}$. This evidently produces a undesirable effect of numerical cancellation and our numerical tests confirm it. If we use Chakalov–Popoviciu quadratures with the same degree of exactness and 3 nodes, $\sigma_3 \in \{(s_1, s_2, s_3) | s_1 + s_2 + s_3 = 3s\}$, for calculating of $I_1(10^{-7})$, the same effect of cancellation is appeared in symmetric cases (see below for an explanation of the "symmetric case"). For instance, for $s = 3$ and $\sigma_3 \in \{(4, 1, 4), (2, 5, 2), (1, 7, 1), (0, 9, 0)\}$, we have a break of calculation, which is an expected fact. But, in all other cases we can calculate the requested integral. For instance, in the case $\sigma_3 = (4, 3, 2)$, we calculate this integral with the relative error of 4.766×10^{-21}. The nodes of the corresponding Chakalov–Popoviciu quadrature are

$$
\begin{aligned}
\tau_1 &= -0.80467294852322334246469581 96,\\
\tau_2 &= 0.22201345409241151787102980 40,\\
\tau_3 &= 0.91633292823003320832510629 54.
\end{aligned}
$$

To avoid the problem with cancellation in these cases, also in the cases when the weight function belongs to the class (1.7), it is possible to use the corresponding Gauss–Turán quadrature formula with an even number of nodes, as it was recommended by Gori and Santi [8,9]. But, what is the outlet for a more general case, for instance, if the weight function do not belong to the just quoted class?

Let us calculate, by using here introduced quadratures with multiple nodes, the following integral:

$$
I_2(t) = \fint_{-1}^{1} \frac{e^x}{x - t}\, dx, \quad t \in (-1, 1),
$$

which has been also calculated earlier by some other methods (cf. Criscuolo [2], Monegato [21], Caliò and Marchetti [1]). It is very suitable for its calculation to use the ChPL quadrature formulae (in this example only the Chakalov–Popoviciu), since we have not any problem with finding the derivatives of e^x.

We consider the calculation of $I_2(10^{-7}) = 2.11450165358548853092951869 7\ldots$. Since $w(x) \equiv 1$ (an even weight function), we expect again a cancellation in all symmetric cases, when we use the corresponding quadratures with odd number of nodes for calculating $I_2(10^{-7})$, since one of nodes has to be 0 and it is "close" to the given singularity $t = 10^{-7}$. For instance, in our quadratures with 5 nodes, we have a cancellation in the calculation of $I_2(10^{-7})$, when σ_5 is $(1, 1, 1, 1, 1)$ and $(0, 0, 5, 0, 0)$. But, if $\mathrm{err} = \mathrm{err}(t)$ denotes the relative error in calculating $I_2(t)$, in some nonsymmetric cases, for $t = 10^{-7}$, we obtain: $\mathrm{err} = 5.412 \times 10^{-25}$ for $\sigma_5 = (5, 0, 0, 0, 0)$; $\mathrm{err} = 5.292 \times 10^{-25}$ for $\sigma_5 = (0, 5, 0, 0, 0)$; $\mathrm{err} = 5.768 \times 10^{-25}$ for $\sigma_5 = (0, 0, 0, 5, 0)$; $\mathrm{err} = 6.407 \times 10^{-25}$ for $\sigma_5 = (0, 0, 0, 0, 5)$. In the case $\sigma_5 = (0, 5, 0, 0, 0)$, the nodes of the corresponding Chakalov–Popoviciu quadrature formula are as follows:

$$
\begin{aligned}
\tau_1 &= -0.95612372495192240568670359 66,\\
\tau_2 &= -0.31823748283936086455627475 34,\\
\tau_3 &= 0.57477280717540240243269239 28,\\
\tau_4 &= 0.82704312538477363627683754 59,\\
\tau_5 &= 0.96697245149771425834072004 93.
\end{aligned}
$$

Table 1
Relative errors of calculating $I_2(10^{-11})$

σ_9	$\mathrm{err}(10^{-11})$
(1, 0, 0, 0, 0, 0, 0, 0, 0)	3.285(−26)
(0, 1, 0, 0, 0, 0, 0, 0, 0)	3.289(−26)
(0, 0, 1, 0, 0, 0, 0, 0, 0)	3.294(−26)
(0, 0, 0, 1, 0, 0, 0, 0, 0)	3.302(−26)
(0, 0, 0, 0, 0, 1, 0, 0, 0)	3.319(−26)
(0, 0, 0, 0, 0, 0, 1, 0, 0)	3.327(−26)
(0, 0, 0, 0, 0, 0, 0, 1, 0)	3.334(−26)
(0, 0, 0, 0, 0, 0, 0, 0, 1)	3.338(−26)

We end this example by calculating the following integral

$$I_2(10^{-11}) = 2.114501750741740433954728301\ldots$$

by certain Chakalov–Popoviciu quadratures with 9 nodes.

Taking $\sigma_9 = (0, 0, 0, 0, 1, 0, 0, 0, 0)$ we have cancellation in the calculation of $I_2(10^{-11})$. But, for some nonsymmetric quadratures we get satisfactory results. The corresponding relative errors of calculating $I_2(t)$ for some selected nonsymmetric quadratures and $t = 10^{-11}$ are displayed in Table 1. Numbers in parentheses indicate decimal exponents.

3. Analysis of the error term $e^{(m)}_{\sigma-1,n,1}(f; t)$

Introduce $\Omega(x; w)$ by

$$\Omega(x; w) = (1 + x)^p (1 - x)^q \prod_{\nu=1}^{n} (x - \tau_\nu)^{2s_\nu+1} = \prod_{\nu=0}^{n+1} (x - \tau_\nu)^{2s_\nu+1},$$

where $\tau_0 = -1$, $\tau_{n+1} = 1$, $s_0 = (p - 1)/2$, $s_{n+1} = (q - 1)/2$. We recall that it is possible to associate, with any system of σ-orthogonal polynomials and with the corresponding ChPL quadrature rule (1.1), the *kernel function* $K_{\sigma-1,n,1}(z; w)$ given by (see, for instance [17])

$$K_{\sigma-1,n,1}(z; w) = \frac{\varrho_{\sigma-1,n,1}(z; w)}{\Omega(z; w)}, \quad z \notin [-1, 1], \tag{3.1}$$

where

$$\varrho_{\sigma-1,n,1}(z; w) = \int_{-1}^{1} w(x) \frac{\Omega(x; w)}{z - x}\, \mathrm{d}x,$$

which plays a fundamental role in a representation of the remainder term of the ChPL quadrature formula (1.1) by means of a contour integral. In fact, when F is analytic in a domain D containing $[-1, 1]$ and Γ

is a curve in D surrounding $[-1, 1]$, then the following expression for the remainder term is well-known (cf. [3]):

$$R_{\sigma_{-1,n,1}}[F] = \frac{1}{2\pi i}\oint_{\Gamma} K_{\sigma_{-1,n,1}}(z; w) F(z)\, dz. \tag{3.2}$$

The kernel can be given alternatively by

$$K_{\sigma_{-1,n,1}}(z; w) = R_{\sigma_{-1,n,1}}\left[\frac{1}{z - \cdot}\right].$$

We recall that the authors of [3] observed that the estimates of the error term of the type (3.2) are good even for small values of n and less conservative than other estimates given in terms of high-order derivatives of the integrand.

Let $K^{(m)}_{\sigma_{-1,n,1}}(z, t; w)$ be the corresponding kernel function of the quadrature formula (2.1). Suppose now, that the function f is a single-valued holomorphic in a domain D. Then, the following representation of the error in (2.1) can be given.

Theorem 3.1. *One has*

$$K^{(m)}_{\sigma_{-1,n,1}}(z, t; w) = \frac{1}{(z-t)^{m+1}} K_{\sigma_{-1,n,1}}(z; w). \tag{3.3}$$

Proof. The proof follows by applying the residue theorem, with respect to z, to the function

$$\frac{f(z)\Omega(x; w)}{(z-t)^{m+1}(z-x)\Omega(z; w)},$$

and then integrating with respect to the variable x on the interval $[-1, 1]$. □

On the basis of (3.3) we can represent the error in (2.1) by

$$e^{(m)}_{\sigma_{-1,n,1}}(f; t) = \frac{1}{2\pi i}\oint_{\Gamma} K^{(m)}_{\sigma_{-1,n,1}}(z, t; w)\, f(z) dz. \tag{3.4}$$

Consider now the *symmetric ChPL quadrature formula*, i.e., the quadrature formula (1.1) in which

$$w(-x) = w(x), \quad p = q, \quad s_\nu = s_{n-\nu+1} \left(\nu = 1, \ldots, \left[\frac{n}{2}\right]\right). \tag{3.5}$$

On the basis of well-known facts for the symmetric ChPL quadrature formula we can almost immediately conclude:

- The nodes satisfy

$$\tau_{n-\nu+1} = -\tau_\nu \quad \left(\nu = 1, \ldots, \left[\frac{n}{2}\right]\right).$$

- There holds $\pi_{\sigma_n}(-x) = (-1)^n \pi_{\sigma_n}(x)$, where $\pi_{\sigma_n}(x) = \prod_{\nu=1}^{n}(x - \tau_\nu)$ is the corresponding σ-orthogonal polynomial with respect to the weight function $w^L(x) = w^L_{p,q}(x) = (1 - x^2)^p w(x)$.

- The coefficients satisfy

$$A_{i,v} = (-1)^i A_{i,n-v+1} \left(v = 0, 1, \ldots, \left[\frac{n}{2}\right]; i = 0, 1, \ldots, 2s_v\right).$$

In particular, $A_{i,[n/2]+1} = 0$, if n is odd and $i = 1, 3, \ldots, 2s_{[n/2]+1} - 1$.

Lemma 3.2. *If for the ChPL quadrature formula* (1.1) *conditions* (3.5) *hold*, *then*

$$R_{\sigma-1,n,1}[x^k] \begin{cases} = 0, & k \text{ is odd}, \\ \text{has the same sign independently of } k, & k \text{ is even}. \end{cases}$$

Proof. By using the above facts for a symmetric ChPL quadrature formula it is easy to conclude that $R_{\sigma-1,n,1}[x^k] = 0$ if k is odd.

Let now k be even. On the basis of conditions (3.5) and (1.3) we have that N is even. Therefore, $k - N$ is even. Now, we have that

$$(x^k)^{(N)} \geqslant 0 \quad \text{on } [-1, 1].$$

Recently, we have introduced the so-called influence function $\Phi(x)$ for the ChPL quadrature formula (1.1) (see [23]) and proved that its sign does not change in the interval $(-1, 1)$, as well as

$$R_{\sigma-1,n,1}[x^k] = \int_{-1}^{1} \Phi(x)(x^k)^{(N)}\, \mathrm{d}x.$$

Therefore, each $R_{\sigma-1,n,1}[x^k]$ (k is even) has the same sign as the influence function. □

3.1. Circular contour

Let Γ be a circle C_ϱ with center at origin and radius ϱ (> 1), i.e., $C_\varrho = \{z : |z| = \varrho\}$, $\varrho > 1$.

Theorem 3.3. *If for the ChPL quadrature formula* (1.1) *conditions* (3.5) *hold*, *then*

$$\max_{z \in C_\varrho} |K_{\sigma-1,n,1}(z; w)| = |K_{\sigma-1,n,1}(\varrho; w)|. \tag{3.6}$$

Proof. Since

$$K_{\sigma-1,n,1}(z; w) = \sum_{k=N}^{+\infty} \frac{R_{\sigma-1,n,1}[x^k]}{z^{k+1}}, \tag{3.7}$$

for $z = \varrho$ we have

$$K_{\sigma-1,n,1}(\varrho; w) = \sum_{k=N}^{+\infty} \frac{R_{\sigma-1,n,1}[x^k]}{\varrho^{k+1}}. \tag{3.8}$$

According to Lemma 3.2, from (3.8) we conclude that

$$|K_{\sigma_{-1},n,1}(\varrho;w)| = \left|\sum_{k=N}^{+\infty} \frac{R_{\sigma_{-1},n,1}[x^k]}{\varrho^{k+1}}\right| = \sum_{k=N}^{+\infty} \frac{|R_{\sigma_{-1},n,1}[x^k]|}{\varrho^{k+1}}.$$

On the other side, from (3.7) it follows:

$$|K_{\sigma_{-1},n,1}(z;w)| \leqslant \sum_{k=N}^{+\infty} \frac{|R_{\sigma_{-1},n,1}[x^k]|}{\varrho^{k+1}}.$$

Therefore,

$$\max_{z\in C_\varrho} |K_{\sigma_{-1},n,1}(z;w)| = \sum_{k=N}^{+\infty} \frac{|R_{\sigma_{-1},n,1}[x^k]|}{\varrho^{k+1}} = |K_{\sigma_{-1},n,1}(\varrho;w)|. \qquad \square$$

Now, from (3.3), (3.4), and (3.6) the estimate below of $|e^{(m)}_{\sigma_{-1},n,1}(f;t)|$ is easily derived.

Corollary 3.4. *If for the ChPL quadrature formula* (1.1) *conditions* (3.5) *hold*, *then*

$$|e^{(m)}_{\sigma_{-1},n,1}(f;t)| \leqslant \frac{\varrho}{(\varrho-|t|)^{m+1}} |K_{\sigma_{-1},n,1}(\varrho;w)| \left(\max_{z\in C_\varrho} |f(z)|\right).$$

Theorem 3.5. *Let* $f \in C^{M+1}[-1,1]$, $M = N+m$. *Then*, *there exists* $\xi \in (-1,1)$ *such that*

$$e^{(m)}_{\sigma_{-1},n,1}(f;t) = \frac{f^{(M+1)}(\xi)}{(M+1)!} \int_{-1}^{1} \left(\prod_{v=1}^{n} (x-\tau_v)^{2s_v+2}\right) (1-x^2)^p w(x)\,\mathrm{d}x.$$

Proof. We have $e^{(m)}_{\sigma_{-1},n,1}(f;t) = R_{\sigma_{-1},n,1}[g]$, where $g \equiv g(x,t)$ is defined above.

Further, if $f \in C^N[-1,1]$, then

$$R_{\sigma_{-1},n,1}[g] = \left[\frac{\partial^N g(x,t)}{\partial x^N}\right]_{x=\xi} \frac{1}{N!} \int_{-1}^{1} w(x)(1-x^2)^p \left(\prod_{v=1}^{n} (x-\tau_v)^{2s_v+2}\right) \mathrm{d}x, \tag{3.9}$$

where $\xi \in (-1,1)$. Since (see [9, p. 113])

$$\left[\frac{\partial^N g(x,t)}{\partial x^N}\right]_{x=\xi} = \frac{1}{m!} f^{(M+1)}(\eta) B(m+1,N+1) = \frac{N!}{(M+1)!} f^{(M+1)}(\eta),$$

where $\eta \in (-1,1)$, by substituting in (3.9), we have that

$$R_{\sigma_{-1},n,1}[g] = \frac{f^{(M+1)}(\eta)}{(M+1)!} \int_{-1}^{1} \left(\prod_{v=1}^{n} (x-\tau_v)^{2s_v+2}\right) (1-x^2)^p w(x)\,\mathrm{d}x.$$

Finally, we obtain

$$e^{(m)}_{\sigma_{-1},n,1}(f;t) = \gamma^{(m)}_{\sigma_{-1},n,1} f^{(M+1)}(\eta), \quad \eta \in (-1,1), \tag{3.10}$$

Table 2
The values of $\gamma^{(m)}_{\sigma-1,n,1}$ for some selected m, p, q

m	2	2	2	4	4	4
p	1	3	5	1	3	5
q	1	3	5	1	3	5
$\gamma^{(m)}_{\sigma-1,n,1}$	4.193(−78)	3.543(−87)	2.177(−92)	1.225(−81)	9.071(−89)	4.922(−98)

where

$$\gamma^{(m)}_{\sigma-1,n,1} = \frac{1}{(M+1)!}\int_{-1}^{1}\left(\prod_{v=1}^{n}(x-\tau_v)^{2s_v+2}\right)(1-x^2)^p w(x)\,\mathrm{d}x. \qquad \square$$

The coefficient $\gamma^{(m)}_{\sigma-1,n,1}$ in (3.10) can be given alternatively in the form

$$\gamma^{(m)}_{\sigma-1,n,1} = \frac{1}{(M+1)!}\left[\int_{-1}^{1} x^N w(x)\,\mathrm{d}x - \sum_{i=0}^{p-1}(-1)^{N-i}A_{i0}\frac{N!}{(N-i)!} - \sum_{i=0}^{q-1}A_{i,n+1}\frac{N!}{(N-i)!} - \sum_{v=1}^{n}\sum_{i=0}^{2s_v}A_{iv}\frac{N!}{(N-i)!}\tau_v^{N-i}\right].$$

Example 3.6. Let $w(x)=1/\sqrt{1-x^2}$, $n=10$, and

$$s_1=s_3=s_4=s_9=s_{10}=1, \quad s_2=s_5=s_6=s_7=2, \quad s_8=3.$$

The values of $\gamma^{(m)}_{\sigma-1,n,1}$ for some m, p, q are displayed in Table 2.

3.2. Elliptic contour

Let now the contour Γ be an ellipse E_ϱ with foci at the points ± 1 and sum of semi-axes $\varrho > 1$, i.e.,

$$E_\varrho = \left\{ z \in \mathbb{C} : \; z = \tfrac{1}{2}(\varrho \mathrm{e}^{\mathrm{i}\theta} + \varrho^{-1}\mathrm{e}^{-\mathrm{i}\theta}), \; 0 \leqslant \theta < 2\pi \right\}. \tag{3.11}$$

When $\varrho \to 1$, then the ellipse shrinks to the interval $[-1, 1]$, while with increasing ϱ it becomes more and more circle-like. The advantage of the elliptical contours, regarding to the circular ones, is that such choice needs the analyticity of f in a smaller region of complex plane, especially when ϱ is near to 1.

According to (3.3), for $z = \frac{1}{2}(\varrho \mathrm{e}^{\mathrm{i}\theta} + \varrho^{-1}\mathrm{e}^{-\mathrm{i}\theta})$ we have

$$|K^{(m)}_{\sigma-1,n,1}(z,t;w)| = \frac{|K_{\sigma-1,n,1}(z;w)|}{[a_1^2 - \sin^2\theta - 2ta_1\cos\theta + t^2]^{(m+1)/2}}, \tag{3.12}$$

where we used the usual notation $a_j = a_j(\varrho) = \frac{1}{2}(\varrho^j + \varrho^{-j})$, $j \in \mathbb{N}$, $\varrho > 1$.

For the remainder in the corresponding quadrature formula (2.1), by using (3.4), we obtain the following error bound:

$$|e^{(m)}_{\sigma-1,n,1}(f;t)| \leqslant L^{(m)}_{\sigma-1,n,1}(E_\varrho,t;w)\left(\max_{z\in E_\varrho}|f(z)|\right), \tag{3.13}$$

where, because of $z=\frac{1}{2}(\xi+\xi^{-1})$, $\xi=\varrho e^{i\theta}$, and $|dz|=2^{-1/2}\sqrt{a_2-\cos 2\theta}\,d\theta$,

$$\begin{aligned} L^{(m)}_{\sigma-1,n,1}(E_\varrho,t;w) &= \frac{1}{2\pi}\oint_{E_\varrho}|K^{(m)}_{\sigma-1,n,1}(z,t;w)||dz| \\ &= \frac{1}{2\pi\sqrt{2}}\int_0^{2\pi}\left|K^{(m)}_{\sigma-1,n,1}\left(\frac{1}{2}(\varrho e^{i\theta}+\varrho^{-1}e^{-i\theta}),t;w\right)\right|(a_2-\cos 2\theta)^{1/2}\,d\theta, \end{aligned}$$

where the kernel is given by (3.12).

Consider the denominator of the fraction in (3.12) which we define as $h(\theta)^{(m+1)/2}$, where $h(\theta)=a_1^2-\sin^2\theta-2ta_1\cos\theta+t^2$ is a continuous-differentiable function of an arbitrary order. Since $h(2\pi-\theta)=h(\theta)$ ($\theta\in[0,\pi]$), for determining of an extremum of the function $h(\theta)$, i.e., $h(\theta)^{-(m+1)/2}$, it is sufficient to consider its behavior on the interval $[0,\pi]$. It is clear that if the function $h(\theta)^{-(m+1)/2}$ attains the maximum value on the interval $[0,\pi]$ at a point $\overline{\theta}$, then it is equivalent to the fact that $h(\theta)$ attains the minimum value at the same point on $[0,\pi]$. We have that $h'(\theta)=2\sin\theta(ta_1-\cos\theta)$. By using this formula and by investigation the sign of the derivative on $[0,\pi]$, we conclude that the point $\overline{\theta}$, in which the function $h(\theta)$ attains the minimum value on $[0,\pi]$, is equal to 0, π, and $\arccos(ta_1)$, if $ta_1>1$, $ta_1<-1$, and $|ta_1|\leqslant 1$, respectively.

Let $\alpha=\alpha(\varrho,t)=\max_{\theta\in[0,\pi]}h(\theta)^{-(m+1)/2}$. On the basis of the previous analysis, we conclude that

$$\alpha=\begin{cases}\dfrac{1}{(a_1-|t|)^{m+1}}, & |t|a_1>1,\\[2ex] \dfrac{1}{[(a_1-|t|)^2-(1-|t|a_1)^2]^{(m+1)/2}}, & |t|a_1\leqslant 1.\end{cases} \tag{3.14}$$

Denoting

$$\begin{aligned} L_{\sigma-1,n,1}(E_\varrho;w) &:= \frac{1}{2\pi}\oint_{E_\varrho}|K_{\sigma-1,n,1}(z;w)||dz| \\ &= \frac{1}{2\pi\sqrt{2}}\int_0^{2\pi}\left|K_{\sigma-1,n,1}\left(\frac{1}{2}(\varrho e^{i\theta}+\varrho^{-1}e^{-i\theta});w\right)\right|(a_2-\cos 2\theta)^{1/2}\,d\theta, \end{aligned}$$

and by using (3.12), (3.14), we obtain

$$L^{(m)}_{\sigma-1,n,1}(E_\varrho,t;w)\leqslant \alpha L_{\sigma-1,n,1}(E_\varrho;w).$$

Substituting the last inequality in (3.13) we obtain the following error bound for (2.1),

$$|e^{(m)}_{\sigma-1,n,1}(f;t)|\leqslant \alpha L_{\sigma-1,n,1}(E_\varrho;w)\left(\max_{z\in E_\varrho}|f(z)|\right). \tag{3.15}$$

The error bounds (3.13) are very precise. For the Gauss quadrature formulae such bounds are considered by Hunter [11]. Another interesting approach has been given by Gautschi and Varga [4]. The case of Gauss–Turán quadratures has been considered in [16].

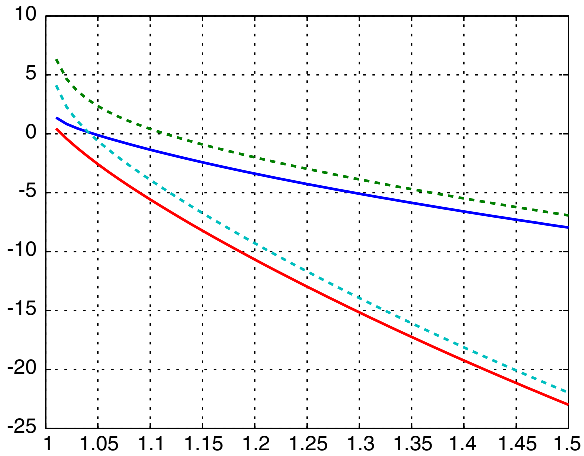

Fig. 1. Log_{10} of the values $L^{(2)}_{\sigma-1,n,1}(E_\varrho, 0; w)$ (solid line) and its bound given by (3.16) (dashed line) for $n = 10$ (top) and $n = 30$ (bottom), when $1 < \varrho \leqslant 1.5$.

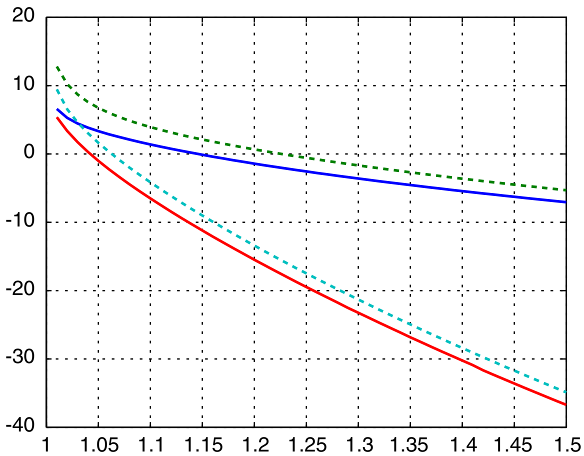

Fig. 2. Log_{10} of the values $L^{(5)}_{\sigma-1,n,1}(E_\varrho, 0; w)$ (solid line) and its bound given by (3.16) (dashed line) for $n = 10$ (top) and $n = 50$ (bottom), when $1 < \varrho \leqslant 1.5$.

The error bounds (3.15) can be easily computed for the Gauss–Turán quadratures formulae and some classes of weight functions, especially if we use upper bounds of $L_{\sigma-1,n,1}(E_\varrho; w)$ which are rather simple for calculation. For more details see the recent papers [17–19].

Example 3.7. The Gauss–Turán quadrature formulae for $s = 1$ and the Gori–Michelli weight functions (1.7) with $\mu = \frac{1}{2}$, i.e.,

$$w(x) = w_{n,1/2}(x) = |U_{n-1}(x)/n|^2\sqrt{1 - x^2},$$

have been considered in [19]. By using the results from [19, Theorem 3.1] and our considerations for the error bounds, when the contour is an ellipse, we obtain in this case

$$L^{(m)}_{\sigma_{-1},n,1}(E_\varrho,t;w)=\frac{1}{2n^2\varrho^{3n}}\int_0^\pi\sqrt{\frac{(a_{2n}-\cos 2n\theta)(b_{2n}+\cos 2n\theta)}{(a_{2n}+\cos 2n\theta)^3(a_1^2-\sin^2\theta-2ta_1\cos\theta+t^2)^{m+1}}}\,\mathrm{d}\theta,$$

where $b_{2n}=\varrho^{2n}+\varrho^{-2n}/4$, as well

$$L^{(m)}_{\sigma_{-1},n,1}(E_\varrho,t;w)\leqslant\frac{\alpha\pi}{2n^2}\sqrt{\frac{1-x-9x^2+29x^3+4x^4}{x(x-1)^5}}, \tag{3.16}$$

where $x=\varrho^{4n}$.

Let $t=0$, for simplicity. The function $\varrho\mapsto\log_{10}(L^{(m)}_{\sigma_{-1},n,1}(E_\varrho,0;w))$, as well as its bound which appear on the right side in (3.16) are displayed in Fig. 1 for $m=2$, i.e., in Fig. 2 for $m=5$, respectively.

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