A method for efficient computation of integrals with oscillatory and singular integrand

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Abstract A method based on modification of numerical steepest descent method to efficiently compute highly oscillatory integrals having endpoint singularities of algebraic and logarithmic type is proposed in this paper. The three-term recursion coefficients for orthogonal polynomials with respect to Gautschi's weight function $w^G(t;s) = t^s(t-1-\log t)e^{-t}$ (s > -1) on $(0, \infty)$, as well as the corresponding quadrature formulas of Gaussian type, are used in this method. Finally, in order to illustrate the efficiency of the presented method a few numerical examples are included. The obtained results show that the proposed method is very efficient and economical in terms of computation time.

Keywords Highly oscillatory integrals · Algebraic and logarithmic singularities · Steepest descent method · Generalized Gauss-Laguerre · Logarithmic Gauss-Gautschi-Laguerre.

1 Introduction

Consider integrals in the following form

$$I[f] = \int_{a}^{b} \frac{[\log(x-a)]^{c_1} [\log(b-x)]^{c_2} f(x) e^{i\omega x}}{(x-a)^{\alpha} (b-x)^{\beta}} dx \quad (\alpha, \beta < 1),$$
(1)

where ω (= frequency) $\gg 1$, $c_1, c_2 \in \{0, 1\}$, $-\infty < a < b < \infty$ and f(z) is non-oscillatory, analytic and of exponential order on the strip

$$S = \{ z \in \mathbb{C} : a \le \operatorname{Re}(z) \le b \}.$$
⁽²⁾

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Here, by f(z) is of exponential order on S, we mean that there exist constants m and M satisfying

$$|f(z)| = |f(x+iy)| \le M e^{m|y|}, \quad z \in S.$$
 (3)

For example, e^z is of exponential order on *S* with constants m = 0 and $M = e^b$ because $|\exp(x+iy)| \le e^b$. The function $\exp(-z^2)$, on the other hand, is not of exponential order.

In this paper, we are interested in the numerical evaluation of integrals of the following form, under the condition of $c_1 = c_2 = 1$ for integral of (1),

$$I[f] = \int_{a}^{b} \frac{\log(x-a)\log(b-x)f(x)e^{i\omega x}}{(x-a)^{\alpha}(b-x)^{\beta}} dx \quad (\alpha, \beta < 1, \ \omega \gg 1).$$

$$\tag{4}$$

Highly oscillatory singular integrals of the form (1) arise in many areas of natural sciences, engineering, applied mathematics and medicine. For $\alpha = \beta = c_1 = c_2 = 0$, there are efficient methods such as Filon method, Clenshaw-Curtis method, asymptotic method, Levin method, numerical steepest descent method, generalized quadrature rule [5,8,9,15,19,20, 22,23,29]. However, they are not suitable in calculating the oscillatory singular integrals. Therefore, different methods have been developed for these type of integrals. These methods are modified Clenshew-Curtis method presented by R. Piessens and M. Branders [31, 32], the methods proposed by G.A. Evans and J.R. Webster [7], the methods suggested by Hongchao Kang, Shuhuang Xiang and Guo He [21], a modification of the steepest descent method presented by Ruyun Chen [4] and A.I. Hasçelik and D. Kılıç [18], and special Gauss-type integration methods proposed by A.I. Hasçelik [16,17]. Also in the case $c_1 = c_2 = 0$, Gauss-Jacobi method [11] gives effective results for small ω . But, none of these methods are efficient for integrals of the form (4), especially for large ω .

In this paper, we develop a new Gauss integration method based on the modification of numerical steepest descent method and a complex integration method proposed by G.V. Milovanović [25]. Otherwise, these methods have been used in many other papers, especially in numerical evaluation of special functions (cf. [3,27,34,33]).

Our method is improved according to Gautschi's weight function [12] and using the so-called logarithmic Gauss-Laguerre quadratures. We also create a MATHEMATICA program to efficiently compute this type of integrals. While existing methods in the literature are not sufficient to solve highly oscillatory integrals with logarithmic and algebraic integrals, the proposed method is suitable and can calculate such integrals efficiently and highly accurately.

The presented paper is structured as follows. We present a method by choosing a contour on the complex plane in Section 2. Integrals given in the second section are reduced in Section 3 to ones along $(0,\infty)$ with respect to the generalized Gauss-Laguerre and logarithmic Gauss-Gautschi-Laguerre weight functions. Gauss quadrature rules for these weight functions are constructed in Section 4. In the last section, some vigorous and robust numerical results verify the accuracy and effectiveness of the presented method.

2 Expressing I[f] as a sum of two nonoscillatory integrals

In this section, we develop a method, based on contour integration on the complex plane, for efficient computation of (4).

Let *c* be any number in (a, b). Then the integral (4) can be written as

$$I[f] = I_a[f] + I_b[f]$$

$$I_a[f] = \int_a^c \frac{\log (x-a) \log (b-x) f(x) e^{i\omega x}}{(x-a)^\alpha (b-x)^\beta} dx$$
(5)

and

$$I_b[f] = \int_c^b \frac{\log(x-a)\log(b-x)f(x)e^{i\omega x}}{(x-a)^{\alpha}(b-x)^{\beta}} dx.$$
 (6)

2.1 $I_a[f]$ as a sum of two nonoscillatory integrals

Using the change of variables u = x - a in (5) we get

$$I_a[f] = e^{i\omega a} \int_0^{c-a} \frac{\log\left(u\right)\log\left(b-a-u\right)f(u+a)e^{i\omega u}}{u^{\alpha}(b-a-u)^{\beta}} du.$$
(7)

Now consider the closed contour

$$C = \bigcup_{k=1}^{5} C_k \tag{8}$$

in the complex plane \mathbb{C} , where

$$C_{1}: \gamma_{1}(t) = re^{it}, \ 0 \le t \le \pi,$$

$$C_{2}: \gamma_{2}(t) = t, \ r \le t \le c - a,$$

$$C_{3}: \gamma_{3}(t) = c - a + it, \ 0 \le t \le R,$$

$$C_{4}: \gamma_{4}(t) = t + iR, \ 0 \le t \le c - a,$$

$$C_{5}: \gamma_{5}(t) = it, \ r \le t \le R,$$
(9)

and let \mathbf{D} be the closure of the region bounded by C, as shown in Figure 1.



Fig. 1 Contour of integration for integral (7)

Lemma 1 If ψ_0 is defined by

$$\psi_0(z) = \frac{\log(z)\log(b - a - z)}{z^{\alpha}(b - a - z)^{\beta}},$$
(10)

then there exist nonnegative constants K and δ such that

$$|\psi_0(t+\mathrm{i}R)| \le K\mathrm{e}^{\delta R} \tag{11}$$

for all $t \in [0, c-a]$, when R is sufficiently large.

Remark 1 For $\alpha, \beta \in (0, 1)$, since $\lim_{R\to\infty} |\psi_0(t + iR)| = 0$ for $t \in [0, c - a]$, it follows that $|\psi_0(t + iR)| < 1$ for sufficiently large *R*.

Now we can state and prove the following theorem:

Theorem 1 If f(z) is of exponential order in the sense (3) with constants $\{m, M\}$ and analytic on the strip S given by (2), then we have

$$I_{a}[f] = i^{1-\alpha} e^{i\omega a} \int_{0}^{\infty} \frac{\log(it)\log(b-a-it)f(a+it)}{(b-a-it)^{\beta}} t^{-\alpha} e^{-\omega t} dt$$
$$-ie^{i\omega c} \int_{0}^{\infty} \frac{\log(c-a+it)\log(b-c-it)f(c+it)}{(b-c-it)^{\beta}(c-a+it)^{\alpha}} e^{-\omega t} dt$$
(12)

for $\omega > \omega_0 = m + \delta$.

Proof Let

$$\psi(z) = \frac{\log(z)\log(b-a-z)f(z+a)\mathrm{e}^{\mathrm{i}\omega z}}{z^{\alpha}(b-a-z)^{\beta}}.$$
(13)

Since $\psi(z)$ is analytic on **D**, by the Cauchy-Goursat theorem [2] we have

$$e^{i\omega a} \oint_C \psi(z) dz = e^{i\omega a} \sum_{k=1}^5 \int_{C_k} \psi(z) dz = 0, \qquad (14)$$

where the orientation is taken in the counter-clockwise direction as shown in Figure 1. Now consider each integral on the right side of (14).

On the quarter circle, centered at 0 with radius r < (b-a)/2, we have

$$\begin{split} \left| \int_{C_1} \psi(z) \mathrm{d}z \right| &= \left| \int_{\pi/2}^0 \frac{\log(r\mathrm{e}^{\mathrm{i}\theta}) \log(b-a-r\mathrm{e}^{\mathrm{i}\theta}) f(a+r\mathrm{e}^{\mathrm{i}\theta}) \mathrm{e}^{\mathrm{i}\omega r\mathrm{e}^{\mathrm{i}\theta}}}{(r\mathrm{e}^{\mathrm{i}\theta})^\alpha (b-a-r\mathrm{e}^{\mathrm{i}\theta})^\beta} r\mathrm{e}^{\mathrm{i}\theta} \mathrm{d}\theta \right| \\ &= r^{1-\alpha} \left| \int_0^{\pi/2} \frac{\log(r\mathrm{e}^{\mathrm{i}\theta}) \log(b-a-r\mathrm{e}^{\mathrm{i}\theta}) f(a+r\mathrm{e}^{\mathrm{i}\theta}) \mathrm{e}^{\mathrm{i}\omega r\mathrm{e}^{\mathrm{i}\theta}}}{\mathrm{e}^{\mathrm{i}\theta(\alpha-1)} (b-a-r\mathrm{e}^{\mathrm{i}\theta})^\beta} \mathrm{d}\theta \right| \\ &\leq r^{1-\alpha} |\log r| \int_0^{\pi/2} |\phi(r,\theta)| \,\mathrm{d}\theta + r^{1-\alpha} \int_0^{\pi/2} \theta \,|\phi(r,\theta)| \,\mathrm{d}\theta, \end{split}$$

where

$$\phi(r,\theta) = \frac{\log(b-a-r\mathrm{e}^{\mathrm{i}\theta})f(a+r\mathrm{e}^{\mathrm{i}\theta})\mathrm{e}^{\mathrm{i}\omega r\mathrm{e}^{\mathrm{i}\theta}}}{\mathrm{e}^{\mathrm{i}\theta(\alpha-1)}(b-a-r\mathrm{e}^{\mathrm{i}\theta})^{\beta}}.$$

It can be shown that the absolute value of $\phi(s,t)$ is continuous on

$$\left\{(s,t): 0 \le s \le r, \ 0 \le t \le \frac{\pi}{2}\right\},\$$

which implies that each integral in the last line of the above inequality exists and is a continuous function of *r*. Taking the limit as $r \to 0$ we get $\int_{C_1} \psi(z) dz \to 0$.

On C_2 , taking z = x, it is easy to show that

$$\lim_{r\to 0}\int_{C_2}\psi(z)\mathrm{d} z=\lim_{r\to 0}\int_r^{c-a}\psi(x)\mathrm{d} x=\mathrm{e}^{-\mathrm{i}\omega a}I_a[f].$$

On C_3 , taking z = c - a + it, $0 \le t \le R$, we obtain

$$e^{i\omega a} \int_{C_3} \Psi(z) dz = e^{i\omega a} \int_0^R \Psi(c - a + it) i dt$$

= $i e^{i\omega c} \int_0^R \frac{\log(c - a + it) \log(b - c - it) f(c + it) e^{-\omega t}}{(c - a + it)^\alpha (b - c - it)^\beta} dt.$

Now consider the integral along the path C_4 . Using the parametrization z = t + iR, $0 \le t \le c - a$, we have

$$-\int_{C_4} \Psi(z) dz = \int_0^{c-a} \Psi(t+iR) dt$$

= $e^{-\omega R} \int_0^{c-a} \frac{\log(t+iR)\log(b-a-t-iR)f(t+a+iR)}{(t+iR)^{\alpha}(b-a-t-iR)^{\beta}e^{-i\omega t}} dt.$

Taking the absolute values of both sides yields

$$\left|\int_{C_4} \Psi(z) \mathrm{d} z\right| \leq M \mathrm{e}^{-R(\omega-m)} \int_0^{c-a} |\Psi_0(t+\mathrm{i} R)| \, \mathrm{d} t,$$

where ψ_0 is defined as in Lemma 1. Consequently, for sufficiently large *R*, we have

$$\left|\int_{C_4} \psi(z) \mathrm{d} z\right| \leq M K \mathrm{e}^{-R(\omega - \omega_0)}(c - a), \quad \omega_0 = m + \delta,$$

where *K* and δ are as in Lemma 1. Note that we can take K = 1 and $\delta = 0$ when $\alpha, \beta \in (0, 1)$. Taking the limit as $R \to \infty$ we obtain

$$\lim_{R\to\infty}\int_{C_4}\psi(z)\mathrm{d} z=0,\quad \omega>\omega_0$$

For the integral along the path C_5 , it can easily be shown that

$$\int_{C_5} \Psi(z) dz = -i^{1-\alpha} \int_r^R \frac{\log(it) \log(b-a-it) f(it+a) e^{-\omega t}}{t^{\alpha} (b-a-it)^{\beta}} dt.$$

Combining the above results and letting $r \to 0$ and $R \to \infty$, we get the assertion of the theorem.

2.2 $I_b[f]$ as a sum of two nonoscillatory integrals

Theorem 2 Under the same conditions as in Theorem 1, we have

$$I_{b}[f] = (-\mathrm{i})^{1-\beta} \mathrm{e}^{\mathrm{i}\omega b} \int_{0}^{\infty} \frac{\log\left(-\mathrm{i}t\right) \log\left(b-a+\mathrm{i}t\right) f\left(b+\mathrm{i}t\right)}{(b-a+\mathrm{i}t)^{\alpha}} t^{-\beta} \mathrm{e}^{-\omega t} \mathrm{d}t$$
$$+\mathrm{i} \mathrm{e}^{\mathrm{i}\omega c} \int_{0}^{\infty} \frac{\log\left(c-a+\mathrm{i}t\right) \log\left(b-c-\mathrm{i}t\right) f\left(c+\mathrm{i}t\right)}{(b-c-\mathrm{i}t)^{\beta} (c-a+\mathrm{i}t)^{\alpha}} \mathrm{e}^{-\omega t} \mathrm{d}t.$$
(15)

Proof Using the change of variables u = b - x in (7) we can write $I_b[f]$ in the form

$$I_b[f] = e^{i\omega b} \int_0^{b-c} \frac{\log(u)\log(b-a-u)f(b-u)e^{-i\omega u}}{u^\beta(b-a-u)^\alpha} du.$$

Therefore, the proof of this theorem is analogues to the proof of Theorem 1, except that the integration path in this case is taken as the union of the curves

$$C_{b1} : \gamma_{1}(t) = re^{it}, \quad -\pi/2 \le t \le 0,$$

$$C_{b2} : \gamma_{2}(t) = -it, \quad r \le t \le R,$$

$$C_{b3} : \gamma_{3}(t) = t - iR, \quad 0 \le t \le b - c,$$

$$C_{b4} : \gamma_{4}(t) = b - c - it, \quad 0 \le t \le R,$$

$$C_{b5} : \gamma_{5}(t) = t, \quad 0 \le t \le b - c.$$
(16)

Notice that the region in this case is below the real axis.

2.3 I[f] as a sum of two nonoscillatory integrals

As a corollary of Theorem 1 and Theorem 2 we have

Theorem 3 If the hypothesis of Theorem 2 is satisfied, then we have

$$I[f] = i^{1-\alpha} e^{i\omega a} \int_0^\infty \frac{\log (it) \log (b-a-it) f(a+it)}{(b-a-it)^\beta} t^{-\alpha} e^{-\omega t} dt$$

+ $(-i)^{1-\beta} e^{i\omega b} \int_0^\infty \frac{\log (-it) \log (b-a+it) f(b+it)}{(b-a+it)^\alpha} t^{-\beta} e^{-\omega t} dt$
= $I_1 + I_2$ (17)

for $\omega > m + \delta$.

Proof Since $I[f] = I_a[f] + I_b[f]$, the result follows from Theorems 1 and 2.

It can be shown that the integrals given in Theorem 3 are nonoscillatory.

3 Computation of the integrals given in Theorem 3

Since the integrands of I_1 and I_2 given by (17) are nonoscillatory, they can be approximated by the double exponential method [30]. However, we will show in the rest of this paper that for moderate and large values of ω these integrals can be computed more efficiently by appropriate Gaussian quadrature rules.

By a change of variables $t = u/\omega$, the first integral I_1 in (17) reduces to a weighted integral with respect to the generalized Laguerre weight function $u \mapsto w^{gL}(u;s) = u^s e^{-u}$ $(s = -\alpha > -1)$,

$$I_1 = p \int_0^\infty \left[\log u + i\frac{\pi}{2} - \log \omega \right] F(u) u^{-\alpha} e^{-u} du$$
(18)

where

$$p = (i/\omega)^{1-\alpha} e^{i\omega a}, \quad F(u) = \frac{\log(b - a - iu/\omega)f(a + iu/\omega)}{(b - a - iu/\omega)^{\beta}}.$$
 (19)

Because of logarithmic singularity of the integrand in (18) at the point u = 0, the corresponding generalized Gauss-Laguerre quadrature (with the parameter $s = -\alpha$) is not feasible. As in a similar problem in [33], we use now the so-called logarithmic Gauss-Laguerre quadrature with the weight function $u \mapsto w^G(u;s) = u^s(u-1-\log u)e^{-u}$ on $(0,\infty)$ recently developed by Gautschi [12], following a paper by Ball and Beebe [1].

Therefore, we rewrite (18) in the form

$$I_1 = p \int_0^\infty \left[\left(u - 1 + \mathrm{i} \frac{\pi}{2} - \log \omega \right) - \left(u - 1 - \log u \right) \right] F(u) u^{-\alpha} \mathrm{e}^{-u} \, \mathrm{d}u,$$

i.e.,

$$I_1 = p\left(\int_0^\infty F_1(u)w^{gL}(u; -\alpha)\mathrm{d}u - \int_0^\infty F(u)w^G(u; -\alpha)\mathrm{d}u\right),\tag{20}$$

where $F_1(u) = (u - 1 + i\pi/2 - \log \omega)F(u)$.

In a similar way, we obtain the integral I_2 in (17) in the following form

$$I_2 = q\left(\int_0^\infty G_1(u)w^{gL}(u;-\beta)\mathrm{d}u - \int_0^\infty G(u)w^G(u;-\beta)\mathrm{d}u\right),\tag{21}$$

where

$$q = (-i/\omega)^{1-\beta} e^{i\omega b}, \quad G(u) = \frac{\log(b - a + iu/\omega)f(b + iu/\omega)}{(b - a + iu/\omega)^{\alpha}}, \tag{22}$$

and $G_1(u) = (u - 1 + i\pi/2 - \log \omega)G(u)$.

Thus, for calculating the integrals I[f], given by (4), regarding Theorem 3 and the previous transformations, we need two kind of quadrature rules:

- the generalized Gauss-Laguerre quadrature formula

$$\int_{0}^{\infty} \varphi(u) w^{gL}(u;s) \mathrm{d}u = \sum_{k=1}^{n} A_{k}^{(n)}(s) \varphi\left(\tau_{k}^{(n)}(s)\right) + R_{n,s}^{gL}[\varphi],$$
(23)

- the logarithmic Gauss-Gautschi-Laguerre quadrature formula

$$\int_{0}^{\infty} \varphi(u) w^{G}(u;s) \mathrm{d}u = \sum_{k=1}^{n} B_{k}^{(n)}(s) \varphi\left(\xi_{k}^{(n)}(s)\right) + R_{n,s}^{G}[\varphi],$$
(24)

when the parameter $s = -\alpha$ and $s = -\beta$. Here, $\tau_k^{(n)}(s)$ and $A_k^{(n)}(s)$ are nodes and weight coefficients of the first quadrature rule, and $\xi_k^{(n)}(s)$ and $B_k^{(n)}(s)$ are ones of the second rule. The corresponding remainder terms are denoted by $R_{n,s}^{gL}$ and $R_{n,s}^{G}$, respectively.

Taking the *n*-point quadrature sums we get an approximation of I[f] by $I_n(\omega)$, where

$$I_{n}(\boldsymbol{\omega}) = \sum_{k=1}^{n} \left\{ p \left[A_{k}^{(n)}(-\alpha) F_{1}(\boldsymbol{\tau}_{k}^{(n)}(-\alpha)) - B_{k}^{(n)}(-\alpha) F(\boldsymbol{\xi}_{k}^{(n)}(-\alpha)) \right] + q \left[A_{k}^{(n)}(-\beta) G_{1}(\boldsymbol{\tau}_{k}^{(n)}(-\beta)) - B_{k}^{(n)}(-\beta) G(\boldsymbol{\xi}_{k}^{(n)}(-\beta)) \right] \right\}, \quad (25)$$

with p, q, F, G, given in (19) and (22), and F_1 and G_1 are defined before as

$$F_1(u) = \left(u - 1 + i\frac{\pi}{2} - \log\omega\right)F(u) \quad \text{and} \quad G_1(u) = \left(u - 1 + i\frac{\pi}{2} - \log\omega\right)G(u).$$

4 Construction of Gaussian quadrature rules

Let \mathcal{P} be the space of real polynomials and $\mathcal{P}_n \subset \mathcal{P}$ be the space of polynomials of degree at most *n*. In general, for a given nonnegative weight function w(t) on $(a,b) \subset \mathbb{R}$, for which all moments $\mu_k = \int_a^b t^k w(t) dt$, $k \ge 0$, exist and are finite and $\mu_0 = \int_a^b w(t) dt > 0$, the inner product

$$(p,q) = \int_{a}^{b} p(t)q(t)w(t)dt$$
(26)

is well defined for any polynomials $p,q \in \mathcal{P}$ and gives rise to a unique system of (monic) orthogonal polynomials $\pi_k(x), k = 0, 1, 2, \dots$ Because of the property (tp,q) = (p,tq), these orthogonal polynomials satisfy a three-term recurrence relation of the form

$$\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t), \quad k = 0, 1, \dots,$$
(27)

with initial values $\pi_0(t) = 1$ and $\pi_{-1}(t) = 0$. For recurrence coefficients α_k and β_k , which depend on the weight function w(t), the following Darboux's formulae

$$\alpha_k = \frac{(t\pi_k, \pi_k)}{(\pi_k, \pi_k)}, \quad \beta_k = \frac{(\pi_k, \pi_k)}{(\pi_{k-1}, \pi_{k-1})}, \quad k = 0, 1, \dots$$
(28)

The coefficient β_0 may be arbitrary, but usually, it is appropriate to define $\beta_0 = \mu_0$.

The coefficients α_k and β_k in (27) are fundamental quantities in the so-called *construc*tive theory of orthogonal polynomials on \mathbb{R} , which was developed by Walter Gautschi in the eighties on the last century (see [10]). This theory includes effective algorithms for numerically generating recursion coefficients α_k and β_k for arbitrary weight functions, strong stability analysis of such algorithms, etc.

There is a close connection between orthogonal polynomials and quadrature formulas of Gaussian type. For each $n \in \mathbb{N}$, there exists the *n*-point quadrature formula of Gaussian type

$$\int_{a}^{b} \varphi(t) w(t) dt = \sum_{k=1}^{n} A_{k}^{(n)} \varphi\left(\tau_{k}^{(n)}\right) + R_{n}[\varphi],$$
(29)

which is exact for all algebraic polynomials of degree $\leq 2n - 1$, i.e., $R_n[\varphi] = 0$ for each $\varphi \in \mathcal{P}_{2n-1}$. Such a quadrature rule can be characterized as an interpolatory formula for which its node polynomial $\omega(t) = \prod_{k=1}^n (t - \tau_k^{(n)}) = \pi_n(t)$ is orthogonal to \mathcal{P}_{n-1} with respect

to the inner product (26). There are many estimates of the remainder term $R_n[\varphi]$ in different classes of functions (cf. [24, pp. 332–345]). The simplest one is the classical result for functions in the class $C^{2n}[a,b]$: *There exists* $\xi \in (a,b)$ *such that*

$$R_n[\varphi] = \frac{\beta_0 \beta_1 \cdots \beta_n}{(2n)!} \varphi^{(2n)}(\xi).$$
(30)

The quadrature nodes $\tau_1^{(n)}, \ldots, \tau_n^{(n)}$ in (29), i.e., the zeros of $\pi_n(t)$, are eigenvalues of the symmetric tridiagonal Jacobi matrix

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

and the weight coefficients (Christoffel numbers) in (29) are given by $A_k^{(n)} = \beta_0 v_{k,1}^2$, k = 1, ..., n, where $v_{k,1}$ is the first component of the normalized eigenvector $\mathbf{v}_k = [v_{k,1} \dots v_{k,n}]^T$ such that $\mathbf{v}_k^T \mathbf{v}_k = 1$. Thus, in order to construct the *n*-point Gauss quadrature rule relative to w(t) on (a, b), we need the three-term recursion coefficients of the polynomials orthogonal with respect to the inner product (26). The most popular method for solving this eigenvalue problem is the Golub-Welsch procedure, obtained by a simplification of the QR algorithm [15]. For details on orthogonal polynomials and Gaussian quadrature rules see, for example, the books [11] and [24].

Thanks to recent progress in variable-precision arithmetic, as well as in symbolic computation, the recursion coefficients in the three-term recurrence relation (27) can be generated directly by using the original Chebyshev method of moments (or by the method of modified moments). Respective symbolic/variable-precision software for orthogonal polynomials and quadrature formulas is available: packages OPQ and SOPQ in MATLAB by Gautschi (see [13], [14] and [26]) and OrthogonalPolynomials package in MATHEMATICA developed by Cvetković and Milovanović (see [6] and [28]), which is downloadable from the Web site in the Mathematical Institute of the Serbian Academy of Sciences and Arts:

http://www.mi.sanu.ac.rs/~gvm/.

As we have seen in the previous section, in order to compute our highly oscillatory singular integrals (4) by using (25), we need two types of quadrature formulas: the generalized Gauss-Laguerre formulas (23) and the corresponding Gaussian formulas with respect to Gautschi's weight function w^G (with the same parameters), given by (24).

4.1 Construction of the generalized Gauss-Laguerre rules relative to the weight $w^{gL}(t;s)$

The monic generalized Laguerre polynomials $\hat{L}_k^s(t)$, orthogonal with respect to the weight $w^{gL}(t;s) = t^s e^{-t}$, satisfy the recurrence relation (cf. [24, p. 141])

$$\hat{L}_{k+1}^{s}(t) = \begin{bmatrix} t - (2k+s+1) \end{bmatrix} \hat{L}_{k}^{s}(t) - k(k+s) \hat{L}_{k-1}^{s}(t), \quad k = 0, 1, \dots,$$
(31)

with $\hat{L}_0^s(t) = 1$ and $\hat{L}_{-1}^s(t) = 0$. Thus, $\alpha_k^{gL}(s) = 2k + s + 1$ $(k \ge 0)$ and $\beta_k^{gL}(s) = k(k+s)$ $(k \ge 1)$. Also, we put $\beta_0^{gL} = \mu_0^{gL} = \int_0^\infty t^{s+1} e^{-t} dt = \Gamma(s+1)$.

The parameters of the generalized Gauss-Laguerre quadrature formula (23) for given s and n can be obtained, with arbitrary precision, very easy by using MATHEMATICA package OrthogonalPolynomials (see [6] and [28]). For example, for s = -1/2, n = 10, and Precision -> 30 (WorkingPrecision must be greater than Precision!), we use the following commands:

It enables us to calculate the parameters $\tau_k^{(n)}(s)$ and $A_k^{(n)}(s)$ (resp. the lists tauk and Ak) for each $n \leq 20$, because the lists of the recurrence coefficients α_k^{gL} and β_k^{gL} (resp. akgL[s] and bkgL[s]) are done for $k \leq 2n_{\max} - 1 = 2 \cdot 20 - 1 = 39$.

Alternatively, it can be realized simpler by only one command:

```
<< orthogonalPolynomials'
{tauk,Ak}=aGaussianNodesWeights[10,{aLaguerreG,-1/2},
WorkingPrecision -> 40, Precision -> 30];
```

4.2 Construction of Gauss rules relative to Gautschi's weight $w^G(t;s)$

For constructing the logarithmic Gauss-Gautschi-Laguerre quadrature formula (24) we need first to obtain the coefficients in the three-term recurrence relation for (monic) polynomials orthogonal with respect to Gautschi's weight function $w^G(t;s)$,

$$G_{k+1}^{s}(t) = \left(t - \alpha_{k}^{G}(s)\right)G_{k}^{s}(t) - \beta_{k}^{G}(s)G_{k-1}^{s}(t), \quad k = 0, 1, \dots,$$
(32)

with $G_0^s(t) = 1$ and $G_{-1}^s(t) = 0$.

For these recurrence coefficients in (32), α_k^G and β_k^G , we use the method of modified moments developed by Gautschi [10] (see also [24, pp. 160–162]). In order to have the first *n* coefficients $\alpha_k^G(s)$ and $\beta_k^G(s)$, k = 0, 1, ..., n-1, the method needs the first 2*n* modified moments of the weight function $w^G(t;s)$ on $(0,\infty)$ with respect to a system of monic polynomials $\{\phi_k\}$ (deg $\phi_k = k$) chosen to be close in some sense to the desired orthogonal polynomials $G_k^s(t)$. In our case an appropriate system is if we take $\phi_k(t) = \hat{L}_k^s(t)$, for which the recurrence relation (31) holds.

The modified moments relative to the system of monic generalized Laguerre polynomials $\hat{L}_k^s(t)$ are

$$m_k(s) = \int_0^\infty w^G(s;t) \hat{L}_k^s(t) \, \mathrm{d}t = \Gamma(1+s) \begin{cases} s - \psi(1+s), & k = 0, \\ s, & k = 1, \\ (-1)^k (k-1)!, & k \ge 2, \end{cases}$$
(33)

where ψ is the logarithmic derivative of the gamma function, given by $\psi(s) = \Gamma'(s)/\Gamma(s)$. These functions, $\Gamma(s)$ and $\psi(s)$, are implemented in MATHEMATICA as Gamma[s] and PolyGamma[s], respectively, and suitable for both symbolic and numerical manipulation, and can be evaluated to arbitrary numerical precision.

The coefficients $\alpha_k^G(s)$ and $\beta_k^G(s)$, as well as the corresponding Gaussian formula (24), with arbitrary precision, can be realized by the following commands:

The first 20 recurrence coefficients $\alpha_k^G(s)$ and $\beta_k^G(s)$ (the lists {akG,bkG}), for s = -1/2, rounded to 30 decimal digits, are given bellow.

```
\{\{0.158355603234739446677507982216, 4.34208148088076361658754048152, \}
 6.06346660759813453494680491424, 7.51167341692391892284992518685, 9.20107973580966183533334809313, 11.3709082541083318493081241813,
  13.6820827866566755962831868955, 15.8839347481331513367512405890,
  17.9491712137437041197883429109, 19.9075910730444038742249438809,
 \texttt{21.7878189386096150572815400925}, \texttt{ 23.6239533583804308694332164149},
  25.4657347372808240823374008720\mbox{, } 27.3673454687383573087148272386\mbox{, }
  29.3585602690189308521620602779, 31.4281808207585759263982394324,
 33.5379679651329537814715470627, 35.6490497427103589022880357502,
 37.7367368279606119430619381467, 39.7906599603540964839744810075},
 {2.59400398146050401328951145647, 0.383279106158901224369399128268,
  4.00964558018994939209970216037, 10.8612004247526083850982352867,
  \verb+20.3913654921158296648188081202, \verb+30.1705825730405458620833524789, \verb+
 39.9949308142528973726121371078, 51.7249071021896738265478244429,
  66.2700141732975527115406636042, 83.7410022304368175123096687708,
  104.091934235457131880664679009, 127.202934031282256772947719544,
  152.716650402246155124335431844,\ 179.967946756007675424386031420,
  208.247436736091109280838174003, 237.254229290351505073049439263,
  267.262355256421742566283181124, 298.855336808019796788880140207
 332.573304622716467186007229523, 368.756359478039270546883164708}}
```

As before, these coefficients enable us to get the quadrature parameters $\xi_k^{(n)}(s)$ and $B_{\scriptscriptstyle L}^{(n)}(s)$ (resp. the lists xik and Bk) for each $n \leq 20$.

The package OrthogonalPolynomials also provides the ability to determine coefficients in symbolic form, using the option Algorithm -> Symbolic in the command aChebyshevAlgorithmModified. Due to complicated expressions, we list here only a few first recurrence coefficients:

$$\begin{aligned} \alpha_0^G &= \frac{s(s+2)-(s+1)\xi}{s-\xi}, \\ \alpha_1^G &= \frac{s^2(s^3+6s^2+9s+3)-s(3s^3+17s^2+24s+8)\xi+A\xi^2-(s+1)(s+3)\xi^3}{(s-\xi)\left[s(1+s)^2-(2s^2+4s+1)\xi+(1+s)\xi^2\right]}, \end{aligned}$$



Fig. 2 Recurrence coefficients $\alpha_k^G(s)$ (top) and $\beta_k^G(s)$ (bottom), for $k \le 6$, as function on *s*

and

$$\begin{split} \beta_0^G &= (s-\xi)\Gamma(s+1), \\ \beta_1^G &= \frac{s(s+1)^2 - (2s^2 + 4s + 1)\xi + (s+1)\xi^2}{(s-\xi)^2}, \\ \beta_2^G &= \frac{(s-\xi)\left[B + C\xi + D\xi^2 - 2(s+1)^2(s+2)\xi^3\right]}{\left[s(s+1)^2 - (2s^2 + 4s + 1)\xi + (s+1)\xi^2\right]^2}, \\ &\vdots \end{split}$$

where $\xi = \psi(s+1)$ and

$$A = 3s^{3} + 15s^{2} + 19s + 5,$$

$$B = 2s^{6} + 14s^{5} + 38s^{4} + 52s^{3} + 35s^{2} + 7s - 1,$$

$$C = -(6s^{5} + 42s^{4} + 108s^{3} + 120s^{2} + 51s + 5),$$

$$D = 2(3s^{4} + 18s^{3} + 36s^{2} + 28s + 7).$$

In Figure 2 we present the recurrence coefficients $\alpha_k^G(s)$ and $\beta_k^G(s)$ for $k \le 6$, when $s \in (-1,5)$. Note that the recurrence coefficients $\alpha_k^{gL}(s)$ and $\beta_k^{gL}(s)$ for the generalized monic Laguerre polynomials are linear functions in *s*.

5 Numerical Examples and Results

In this section, some numerical examples are presented to test the performance of the proposed method (25), which gives a quadrature approximation $I_n(\omega)$ of the the highly oscillatory singular integral $I(\omega) (= I[f])$, with the relative error

$$\operatorname{err}_{n}(\boldsymbol{\omega}) = \left| \frac{I_{n}(\boldsymbol{\omega}) - I(\boldsymbol{\omega})}{I(\boldsymbol{\omega})} \right|.$$
(34)

Integrals of the form (4) are calculated for various values of ω , α , β and *n* nodes.

Example 1 Let $f(x) = (2x^6 - 5x^3 + 7x + 3)/(x - 100)^2$, a = -1, b = 1/2, i.e., $I(\omega) = \int_{-1}^{1/2} \frac{\log(x+1)\log(\frac{1}{2}-x)f(x)e^{i\omega x}}{(x+1)^{\alpha}(\frac{1}{2}-x)^{\beta}} dx, \quad \alpha, \beta < 1, \ \omega \gg 1.$

Exact values of the integral $I(\omega)$, rounded to 30 decimal digits, are shown in Table 1 for different values of of α , β and ω .

ω	$\{\alpha, \beta\} = \{1/100, 1/300\}$
10^{3}	$3.01134865574957282241979012467 \times 10^{-8} - i 1.79871927840133855809100118541 \times 10^{-8}$
10^{4}	$2.95252144690242617839569827179 \times 10^{-7} + i 1.92915243847152481922059057191 \times 10^{-7}$
10^{5}	$3.21714532823195758804684419317 \times 10^{-8} \ + \ i 1.98665646307200830224278882327 \times 10^{-8}$
10^{6}	$2.23449908235971149231081725170 \times 10^{-10} - \ i \ 5.59251660888956391435954761090 \times 10^{-9}$
	$\{\alpha, \beta\} = \{1/2, 1/4\}$
10^{3}	$4.10358237622214636852662703582 \times 10^{-5} + i1.42204094064731296764984070055 \times 10^{-5}$
10^{4}	$2.22813904098044943114581257244 \times 10^{-5} \ + \ i 8.70396944941118137943442145903 \times 10^{-6}$
10^{5}	$6.71993058366476730030106708878 \times 10^{-6} + i 5.57186683782947190248781857547 \times 10^{-6}$
10^{6}	$-1.48728318176985557957728903939 \times 10^{-6} - i 2.72626279562357616684089767707 \times 10^{-6}$
	$\{\alpha, \beta\} = \{99/100, 99/100\}$
10^{3}	$9.79736097316431469797626227503 \times 10^{-1} + \text{i} 1.41162325303922419159778188717$
10^{4}	$5.09858444495283779206531476712 \times 10^{-1} + i1.35110478417875752971413921607$
10^{5}	$8.23743182254793379431170581307 \times 10^{-1} \ + \ i1.63766580155235539029294914330$
10^{6}	$8.37697937352336393554945738394 \times 10^{-1} - i 5.66552013941884740340478259594 \times 10^{-1}$

Using MATHEMATICA package OrthogonalPolynomials (see [6] and [28]) we construct quadrature formulas (23) and (24) for a given *n* and two values of the parameter *s* ($s = -\alpha$ and $s = -\beta$), in order to get the quadrature sum $I_n(\omega)$, given by (25). Such a constructive procedure, including (numerical or symbolic) construction of the recurrence coefficients $\alpha_k^G(s)$ and $\beta_k^G(s)$ in (32) from the modified moments $m_k(s)$, given by (33), has been explained in Section 4.

After this construction, we approximate the integral $I(\omega)$ by (25). The obtained relative errors (34) for n = 2, 4, 6, and 8 nodes are presented in Table 2. All computations were performed in MATHEMATICA, Ver. 12, on MacBook Pro (15-inch, 2017), OS X 10.14.6, and they are very fast. For example, for computing $I_n(\omega)$, for $\omega = 10^3$, $\alpha = 1/100$, $\beta = 1/300$

and n = 8, we need about 20 ms when WP=WorkingPrecision->35, and 22 ms for WP->60. Very similar times are for other values of α , β , and ω . The running time is evaluated by the function Timing in MATHEMATICA and it includes only CPU time spent in the MATHEMATICA kernel. Such a way may give different results on different occasions within a session, because of the use of internal system caches. In order to generate worst-case timing results independent of previous computations we used the command ClearSystemCache[].

ω	α	β	$err_2(\omega)$	$err_4(\omega)$	$err_6(\omega)$	$err_8(\omega)$
	1/100	1/300	1.00×10^{-8}	2.15×10^{-20}	3.57×10^{-31}	1.15×10^{-40}
10^{3}	1/2	1/4	6.61×10^{-9}	2.56×10^{-21}	3.66×10^{-31}	1.66×10^{-40}
	99/100	99/100	1.94×10^{-12}	$3.39 imes 10^{-24}$	$5.92 imes 10^{-34}$	$3.30 imes 10^{-43}$
	1/100	1/300	5.47×10^{-12}	9.70×10^{-28}	1.54×10^{-42}	5.15×10^{-56}
10^{4}	1/2	1/4	3.88×10^{-12}	1.02×10^{-28}	1.26×10^{-42}	5.38×10^{-56}
	99/100	99/100	$2.22 imes 10^{-15}$	$3.60 imes 10^{-31}$	7.15×10^{-45}	3.95×10^{-58}
	1/100	1/300	5.01×10^{-15}	1.10×10^{-34}	1.95×10^{-53}	6.71×10^{-71}
10^{5}	1/2	1/4	3.34×10^{-15}	9.60×10^{-36}	1.24×10^{-53}	$5.38 imes 10^{-71}$
	99/100	99/100	$1.76 imes 10^{-18}$	$3.27 imes 10^{-38}$	4.94×10^{-56}	2.64×10^{-73}
	1/100	1/300	3.72×10^{-18}	4.85×10^{-42}	5.65×10^{-65}	1.63×10^{-86}
10^{6}	1/2	1/4	$2.97 imes 10^{-18}$	$8.88 imes 10^{-43}$	$1.16 imes 10^{-64}$	$5.10 imes10^{-86}$
	99/100	99/100	2.94×10^{-21}	4.01×10^{-45}	1.05×10^{-66}	5.95×10^{-88}

Table 2 Relative errors for various values of α , β , ω and n



Fig. 3 Relative errors $\operatorname{err}_n(\omega)$ in the quadrature sums $I_n(\omega)$ for n = 5, 10, 15, 20 nodes and several values of ω ($\alpha = 1/2, \beta = 1/4$)

As we can see the convergence of these approximations is very fast, especially for larger ω . For example, for $\omega = 10^3$, with only two nodes (n = 2) we obtain results with about

8, 9, and 12 exact decimal digits, when (α, β) is equal to (1/100, 1/300), (1/2, 1/4), and (99/100, 99/100), respectively. But, for $\omega = 10^6$ this number of exact digits in results is 18, 18, and 21 respectively. In Figure 3 we present the corresponding relative errors for n = 5, 10, 15, 20, when $\omega = 10^k$, $k = 0, 1, \dots, 6$ in the case $(\alpha, \beta) = (1/2, 1/4)$. Note that for $\omega = 10^6$ and n = 20 nodes we obtain the result with more than 200 exact digits (of course, WP must be of this order). In Table 3 we give the corresponding relative errors for n = 5, 10, 15, 20 nodes for all cases of parameters considered earlier.

ω	α	β	$\operatorname{err}_5(\boldsymbol{\omega})$	$\operatorname{err}_{10}(\boldsymbol{\omega})$	$\operatorname{err}_{15}(\boldsymbol{\omega})$	$err_{20}(\boldsymbol{\omega})$
	1/100	1/300	4.23×10^{-26}	1.23×10^{-49}	1.29×10^{-70}	3.56×10^{-90}
10^{3}	1/2	1/4	$2.84 imes10^{-26}$	2.09×10^{-49}	$2.91 imes10^{-70}$	1.11×10^{-89}
	99/100	99/100	$3.84 imes10^{-29}$	4.79×10^{-52}	9.00×10^{-73}	4.71×10^{-92}
	1/100	1/300	1.84×10^{-35}	$5.95 imes 10^{-69}$	3.85×10^{-100}	3.75×10^{-129}
10^{4}	1/2	1/4	$1.05 imes 10^{-35}$	$6.46 imes 10^{-69}$	$8.51 imes 10^{-100}$	3.44×10^{-129}
	99/100	99/100	4.57×10^{-38}	5.60×10^{-71}	9.71×10^{-102}	$4.72 imes 10^{-131}$
	1/100	1/300	2.25×10^{-44}	$7.67 imes 10^{-88}$	1.03×10^{-128}	4.46×10^{-168}
10^{5}	1/2	1/4	$1.00 imes 10^{-44}$	$6.59 imes 10^{-88}$	9.09×10^{-129}	$3.83 imes 10^{-168}$
	99/100	99/100	3.33×10^{-47}	3.70×10^{-90}	$6.40 imes 10^{-131}$	3.14×10^{-170}
	1/100	1/300	$7.83 imes 10^{-54}$	1.96×10^{-107}	3.06×10^{-158}	1.42×10^{-207}
10^{6}	1/2	1/4	$9.37 imes10^{-54}$	$6.29 imes 10^{-107}$	$8.82 imes 10^{-158}$	3.77×10^{-207}
	99/100	99/100	6.50×10^{-56}	8.51×10^{-109}	$1.50 imes 10^{-159}$	7.39×10^{-209}

Table 3 Relative errors for various values of α , β , ω and n

Finally, note that the command NIntegrate in MATHEMATICA can be applied directly to the integral (4), only for smaller values of ω , but the corresponding running time is several dozen times greater than with our method. However, for the larger ω (e.g. > 10⁴) it fails to solve the problem.

Example 2 Here we consider integral (4) for several different functions, intervals and $\omega = 10^4$. Relative errors for n = 3, n = 4 and n = 5 nodes are presented in Table 4.

f(x)	[a,b]	α	β	$err_3(10^4)$	$err_4(10^4)$	$err_5(10^4)$
$r \perp 1$		1/100	1/300	3.45×10^{-21}	6.42×10^{-29}	2.20×10^{-35}
$\frac{x+1}{5+00}\log(x+6)$	[-1, 1/2]	1/2	1/4	$1.30 imes 10^{-20}$	$6.37 imes 10^{-28}$	2.32×10^{-35}
$x^{3} + 90$		99/100	99/100	5.29×10^{-24}	3.69×10^{-31}	3.70×10^{-38}
r (1)	[1/3,2]	1/100	1/300	3.82×10^{-7}	1.27×10^{-9}	3.85×10^{-12}
$\frac{x}{5+75}\sin\left(\frac{1}{4}\right)$		1/2	1/4	$8.07 imes10^{-8}$	$2.29 imes10^{-10}$	$6.02 imes 10^{-13}$
$x^{3} + 75$ (x^{4})		99/100	99/100	$6.52 imes 10^{-11}$	1.56×10^{-13}	3.52×10^{-16}
aroton (15)		1/100	1/300	$1.75 imes 10^{-19}$	$1.78 imes 10^{-25}$	2.98×10^{-32}
$\frac{\operatorname{alctall}(x^*)}{(10)^2 + 1}$	[-1/2, 3/2]	1/2	1/4	$9.20 imes 10^{-20}$	$5.25 imes10^{-26}$	2.71×10^{-33}
$(10x)^3 + 1$		99/100	99/100	6.93×10^{-23}	1.97×10^{-29}	$1.74 imes10^{-36}$

Table 4 Relative errors for various values of α , β , f(x) and intervals

As we can see the convergence of the quadrature process is fast, except the case for the function $f(x) = x \sin(1/x^4)/(x^5 + 75)$. Then, for example, for $\alpha = 1/100$ and $\beta = 1/300$, we get about 7, 9, and 12 exact decimal digis in quadrature approximation $I_n(10^4)$ with

n = 3,4, and 5 nodes, respectively. However, if we take n = 6,7, and 8 nodes, this number of exact digits is about 14, 17, and 19, respectively (see Table 5).

Table 5 Relative errors for various values of α , β , and n = 6,7 and 8 nodes

f(x)	[a,b]	α	β	$err_6(10^4)$	$err_7(10^4)$	$err_8(10^4)$
$\frac{x}{x^5 + 75} \sin\left(\frac{1}{x^4}\right)$	[1/3,2]	1/100 1/2 99/100	1/300 1/4 99/100	$\begin{array}{c} 1.26\times10^{-14}\\ 1.77\times10^{-15}\\ 9.13\times10^{-19} \end{array}$	$\begin{array}{c} 5.06 \times 10^{-17} \\ 6.78 \times 10^{-18} \\ 3.31 \times 10^{-21} \end{array}$	$\begin{array}{c} 2.15\times10^{-19}\\ 2.78\times10^{-20}\\ 1.30\times10^{-23} \end{array}$

6 Conclusion

In this paper, we have presented a numerical integration method to efficiently compute highly oscillatory singular integrals of the form (4). Results of this method have been obtained with MATHEMATICA 12.0. The proposed method has been verified using various numerical examples by changing parameters of integrals. Numerical examples show that when proposed method is used for given integrals, desired precision is obtained and computation is very fast. It can be concluded from all results that presented method is very efficient, stable and economical for highly oscillatory integrals with logarithmic and algebraic integrand.

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