Explicit error bound for the tanh rule and the DE formula for integrals with logarithmic singularity

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Abstract

The tanh rule and the double-exponential (DE) formula are known empirically and theoretically as quite efficient quadrature formulas, especially for integrals with endpoint singularity, including algebraic singularity and logarithmic singularity. Furthermore, in the case of integrals with algebraic singularity, explicit error bounds have been given for those formulas, which enables us to guarantee their approximation accuracy. In the case of integrals with logarithmic singularity, however, such explicit error bounds have not ever given thus far, although those formulas should work accurately in this case as well. This paper presents the desired theoretical explicit error bounds, with numerical experiments.

Keywords  Sinc quadrature, trapezoidal rule, numerical integration, weakly singular kernel

Research Activity Group  Quality of Computations

1. Introduction

This paper is concerned with efficient approximation of the integral with logarithmic singularity of the form

\[ I = \int_0^T \log(t) f(t) \, dt, \]

with its explicit error bound. The function \( f \) may have endpoint singularity. Due to those singularities, we cannot assume that the integrand is continuously differentiable over the given interval \([0, T]\), or is analytic on the complex domain that includes \([0, T]\). This causes a problem to construct an efficient numerical integration library with guaranteed accuracy.

One idea to avoid the difficulty was shown by Yamana et al. [1], where \( f \) is approximated by a power series as

\[ f(t) \approx a_0 + a_1 t + a_2 t^2 + \cdots + a_n t^n, \]

with guaranteed accuracy. Then, the integration of each term of the approximated integrand \((\log(t) a_k t^k)\) is analytically obtained. This approach should work fine when \( T \) is sufficiently small, but not so fine otherwise, since (2) is the Taylor expansion. In addition, such an approximation performs badly in the case where \( f \) also has singularity at the endpoint, e.g., \( f(t) = \cos(t^{1/\pi}) \).

In order to treat those endpoint singularities, this paper considers the tanh rule [2] and the double-exponential (DE) formula [3], which are well known as efficient quadrature rules for integrals with such singularities. The idea of those rules is the combination of the following two techniques: (i) apply a variable transformation using a map \( \psi : \mathbb{R} \to [0, T] \) as

\[ \int_0^T F(t) \, dt = \int_{-\infty}^{\infty} F(\psi(\tau)) \psi'(\tau) \, d\tau, \]

where \( |\psi'(\tau)| \) decays quickly enough as \( \tau \to \pm \infty \) to suppress the divergence of \([F(\psi(\tau))]\), and (ii) apply the (truncated) trapezoidal rule as

\[ \int_{-\infty}^{\infty} F(\psi(\tau)) \psi'(\tau) \, d\tau \approx h \sum_{k=-N}^{M} F(\psi(kh)) \psi'(kh). \]

As the map \( \psi \), the tanh transformation

\[ t = \psi_{\text{SE}}(\tau) = \frac{T}{2} \tanh \left( \frac{\tau}{2} \right) + \frac{T}{2} \]

is used in the tanh rule, and the DE transformation

\[ t = \psi_{\text{DE}}(\tau) = \frac{T}{2} \tanh \left( \frac{\pi}{2} \frac{\tau}{\sinh \tau} \right) + \frac{T}{2} \]

is used in the DE formula. Both quadrature rules work accurately (more precisely, can converge exponentially) even though \( T \) is large, and even in any of the following cases: the integrand has logarithmic singularity as in (1), and the integrand has algebraic singularity of the form

\[ \int_0^T t^{\alpha-1} (T-t)^{\beta-1} f(t) \, dt, \]

where \( \alpha \) and \( \beta \) are positive constants. Actually, those are theoretically supported in the literature [4, 5]. Furthermore, in the case of algebraic singularity (3), explicit (computable) error bounds of those rules have been recently given [6], and the results were utilized to construct a verified numerical integration library [7] in that case.

The objective of this paper is to give such explicit error bounds for the two rules in the case of logarithmic singularity (1). Although it is known empirically and theoretically that those rules can converge exponentially in that case, still any explicit error bound has not been given thus far. In order to construct a verified numerical integration library, computable, mathematically rigorous
error bounds are desired, which are given by this paper. This paper is organized as follows. Main results are stated in Section 2, and those proofs are given in Section 4. Numerical results are shown in Section 3.

2. Main results: explicit error bounds

The following function space should be introduced to state the main results. In this paper, $\mathcal{D}$ is supposed to be either $\psiSE(\mathcal{D})$ or $\psiDE(\mathcal{D})$, which is a translated domain from the strip domain $\mathcal{D}_d = \{ \zeta \in \mathbb{C} : |\Im \zeta| < d \}$.

**Definition 1** Let $\mathcal{D}$ be a bounded and simply connected domain (or Riemann surface), and let $K$ be a positive constant. Then $H_{\mathcal{D}}^\infty(\mathcal{D})$ denotes the family of all functions $f$ that are analytic on $\mathcal{D}$, and satisfy $|f(z)| \leq K$ for all $z \in \mathcal{D}$.

The main results of this paper are stated as follows.

**Theorem 2** Let $f \in H_{\mathcal{D}}^\infty(\psiSE(\mathcal{D})_d)$ with $0 < d < \pi$. Let $\alpha = (2\pi - 1)/(2\pi)$, let $N$ be a positive integer, and let $h$ and $M$ be selected by

$$h = \frac{2\pi d}{\alpha N}, \quad M = \lfloor \alpha N \rfloor. \quad (4)$$

Then it holds that

$$\left| I - h \sum_{k=-N}^{M} \log(\psiSE(kh)) f(\psiSE(kh)) \psi'_SE(kh) \right| \leq C_0 C_1 \left( \frac{T}{\cos \left( \frac{d}{2} \right)} \right)^{\frac{1}{2}} \left( \pi^2 + \log^2 \left( \frac{T}{\cos \left( \frac{d}{2} \right)} \right) \right)^{\frac{1}{2}}, \quad (5)$$

where $C_0 = 2KT^\alpha/\alpha$ and

$$C_1 = \left( \frac{T}{\cos \left( \frac{d}{2} \right)} \right)^{\frac{1}{2}} \left( \pi^2 + \log^2 \left( \frac{T}{\cos \left( \frac{d}{2} \right)} \right) \right)^{\frac{1}{2}}.$$

**Theorem 3** Let $f \in H_{\mathcal{D}}^\infty(\psiDE(\mathcal{D})_d)$ with $0 < d < \pi/2$. Let $\alpha = (2\pi - 1)/(2\pi)$, let $N$ be a positive integer, and let $h$ and $M$ be selected by

$$h = \frac{\log(4d)}{\alpha}, \quad M = -\left\lfloor \frac{\log(\frac{1}{2})}{h} \right\rfloor. \quad (6)$$

Then it holds that

$$\left| I - h \sum_{k=-N}^{M} \log(\psiDE(kh)) f(\psiDE(kh)) \psi'_DE(kh) \right| \leq C_0 C_1 \left[ \frac{C_2}{1 - e^{-\pi \alpha c/2}} + e^{\pi/2} \right] e^{-2\pi dN/\log(4dN/\alpha)}, \quad (7)$$

where $C_0 = 2KT^\alpha/\alpha$ and

$$C_1 = \left( \frac{T}{\cos \left( \frac{d}{2} \sin d \right)} \right)^{\frac{1}{2}} \left( \pi^2 + \log^2 \left( \frac{T}{\cos \left( \frac{d}{2} \sin d \right)} \right) \right)^{\frac{1}{2}}, \quad (8)$$

$$C_2 = \frac{2}{\cos^{1+\alpha}(\frac{d}{2} \sin d \cos d)}.$$

3. Numerical results

As an example that $T$ is not sufficiently small and $f(t)$ has derivative singularity at the origin, consider $f(t) = \cos(t^{1/3})\sqrt{t^2 - 2t + 2}$ and the following integral

$$\int_0^T \log(t)f(t) \, dt = -0.870621268307117216836724471909871167 \cdots, \quad (9)$$

where the value on the right hand side was calculated by Mathematica with WorkingPrecision→50. The function $f$ satisfies the assumptions in Theorem 2 with $d = \pi/2$ and $K = 2$, and also satisfies the assumptions in Theorem 3 with $d = \pi/6$ and $K = 2\pi/3$ (in both cases, $d$ is determined by the branch points of $\sqrt{t^2 - 2t + 2}$, and $K$ can be found by using the maximum-modulus principle). Therefore, we can compute those error bounds according to the theorems, which can be confirmed in Fig. 1. All computation programs were written in C with quadruple-precision floating-point arithmetic by using "long double" type on a PowerPC CPU.

4. Proofs

The important function space for the error analysis is defined as follows.

**Definition 4** Let $\mathcal{D}$ be a bounded and simply connected domain (or Riemann surface), and let $K$, $\alpha$, $\beta$ be positive constants. Then $L_{\mathcal{D},\alpha,\beta}(\mathcal{D})$ denotes the family of all functions $f$ that are analytic on $\mathcal{D}$, and satisfy $|f(z)| \leq L_{\mathcal{D},\alpha,\beta}(z)$ for all $z \in \mathcal{D}$, where $Q_{\alpha,\beta}(z) = z^\alpha(T - z)^\beta$.

For functions that belong to this function space, the following error estimates are known.

**Theorem 5** (Okayama et al. [6, Theorem 2.6]) Let $F,Q_1,1 \in L_{\mathcal{D},\alpha,\beta}(\psiSE(\mathcal{D})_d)$ for $d$ with $0 < d < \pi$ and $\alpha \leq 1$. Let $N$ be a positive integer, and let $h$ and $M$ be selected by (4). Then it holds that

$$\left| \int_0^T F(t) \, dt - h \sum_{k=-N}^{M} F(\psiSE(kh)) \psi'(SE(kh)) \right| \leq C_0 \left[ \frac{2}{1 - e^{-2\pi d/\alpha}} \cos^{1+\alpha}(\frac{d}{2}) + 1 \right] e^{-\sqrt{2\pi dN}}, \quad (10)$$

where $C_0 = 2LT^\alpha/\alpha$. 

![Fig. 1. Errors of the tanh rule and the DE formula for the integral (9) and their error bounds.](image-url)
Theorem 6 (Okayama et al. [6, Theorem 2.14])
Let $FQ_{1,1} \in L_{L,0,1}(\psi_{SE}(\mathcal{D}))$ for $d \in (0, \pi/2)$ and $1/(2\pi) \leq \alpha \leq 1$. Let $N$ be a positive integer, and let $h$ and $M$ be selected by (6). Then it holds that
\[
\left| \int_0^T F(t) \, dt - h \sum_{k=-N}^M F(\psi_{DE}(kh))\psi_{DE}(kh) \right| 
\leq C_0 \left( \frac{C_2}{1 - e^{-\pi e/2}} + e^{\pi/2} \right) e^{-2\pi dN/\log(4dN/\alpha)},
\]
where $C_0 = 2LT^\alpha/\alpha$ and $C_2$ is a constant defined in (8).

In view of these theorems, we find that the main task here is to show $F \in L_{L,0,1}(\mathcal{D})$ with $F(t) = \log(t)f(t)$ under the assumptions in Theorems 2 and 3. The following lemmas state the desired results.

Lemma 7 Let the assumptions in Theorem 2 be fulfilled, and let $F(t) = \log(t)f(t)$. Then $F \in L_{L,0,1}(\psi_{SE}(\mathcal{D}))$ with $L = KC_1$, where $C_1$ is a constant defined in (5).

Lemma 8 Let the assumptions in Theorem 3 be fulfilled, and let $F(t) = \log(t)f(t)$. Then $F \in L_{L,0,1}(\psi_{DE}(\mathcal{D}))$ with $L = KC_1$, where $C_1$ is a constant defined in (7).

In order to prove these lemmas above, what we need to show is the following inequalities.

Lemma 9 Let $0 < d < \pi$. Then for all $z \in \psi_{SE}(\mathcal{D})$
\[
|\log z| \leq C_1 \frac{1}{|z|^{\pi}},
\]
holds, where $C_1$ is a constant defined in (5).

Lemma 10 Let $0 < d < \pi/2$. Then for all $z \in \psi_{DE}(\mathcal{D})$
\[
|\log z| \leq C_1 \frac{1}{|z|^{\pi}},
\]
holds, where $C_1$ is a constant defined in (7).

The next lemma essentially shows those inequalities.

Lemma 11 Let $R$ be a positive constant, and $z \in \mathbb{C}$ be bounded as $|z| \leq R$. Then it holds that
\[
|z|^{1/(2\pi)} \log |z| \leq R^{\frac{1}{2\pi}} \sqrt{\log^2 R + \pi^2}.
\]

Proof Let $z = re^{i\theta}$, where $r$ and $\theta$ be real numbers with $0 \leq r \leq R$ and $-\pi \leq \theta < \pi$. Then we have
\[
|z|^{1/(2\pi)} \log |z|^2 = r^{\frac{1}{\pi}} (\log^2 r + \theta^2)
\leq r^{\frac{1}{\pi}} (\log^2 r + \pi^2)
\leq R^{\frac{1}{\pi}} (\log^2 R + \pi^2),
\]
which shows the desired result. (QED)

What is left here is to reveal the explicit bound $R$ of Lemma 11, which are done by the following lemmas.

Lemma 12 Let $0 < d < \pi$. Then it holds for all $z \in \psi_{SE}(\mathcal{D})$ that
\[
|z| \leq \frac{T}{\cos(\frac{\pi}{2})}.
\]

Proof From $z \in \psi_{SE}(\mathcal{D})$, we can put $z = \psi_{SE}(x + iy)$ with $x \in \mathbb{R}$ and $y \in [-d, d]$. Then we have
\[
|z| = |\psi_{SE}(x + iy)| = \frac{T}{1 + e^{-x - iy}} 
\leq \frac{T}{1 + e^{-x}} \cos(\frac{\pi}{2}) \leq \frac{T}{\cos(\frac{\pi}{2})}.
\]
The non-trivial inequality here is the first one, which is shown in Okayama et al. [6, Lemma 4.21]. (QED)

Lemma 13 Let $0 < d < \pi/2$. Then it holds for all $z \in \psi_{DE}(\mathcal{D})$ that
\[
|z| \leq \frac{T}{\cos(\frac{\pi}{2} \sin d)}.
\]

Proof From $z \in \psi_{DE}(\mathcal{D})$, we can put $z = \psi_{DE}(x + iy)$ with $x \in \mathbb{R}$ and $y \in [-d, d]$. Then we have
\[
|z| = |\psi_{DE}(x + iy)| = \frac{T}{1 + e^{-\pi \sinh(x + iy)}} 
\leq \frac{T}{1 + e^{-\pi \sinh(x)}} \cos(\frac{\pi}{2} \sin y) \leq \frac{T}{\cos(\frac{\pi}{2} \sin d)}.
\]
The non-trivial inequality here is the first one, which is shown in Okayama et al. [6, Lemma 4.22]. (QED)

These lemmas give the desired $R$, which completes the proofs.

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