APPROXIMATING AND BOUNDING FRACTIONAL STIELTJES CONSTANTS

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Abstract. We discuss evaluating fractional Stieltjes constants $\gamma_\alpha(a)$, arising naturally from the Laurent series expansions of the fractional derivatives of the Hurwitz zeta functions $\zeta^{(\alpha)}(s,a)$. We give an upper bound for the absolute value of $C_\alpha(a) = \gamma_\alpha(a) - \log^\alpha(a)/a$ and an asymptotic formula $\widetilde{C}_\alpha(a)$ for $C_\alpha(a)$ that yields a good approximation even for most small values of α. We bound $|\widetilde{C}_\alpha(a)|$ and based on this conjecture a tighter bound for $|C_\alpha(a)|$

1. Introduction

The Hurwitz zeta function is defined, for $\Re(s) > 1$ and $0 < a \leq 1$, as

$$\zeta(s,a) = \sum_{n=0}^{\infty} \frac{1}{(n+a)^s}.$$

For fixed a, it can be extended to a meromorphic function with a simple pole at $s = 1$ with residue 1 (see [4], [10]). Moreover, the function has a Laurent series expansion

$$\zeta(s,a) = \frac{1}{s-1} + \sum_{n=0}^{\infty} \frac{(-1)^n \gamma_n(a)(s-1)^n}{n!}, \tag{1}$$

about $s = 1$ where $\gamma_n(a)$ are the generalized Stieltjes constants. Kreminski [20] has given a generalization of $\gamma_\alpha(a)$ to all positive real numbers α, the so-called *fractional Stieltjes constants*, which can be defined as the coefficients of the Laurent expansion of the α-th Grünwald-Letnikov fractional derivative [15] of $\zeta(s,a) - 1/a^s$ for $s \neq 1$ (see [12]):

$$D_s^\alpha\left[\zeta(s,a) - 1/a^s\right] = (-1)^\alpha \sum_{n=1}^{\infty} \frac{\log^\alpha(n+a)}{(n+a)^s} = (-1)^\alpha \left(\frac{\Gamma(\alpha+1)}{(s-1)^{\alpha+1}} + \sum_{n=1}^{\infty} \frac{(-1)^n \gamma_{\alpha+n}(a)}{n!}(s-1)^n \right).$$

In [12, Corollary 3.2] we have shown that

$$\gamma_\alpha(1) \to \gamma - 1 = -0.42278\,43350\ldots \text{ as } \alpha \to 0^+, \tag{2}$$

where $\gamma = \gamma_0 = \gamma_0(1) = 0.57721\,46649\ldots$ is Euler's constant. Also in [12] we have also given a short proof of a conjecture of Kreminski, stated in [20, Conjecture IIIa]:

> Let $0 < \alpha \in \mathbb{R}$ and let $C_\alpha(a) := \gamma_\alpha(a) - \frac{\log^\alpha(a)}{a}$ and $h_a(s) := \zeta(s,a) - \frac{1}{s-1} - \frac{1}{a^s}$, then $C_\alpha(a) = (-1)^{-\alpha} D_s^\alpha[h_a](1)$.

The goal of this paper is to approximate $\gamma_\alpha(a)$ by evaluating $C_\alpha(a)$, to find an upper bound for $|C_\alpha(a)|$, and give an asymptotic formula for $C_\alpha(a)$..

Research on related questions dates back to Stieltjes [26], Jensen [17], and Ramanujan [22], and more recently it has received a lot of renewed attention in the works of Adell [2], Adell & Lekuona [3], Blagouchine [6], Coffey [7], Coffey & Knessl [8], and others. In our recent paper [13], we have been able to apply some of the properties of the fractional Stieltjes constants to prove that $D_s^\alpha\left[\zeta(s)\right] \neq 0$ for $|s-1| < 1$.

Here (in Section 2 below) we start with a method for evaluating $C_\alpha(a)$ using the Euler-Maclaurin summation technique; it was chosen because it is closely related to our bound for $C_\alpha(a)$ for $\alpha > 1$ (derived in Section 3), which is a generalization of [27, Theorem 3] to the fractional Stieltjes constants. In Section 4 we then show how this bound can be minimized. Numerical experiments suggest that it improves upon the bounds by Berndt [5], Williams and Zhang [27] and Matsuoka [21]. An asymptotic expression for $C_\alpha(a)$

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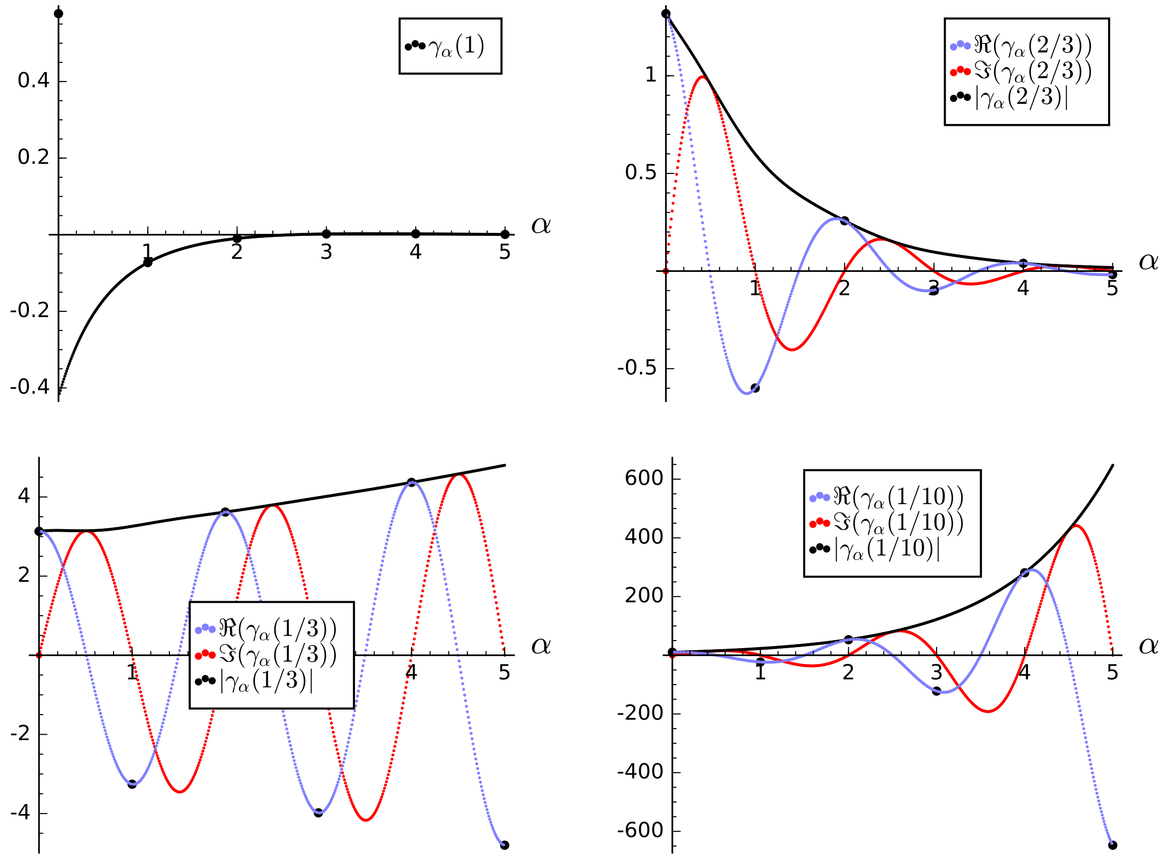

FIGURE 1. Fractional Stieltjes constants $\gamma_\alpha(a)$ for $a \in \{1, 2/3, 1/3, 1/10\}$ plotted for $\alpha \in [0,5]$ with integral Stieltjes constants ($\bullet$). The first plot shows the discontinuity of $\gamma_\alpha(1)$ at $\alpha = 0$ (compare [12, Corollary 3.2]). The values for α are 1/100 apart.

based on the work of Coffey and Knessl [8] for Stieltjes constants is proved in Section 5 and is basis for a conjectured bound in Section 6.

2. Evaluating Fractional Stieltjes Constants

Johansson [18] evaluates generalized Stieltjes constants by computing the series expansion of $\zeta(s,a) - \frac{1}{s-1}$ at $s = 1$ obtained with Euler-Maclaurin summation. To evaluate $\gamma_\alpha(a)$ we approximate $C_\alpha(a)$ with Euler-Maclaurin summation and then use that $\gamma_\alpha(a) = C_\alpha(a) + \frac{\log^\alpha(a)}{a}$. A different approach, namely Newton-Cotes approximation, was chosen by Kreminski in [20].

Let $f_\alpha(x) = \frac{\log^\alpha(x+a)}{x+a}$. By [12, Theorem 3.1] for real $\alpha > 0$, $0 < a \leq 1$ and $m \in \mathbb{N}$, we have

$$\gamma_\alpha(a) = \sum_{r=0}^{m} \frac{\log^\alpha(r+a)}{r+a} - \frac{\log^{\alpha+1}(m+a)}{\alpha+1} - \frac{\log^\alpha(m+a)}{2(m+a)} + \int_m^\infty P_1(x) f'_\alpha(x)dx, \tag{3}$$

where $P_1(x) = x - \lfloor x \rfloor - \frac{1}{2}$. All but the first term of the sum are real, that is,

$$C_\alpha(a) = \sum_{r=1}^{m} \frac{\log^\alpha(r+a)}{r+a} - \frac{\log^{\alpha+1}(m+a)}{\alpha+1} - \frac{\log^\alpha(m+a)}{2(m+a)} + \int_m^\infty P_1(x) f'_\alpha(x)dx \in \mathbb{R}. \tag{4}$$

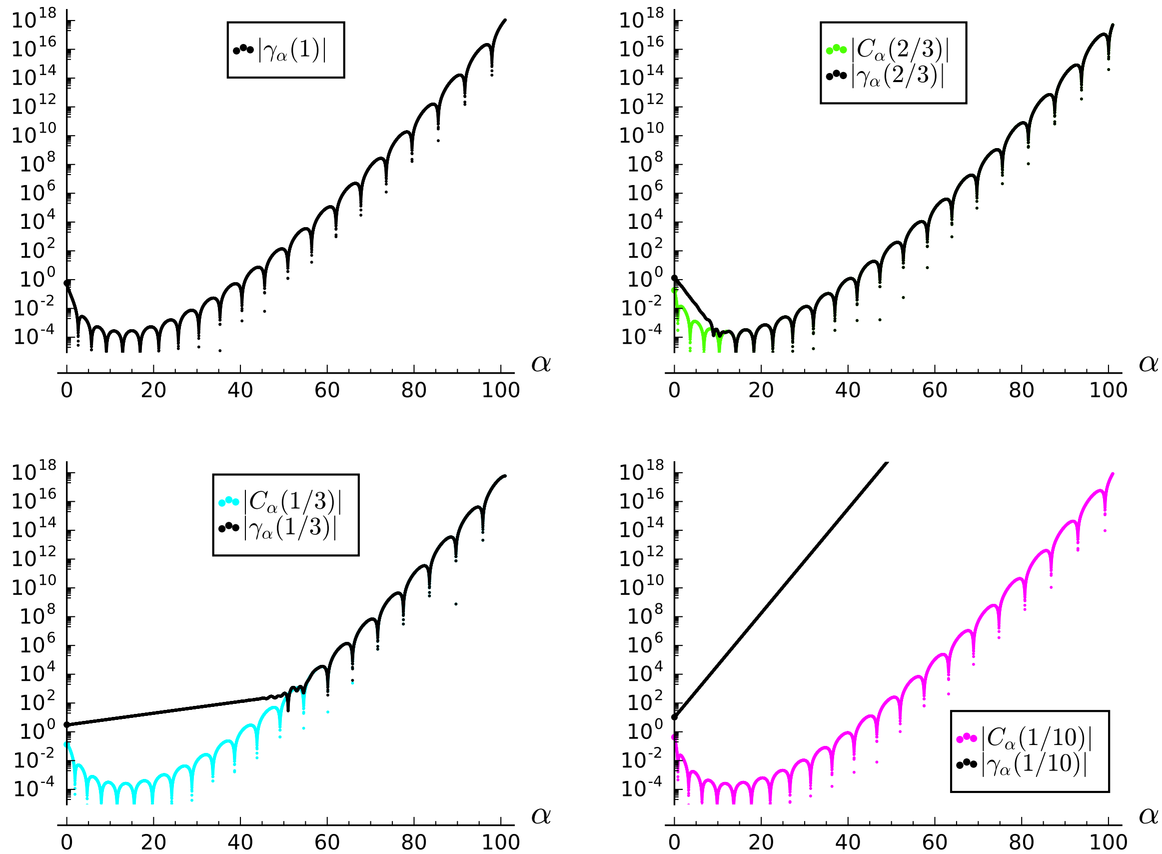

FIGURE 2. Absolute values of fractional Stieltjes constants $\gamma_\alpha(a)$ and $C_\alpha(a)$ for $a \in \{1, 2/3, 1/3, 1/10\}$ plotted for $\alpha \in [0, 100]$. The values for α are $1/100$ apart.

and $\Im(\gamma_\alpha(a)) = \frac{1}{a}\Im(\log^\alpha(a))$. To evaluate $C_\alpha(a)$ we integrate by parts v times and obtain

$$(5)\qquad \int_m^\infty P_1(x) f'_\alpha(x)dx = \sum_{j=1}^{v}\left[P_j(x) f_\alpha^{(j-1)}(x)\right]_{x=m}^{\infty} + (-1)^{v-1}\int_m^\infty P_v(x) f_\alpha^{(v)}(x)dx,$$

where $P_k(x) = \frac{B_k(x-\lfloor x \rfloor)}{k!}$ is the k^{th} periodic Bernoulli polynomial and B_j is the j^{th} Bernoulli number (with $B_1 = \frac{1}{2}$ and $B_j = 0$, for all odd $j > 1$).

We will soon see that letting $m > 0$ forces the integral on the right hand side of (5) to converge for any $v \in \mathbb{N}$. Specializing [16, Theorem 1] we obtain:

$$(6)\qquad f_\alpha^{(n)}(x) = \sum_{i=0}^{n} s(n+1, i+1)(\alpha)_i \frac{\log^{\alpha-i}(x+a)}{(x+a)^{n+1}},$$

where $s(i,j)$ denotes the signed Stirling numbers of the first kind and $(\alpha)_i = \frac{\Gamma(\alpha+1)}{\Gamma(\alpha-i+1)}$ the falling factorial of α. It follows that $f_\alpha^{(n)}(x) \to 0$, as $x \to \infty$, for any $n \in \mathbb{N}$. Thus, we can rewrite (5) as

$$(7)\qquad \int_m^\infty P_1(x) f'_\alpha(x)dx = -\sum_{j=1}^{v} P_j(m) f_\alpha^{(j-1)}(m) + (-1)^{v-1}\int_m^\infty P_v(x) f_\alpha^{(v)}(x)dx.$$

For any $j \in \mathbb{N}$ and $m \in \mathbb{N}$ we have $P_j(m) = \frac{B_j}{j!}$. We now approximate $C_\alpha(a)$ by

$$C_\alpha(a) \approx \sum_{r=1}^{m} \frac{\log^\alpha(r+a)}{r+a} - \frac{\log^{\alpha+1}(m+a)}{\alpha+1} - \frac{\log^\alpha(m+a)}{2(m+a)} - \sum_{j=1}^{\lfloor v/2 \rfloor} \frac{B_{2j}}{(2j)!} f_\alpha^{(2j-1)}(m). \tag{8}$$

The error made in approximating $C_\alpha(a)$ by (8) is given by

$$R_v = (-1)^{v-1} \int_m^\infty P_v(x) f_\alpha^{(v)}(x) dx.$$

We now show that we can choose m and v so that this error is arbitrarily small. Let us choose $v > 1$. As $|P_n(x)| \leq \frac{3+(-1)^n}{(2\pi)^n}$ for any $n > 1$ (see [27] or [5]) we have

$$|R_v| = \left| (-1)^{v-1} \int_m^\infty P_v(x) f_\alpha^{(v)}(x)\, dx \right| \leq \frac{3+(-1)^v}{(2\pi)^v} \int_m^\infty \left| f_\alpha^{(v)}(x) \right| dx. \tag{9}$$

Applying (6) and the triangle inequality in (9) we get

$$|R_v| \leq \frac{3+(-1)^v}{(2\pi)^v} \sum_{i=0}^{v} |s(v+1, i+1)| \frac{\Gamma(\alpha+1)}{|\Gamma(\alpha-i+1)|} \int_m^\infty \frac{\log^{\alpha-i}(x+a)}{(x+a)^{v+1}} dx. \tag{10}$$

Here note that we rewrite the integral in terms of the upper incomplete Gamma function (see [14, p. 346] and [1, 6.5.3])

$$\int_m^\infty \frac{\log^{\alpha-i}(x+a)}{(x+a)^{v+1}} dx = \frac{\Gamma(\alpha-i+1, v\log(m+a))}{v^{\alpha-i+1}}. \tag{11}$$

Applying (11) in (10) we find an upper bound for the error:

$$|R_v| \leq \frac{(3+(-1)^v)\Gamma(\alpha+1)}{(2\pi)^v v^{\alpha+1}} \sum_{i=0}^{v} |s(v+1, i+1)| \frac{\Gamma(\alpha-i+1, v\log(m+a)) v^i}{|\Gamma(\alpha-i+1)|}. \tag{12}$$

The error term R_v in (10) converges for all v. To find suitable parameters v and m so that R_v is smaller than a given bound we follow a method similar to that used in [11] to evaluate $\zeta^{(k)}$. We first choose a large $v \in \mathbb{N}$ and then iteratively increase the value of m. The values for $\gamma_\alpha(a)$ in Figures 1, 2, 3, and the Tables 1 and 2 were computed with an implementation of the method described above in SageMath [24] using mpmath [19].

3. An Upper Bound For $C_\alpha(a)$

We present a bound for $C_\alpha(a)$, for real numbers $\alpha > 1$, that is a generalization of [27, Theorem 3] to fractional Stieltjes constants.

Theorem 1. *Let $0 < a \leq 1$, $\alpha > 1$ and $C_\alpha(a) = \gamma_\alpha(a) - \frac{\log^\alpha(a)}{a}$. Then,*

$$|C_\alpha(a)| \leq \frac{(3+(-1)^{n+1})\Gamma(\alpha+1)}{(2\pi)^{n+1}(n+1)^{\alpha+1}} \frac{(2(n+1))!}{(n+1)!}$$

where n is any positive integer satisfying $1 \leq n < \alpha$.

Proof. Setting $m = 1$ in (3) and making some minor simplifications we obtain

$$\gamma_\alpha(a) = \frac{\log^\alpha(a)}{a} + \frac{\log^\alpha(1+a)}{2(1+a)} - \frac{\log^{\alpha+1}(1+a)}{\alpha+1} + \int_1^\infty P_1(x) f'_\alpha(x) dx. \tag{13}$$

α	$\gamma_\alpha(0.1)$	$\gamma_\alpha(1/3)$	$\gamma_\alpha(2/3)$	$\gamma_\alpha(1)$
0.1	$10.65 + 3.359i$	$3.009 + 0.9358i$	$1.172 + 0.4235i$	-0.3495
0.2	$9.782 + 6.945i$	$2.593 + 1.797i$	$0.9194 + 0.736i$	-0.2907
0.3	$7.704 + 10.39i$	$1.923 + 2.497i$	$0.6074 + 0.9256i$	-0.243
0.4	$4.418 + 13.28i$	$1.06 + 2.963i$	$0.2794 + 0.9942i$	-0.2038
0.5	$0.06524 + 15.17i$	$0.08545 + 3.144i$	$-0.02734 + 0.9551i$	-0.1714
0.6	$-5.06 + 15.69i$	$-0.907 + 3.019i$	$-0.2848 + 0.83i$	-0.1444
0.7	$-10.52 + 14.5i$	$-1.82 + 2.592i$	$-0.4746 + 0.6451i$	-0.1217
0.8	$-15.77 + 11.45i$	$-2.564 + 1.901i$	$-0.5885 + 0.4282i$	-0.1026
0.9	$-20.16 + 6.546i$	$-3.061 + 1.009i$	$-0.6273 + 0.2057i$	-0.08651
1.0	-23.04	-3.26	-0.5989	-0.07282
10.0	$4.189\cdot 10^4$	7.683	0.0002643	0.0002053
10.1	$4.331\cdot 10^4 + 1.407\cdot 10^4 i$	$7.376 + 2.397i$	$0.0002155 + 5.086\cdot 10^{-5} i$	0.0002203
10.2	$4.005\cdot 10^4 + 2.91\cdot 10^4 i$	$6.334 + 4.602i$	$0.0001556 + 8.84\cdot 10^{-5} i$	0.0002334
10.3	$3.163\cdot 10^4 + 4.353\cdot 10^4 i$	$4.645 + 6.394i$	$8.997\cdot 10^{-5} + 0.0001112i$	0.0002446
10.4	$1.807\cdot 10^4 + 5.562\cdot 10^4 i$	$2.465 + 7.588i$	$2.381\cdot 10^{-5} + 0.0001194i$	0.0002539
10.5	$0.0001501 + 6.357\cdot 10^4 i$	$-0.0002227 + 8.054i$	$-3.856\cdot 10^{-5} + 0.0001147i$	0.0002612
10.6	$-2.135\cdot 10^4 + 6.572\cdot 10^4 i$	$-2.512 + 7.732i$	$-9.379\cdot 10^{-5} + 9.968\cdot 10^{-5} i$	0.0002667
10.7	$-4.415\cdot 10^4 + 6.077\cdot 10^4 i$	$-4.824 + 6.639i$	$-0.0001397 + 7.747\cdot 10^{-5} i$	0.0002703
10.8	$-6.605\cdot 10^4 + 4.799\cdot 10^4 i$	$-6.702 + 4.869i$	$-0.0001752 + 5.143\cdot 10^{-5} i$	0.0002721
10.9	$-8.44\cdot 10^4 + 2.742\cdot 10^4 i$	$-7.953 + 2.584i$	$-0.0002004 + 2.47\cdot 10^{-5} i$	0.000272
11.0	$-9.647\cdot 10^4$	-8.441	-0.0002163	0.0002702
100.0	$1.666\cdot 10^{37}$	$4.349\cdot 10^{17}$	$-9.528\cdot 10^{15}$	$-4.253\cdot 10^{17}$
100.1	$1.722\cdot 10^{37} + 5.595\cdot 10^{36} i$	$4.576\cdot 10^{17} + 1.137\cdot 10^4 i$	$1.651\cdot 10^{16} + 2.644\cdot 10^{-40} i$	$-4.741\cdot 10^{17}$
100.2	$1.592\cdot 10^{37} + 1.157\cdot 10^{37} i$	$4.799\cdot 10^{17} + 2.182\cdot 10^4 i$	$4.692\cdot 10^{16} + 4.595\cdot 10^{-40} i$	$-5.268\cdot 10^{17}$
100.3	$1.257\cdot 10^{37} + 1.731\cdot 10^{37} i$	$5.015\cdot 10^{17} + 3.032\cdot 10^4 i$	$8.215\cdot 10^{16} + 5.778\cdot 10^{-40} i$	$-5.836\cdot 10^{17}$
100.4	$7.185\cdot 10^{36} + 2.211\cdot 10^{37} i$	$5.22\cdot 10^{17} + 3.598\cdot 10^4 i$	$1.227\cdot 10^{17} + 6.206\cdot 10^{-40} i$	$-6.447\cdot 10^{17}$
100.5	$-4.484\cdot 10^{17} + 2.527\cdot 10^{37} i$	$5.41\cdot 10^{17} + 3.819\cdot 10^4 i$	$1.692\cdot 10^{17} + 5.962\cdot 10^{-40} i$	$-7.102\cdot 10^{17}$
100.6	$-8.489\cdot 10^{36} + 2.613\cdot 10^{37} i$	$5.581\cdot 10^{17} + 3.667\cdot 10^4 i$	$2.221\cdot 10^{17} + 5.181\cdot 10^{-40} i$	$-7.802\cdot 10^{17}$
100.7	$-1.755\cdot 10^{37} + 2.416\cdot 10^{37} i$	$5.728\cdot 10^{17} + 3.149\cdot 10^4 i$	$2.82\cdot 10^{17} + 4.027\cdot 10^{-40} i$	$-8.549\cdot 10^{17}$
100.8	$-2.626\cdot 10^{37} + 1.908\cdot 10^{37} i$	$5.846\cdot 10^{17} + 2.309\cdot 10^4 i$	$3.497\cdot 10^{17} + 2.673\cdot 10^{-40} i$	$-9.343\cdot 10^{17}$
100.9	$-3.356\cdot 10^{37} + 1.09\cdot 10^{37} i$	$5.928\cdot 10^{17} + 1.225\cdot 10^4 i$	$4.258\cdot 10^{17} + 1.284\cdot 10^{-40} i$	$-1.019\cdot 10^{18}$
101.0	$-3.835\cdot 10^{37}$	$5.967\cdot 10^{17}$	$5.111\cdot 10^{17}$	$-1.108\cdot 10^{18}$

Table 1. Fractional Stieltjes constants approximated to a precision of four decimal digits.

Since $0 < a \le 1$ and $P_1(x) = x - \frac{1}{2}$ on $(0,1)$ integration by parts yields

$$\int\limits_{1-a}^{1} P_1(x) f'_\alpha(x)dx = \int\limits_{1-a}^{1} \left(x - \frac{1}{2}\right) f'_\alpha(x)dx = \frac{\log^\alpha(1+a)}{2(1+a)} - \frac{\log^{\alpha+1}(1+a)}{\alpha+1}.$$

Using this in (13), allows us to see that

$$\gamma_\alpha(a) = \frac{\log^\alpha(a)}{a} + \int\limits_{1-a}^{\infty} P_1(x) f'_\alpha(x)dx = \frac{\log^\alpha(a)}{a} + C_\alpha(a).$$

By (6) we have for any positive integer n,

$$f_\alpha^{(n)}(x) = \sum_{i=0}^{n} s(n+1, i+1)(\alpha)_i \frac{\log^{\alpha-i}(x+a)}{(x+a)^{n+1}}.$$

Assume $\alpha > 1$ is real, and n and k are integers that satisfy $1 \le k \le n < \alpha$. Then $f_\alpha^{(k)}(x-a)$ is a combination of positive powers of $\log(x)$, and therefore $f_\alpha^{(k)}(1-a) = 0$. Also, $f_\alpha^{(k)}(x-a) \to 0$, as $x \to \infty$. These observations, and integrating by parts n times, yield

$$\begin{aligned} C_\alpha(a) &= P_2(x)f'_\alpha(x)|_{x=1-a}^{\infty} + \ldots + (-1)^{n+1}P_{n+1}(x)f_\alpha^{(n)}(x)|_{x=1-a}^{\infty} + (-1)^n\int_{1-a}^{\infty} P_{n+1}(x)f_\alpha^{(n+1)}(x)dx \\ &= (-1)^n\int_{1-a}^{\infty} P_{n+1}(x)f_\alpha^{(n+1)}(x)dx. \end{aligned}$$

Substituting x by $x-a$ we get

$$C_\alpha(a) = (-1)^n\int_1^{\infty} P_{n+1}(x-a)f_\alpha^{(n+1)}(x-a)dx.$$

With $|P_n(x)| \le \frac{3+(-1)^n}{(2\pi)^n}$, for all $n>1$ we obtain

$$\begin{aligned} |C_\alpha(a)| &= \left|(-1)^n\int_1^{\infty} P_{n+1}(x-a)f_\alpha^{(n+1)}(x-a)dx\right| \\ &\le \frac{3+(-1)^{n+1}}{(2\pi)^{n+1}}\int_1^{\infty}\left|f_\alpha^{(n+1)}(x-a)\right|dx \\ &\le \frac{3+(-1)^{n+1}}{(2\pi)^{n+1}}\sum_{i=0}^{n+1}|s(n+2,i+1)|(\alpha)_i\int_1^{\infty}\frac{\log^{\alpha-i}(x)}{x^{n+2}}dx. \end{aligned} \tag{14}$$

It remains to evaluate the integral in (14). After a change of variables we have

$$\int_1^{\infty}\frac{\log^{\alpha-i}(x)}{x^{n+2}}dx = \frac{1}{(n+1)^{\alpha-i+1}}\int_0^{\infty}x^{\alpha-i}e^{-x}dx = \frac{\Gamma(\alpha-i+1)}{(n+1)^{\alpha-i+1}}, \tag{15}$$

since $\alpha - i \ge \alpha - n > 0$, and the integral converges for all $0 \le i \le n+1$. Thus, (14) becomes

$$|C_\alpha(a)| \le \frac{3+(-1)^{n+1}}{(2\pi)^{n+1}}\sum_{i=0}^{n+1}|s(n+2,i+1)|(\alpha)_i\frac{\Gamma(\alpha-i+1)}{(n+1)^{\alpha-i+1}}. \tag{16}$$

Since $1 \le n < \alpha$, we can write $(\alpha)_i = \frac{\Gamma(\alpha+1)}{\Gamma(\alpha-i+1)}$ for each $0 \le i \le n+1$, so from (16) we get

$$\begin{aligned} |C_\alpha(a)| &\le \frac{3+(-1)^{n+1}}{(2\pi)^{n+1}}\sum_{i=0}^{n+1}|s(n+2,i+1)|\frac{\Gamma(\alpha+1)}{(n+1)^{\alpha-i+1}} \\ &= \frac{(3+(-1)^{n+1})\Gamma(\alpha+1)}{(2\pi)^{n+1}(n+1)^{\alpha+1}}\sum_{i=0}^{n+1}|s(n+2,i+1)|(n+1)^i \\ &= \frac{(3+(-1)^{n+1})\Gamma(\alpha+1)}{(2\pi)^{n+1}(n+1)^{\alpha+2}}\sum_{j=1}^{n+2}|s(n+2,j)|(n+1)^j. \end{aligned}$$

By [27, 6.14] we have $\sum_{i=1}^{n+2}|s(n+2,j)|(n+1)^j = \frac{(2n+2)!}{n!}$. Using this identity, we arrive at

$$|C_\alpha(a)| \le \frac{(3+(-1)^{n+1})\Gamma(\alpha+1)}{(2\pi)^{n+1}(n+1)^{\alpha+2}}\frac{(2n+2)!}{n!} = \frac{(3+(-1)^{n+1})\Gamma(\alpha+1)}{(2\pi)^{n+1}(n+1)^{\alpha+1}}\frac{(2(n+1))!}{(n+1)!},$$

which concludes the proof. □

4. Minimizing the Bound

The inequality in Theorem 1 holds for any positive integer $n < \alpha$. It is natural to wonder what value of n minimizes the upper bound. The Lambert W function, that is the complex values $W(z)$ for which $W(z)e^{W(z)} = z$, helps us answer this question. In particular we use the principal branch W_0.

Lemma 1. *Fix $0 < a \leq 1$ and $\alpha > 0$ and set $q(x) := \frac{4\sqrt{2}\Gamma(\alpha+1)}{(x+1)^{\alpha+1}} \left(\frac{2(x+1)}{e\pi}\right)^{x+1}$. Then*

1. *For integers $1 \leq n < \alpha$ we have: $|C_\alpha(a)| \leq q(n)$.*
2. *$q(x)$ is minimal when $x = \frac{\pi}{2}e^{W_0\left(\frac{2(\alpha+1)}{\pi}\right)} - 1$.*

Proof. (1) With the sharp version of Stirling's formula given by Robbins [23]:

$$\left(\frac{n}{e}\right)^n \sqrt{2\pi n} e^{\frac{1}{12n+1}} \leq n! \leq \left(\frac{n}{e}\right)^n \sqrt{2\pi n} e^{\frac{1}{12n}}.$$

we obtain for all $n \geq 1$ that

$$\frac{(2n)!}{n!} \leq \sqrt{2}\left(\frac{4n}{e}\right)^n e^{\frac{1}{24n}-\frac{1}{12n+1}} < \sqrt{2}\left(\frac{4n}{e}\right)^n \tag{17}$$

Applying (17) to the right hand side of the inequality in Theorem 1 we obtain

$$|C_\alpha(a)| \leq \frac{(3+(-1)^{n+1})\Gamma(\alpha+1)}{(2\pi)^{n+1}(n+1)^{\alpha+1}} \frac{(2(n+1))!}{(n+1)!} < \frac{4\sqrt{2}\Gamma(\alpha+1)}{(n+1)^{\alpha+1}} \left(\frac{2(n+1)}{e\pi}\right)^{n+1} = q(n).$$

(2) It is our goal to find x on the closed interval $[1, \alpha]$ that minimizes $q(x)$. Once x is found, we let n be the nearest integer to x in $[1, \alpha)$. Let $g_\alpha = 4\sqrt{2}\Gamma(\alpha+1)$. Since we are working on a closed interval and q is continuous on $[1, \alpha]$, q must attain a minimum on $[1, \alpha]$. We write

$$q(x) = \frac{g_\alpha}{(x+1)^{\alpha+1}} \left[\frac{2(x+1)}{\pi e}\right]^{x+1} = g_\alpha \exp\left[-(\alpha+1)\log(x+1) + (x+1)\log\left(\frac{2(x+1)}{\pi e}\right)\right].$$

Differentiating, we find

$$q'(x) = f_\alpha \left[\frac{-(\alpha+1)}{x+1} + 1 + \log\left(\frac{2(x+1)}{\pi e}\right)\right] \exp\left[-(\alpha+1)\log(x+1) + (x+1)\log\left(\frac{2(x+1)}{\pi e}\right)\right].$$

Setting $q'(x) = 0$ and dividing both sides by the constant and exponential terms, we get

$$\frac{-(\alpha+1)}{x+1} + 1 + \log\left(\frac{2(x+1)}{\pi e}\right) = \frac{-(\alpha+1)}{x+1} + \log\left(\frac{2(x+1)}{\pi}\right) = 0.$$

This implies that $\frac{2(x+1)}{\pi}\log\left(\frac{2(x+1)}{\pi}\right) = \frac{2(\alpha+1)}{\pi}$, and if we let $y = \log\left(\frac{2(x+1)}{\pi}\right)$, then the previous equation becomes $ye^y = \frac{2(\alpha+1)}{\pi}$. Applying the Lambert W function, we see that we must have $y = W_0\left(\frac{2(\alpha+1)}{\pi}\right)$. Solving for x, using this relation we then have $x = \frac{\pi}{2}e^{W_0\left(\frac{2(\alpha+1)}{\pi}\right)} - 1$.

□

To apply Lemma 1 to the bound from Theorem 1 we choose $1 < n < \alpha$ in the following manner. If $x := \frac{\pi}{2}e^{W_0\left(\frac{2(\alpha+1)}{\pi}\right)} < \alpha$, then let n be the nearest integer to x. Since $x \geq \alpha$ implies that $q(x)$ is monotonically decreasing on the interval $(1, \alpha)$ we set $n := \lceil \alpha - 1 \rceil$ in this case. In summary this gives us the bound

$$|C_\alpha(a)| \leq \frac{(3+(-1)^{n+1})\Gamma(\alpha+1)}{(2\pi)^{n+1}(n+1)^{\alpha+1}} \frac{(2(n+1))!}{(n+1)!} \text{ with } n = \begin{cases} \lfloor x \rceil & \text{if } x < \alpha \\ \lceil \alpha - 1 \rceil & \text{else} \end{cases} \quad \text{where } x = \frac{\pi}{2}e^{W_0\left(\frac{2(\alpha+1)}{\pi}\right)}. \tag{18}$$

The upper bound for the fractional Stieltjes constants also is a bound for the integral Stieltjes constants. In Figure 3 we compare our bound from (18) to previously known bounds for integral Stieltjes constants $|\gamma_m| = |C_m(1)|$:

1. the bound by Berndt [5]:

$$|\gamma_m| \leq \frac{(3+(-1)^m)(m-1)!}{\pi^m}$$

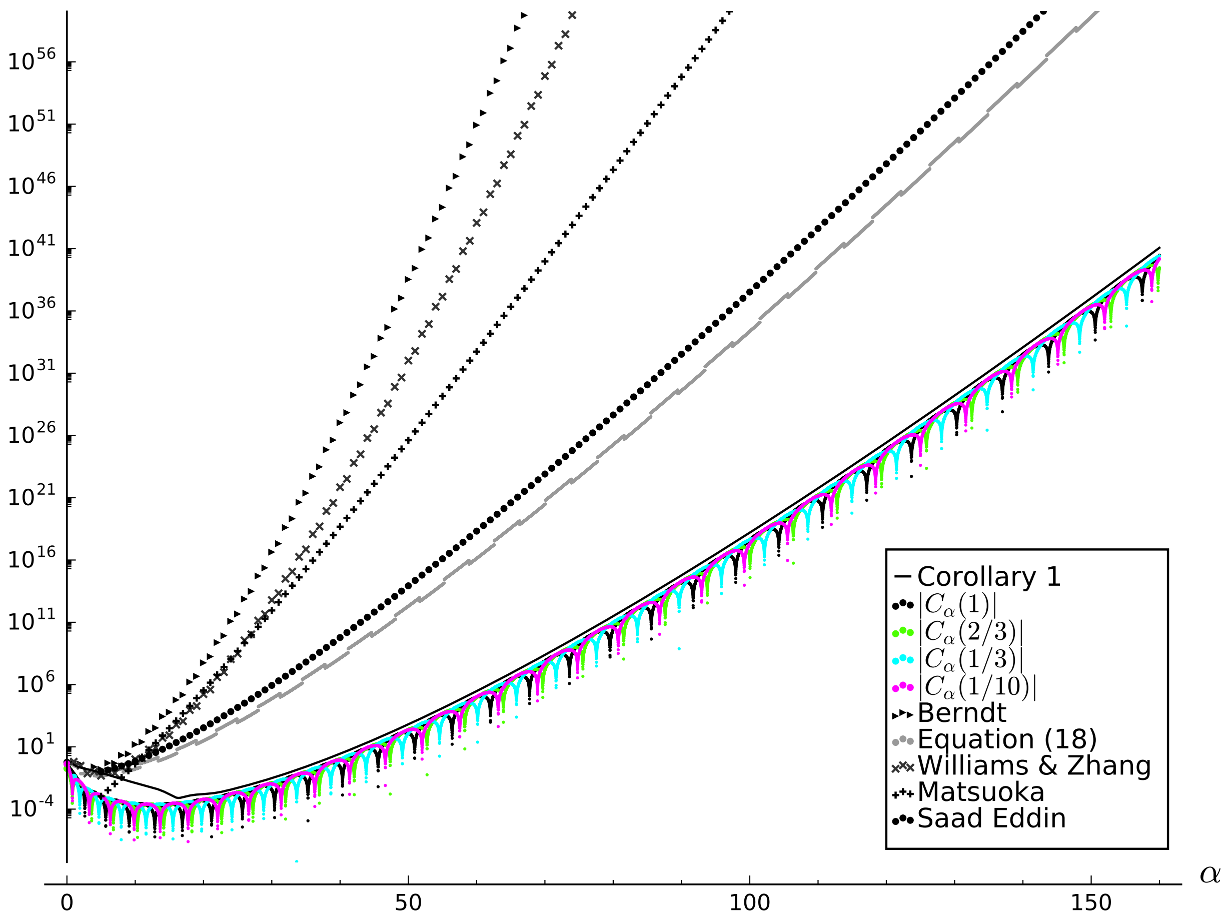

FIGURE 3. Absolute values of $C_\alpha(1/3)$ $1 \le \alpha \le 140$ with the bounds by Berndt [5], by Williams and Zhang [27], and by Matsuoka [21], and by Saad Eddin [25], and the bound from (18) and the bound for the asymptotic formula from Corollary 1.

(2) the bound by Williams and Zhang [27] which we can also obtain from Theorem 1 with $n = m - 1$ and $\alpha = m$:

$$|\gamma_m| \le \frac{(3 + (-1)^m)(2m)!}{m^{m+1}(2\pi)^m}$$

(3) the bound by Matsuoka [21] which holds for $m > 4$:

$$|\gamma_m| < 10^{-4}(\log m)^m$$

(4) the bound by Saad Eddin [25]:

$$|\gamma_m| \le m! \cdot 2\sqrt{2}e^{-(n+1)\log\theta(m)+\theta(m)\left(\log\theta(m)+\log\frac{2}{\pi e}\right)}\left(1 + 2^{-\theta(m)-1}\frac{\theta(m)+1}{\theta(m)-1}\right)$$

where $\theta(m) = \frac{m+1}{\log\frac{2(m+1)}{\pi}} - 1$.

The plot also contains the bound from Corollary 1 for the asymptotic formula given in the next section.

5. An Asymptotic Formula

Coffey and Knessl [8] give an effective asymptotic formula for the Stieltjes constants. We generalize their work to the fractional Stieltjes constants.

Theorem 2. *Let $\alpha > 0$ and set $w(\alpha) = W_0\left(\frac{\alpha i}{2\pi}\right)$ and let*

$$\widetilde{C}_\alpha(a) := \frac{\log^\alpha(1+a)}{2(1+a)} - \frac{\log^{\alpha+1}(1+a)}{\alpha+1} - \Im\left(\sqrt{\frac{2\alpha}{\pi(w(\alpha)+1)}}e^{-w(\alpha)+h(w(\alpha))}\right)$$

where $h(t) = 2\pi i(e^t - a) + \alpha \log t$. Then $C_\alpha(a) \sim \widetilde{C}_\alpha(a)$.

Proof. Again we set $f_\alpha(x) = \frac{\log^\alpha(x+a)}{x+a}$. As in (13) we set $m = 1$ in (3) and get

$$\gamma_\alpha(a) = \frac{\log^\alpha(a)}{a} + \frac{\log^\alpha(1+a)}{2(1+a)} - \frac{\log^{\alpha+1}(1+a)}{\alpha+1} + \int_1^\infty P_1(x) f'_\alpha(x) dx \tag{19}$$

for $\alpha \in \mathbb{R}$ with $\alpha > 0$ and $0 < a \leq 1$. The first periodized Bernoulli polynomial P_1 has the Fourier series [1, page 805]

$$P_1(x) = \frac{-1}{\pi} \sum_{j=1}^\infty \frac{\sin(2\pi j x)}{j}.$$

With the above and the change of variable $t = \log(x+a)$ and setting $b = \log(1+a)$, we obtain

$$\begin{aligned}
\int_1^\infty P_1(x) f'_\alpha(x) dx &= \sum_{j=1}^\infty \frac{-1}{\pi j} \int_1^\infty \sin(2\pi j x) \frac{\log^{\alpha-1}(x+a)}{(x+a)^2}(\alpha - \log(x+a)) dx \\
&= \sum_{j=1}^\infty \frac{-1}{\pi j} \int_1^\infty \Im\left(e^{2\pi i j x}\right) \frac{\log^{\alpha-1}(x+a)}{(x+a)^2}(\alpha - \log(x+a)) dx \\
&= \sum_{j=1}^\infty \frac{-1}{\pi j} \int_b^\infty \Im\left(e^{2\pi i j(e^t - a)}\right) e^t \frac{t^{\alpha-1}(\alpha - t)}{e^{2t}} dt \\
&= \Im\left(\sum_{j=1}^\infty \frac{-1}{\pi j} \int_b^\infty e^{2\pi i j(e^t-a)} e^{-t+\alpha\log t} \frac{\alpha - t}{t} dt\right).
\end{aligned}$$

Comparing the Fourier series for P_1 with the Fourier series expansion of $x - [x]$ one sees that the series is dominated by the $j = 1$ term.

To approximate the integral we apply the saddle point method. We set $h(t) = 2\pi i(e^t - a) + \alpha \log t$. We have saddle points where $h'(w(\alpha)) = 2\pi i e^{w(\alpha)} + \alpha/w(\alpha) = 0$. The Lambert W function yields $w(\alpha) = W_0\left(\frac{\alpha i}{2\pi}\right)$. We have $h''(t) = 2\pi i e^t - \alpha/t^2$, so $h''(w(\alpha)) = -\alpha/w(\alpha) - \alpha/w(\alpha)^2$. We get

$$\begin{aligned}
\int_b^\infty e^{2\pi i(e^t-a)+\alpha\log t} e^{-t} \frac{\alpha - t}{t} dt &= \int_b^\infty e^{h(t)} e^{-t} \frac{\alpha - t}{t} dt \\
&\sim \left(\frac{\alpha}{w(\alpha)} - 1\right) \frac{\sqrt{2\pi}}{\sqrt{-h''(w(\alpha))}} e^{h(w(\alpha))} e^{-w(\alpha)} \\
&= \frac{1}{w(\alpha)} (\alpha - w(\alpha)) \frac{\sqrt{2\pi}}{\sqrt{\alpha/w(\alpha) + \alpha/w(\alpha)^2}} e^{h(w(\alpha)) - w(\alpha)} \\
&= \sqrt{\frac{2\pi}{\alpha(w(\alpha)+1)}} e^{-w(\alpha)+h(w(\alpha))}(\alpha - w(\alpha)) \\
&\sim \sqrt{\frac{2\pi\alpha}{w(\alpha)+1}} e^{-w(\alpha)+h(w(\alpha))}.
\end{aligned}$$

Thus

$$\int_1^\infty P_1(x) f'_\alpha(x) dx \sim \Im\left(\frac{-1}{\pi}\sqrt{\frac{2\pi\alpha}{w(\alpha)+1}} e^{-w(\alpha)+h(w(\alpha))}\right) = \Im\left(-\sqrt{\frac{2\alpha}{\pi(w(\alpha)+1)}} e^{-w(\alpha)+h(w(\alpha))}\right)$$

α	$C_\alpha(1/10)$	$\widetilde{C}_\alpha(1/10)$	$C_\alpha(1/3)$	$\widetilde{C}_\alpha(1/3)$	$C_\alpha(2/3)$	$\widetilde{C}_\alpha(2/3)$
1.0	-0.0164038	0.0123545	0.0362794	0.0993116	0.00929138	0.0323691
1.2	-0.0229109	-0.00134172	0.0231650	0.0734673	0.0131505	0.0451311
10.0	0.0000403022	0.0000415881	-0.000289500	-0.000293600	0.0000841476	0.000391183
10.8	0.000199793	0.000204245	-0.000167717	-0.000169532	-0.000104421	0.0000731472
23.7	-0.00143802	-0.00145190	0.000508309	0.000514185	0.00104436	0.00105405
50.0	227.785	228.832	121.028	121.343	-247.852	-248.893
50.5	253.979	255.226	237.558	238.340	-318.319	-319.726
100.0	$-1.93298 \cdot 10^{17}$	$-1.93351 \cdot 10^{17}$	$4.34868 \cdot 10^{17}$	$4.35806 \cdot 10^{17}$	$-9.52803 \cdot 10^{15}$	$-9.86540 \cdot 10^{15}$
100.2	$-2.79276 \cdot 10^{17}$	$-2.79448 \cdot 10^{17}$	$4.79917 \cdot 10^{17}$	$4.80992 \cdot 10^{17}$	$4.69177 \cdot 10^{16}$	$4.66277 \cdot 10^{16}$
210.3	$-3.73494 \cdot 10^{61}$	$-3.73554 \cdot 10^{61}$	$4.70921 \cdot 10^{61}$	$4.71397 \cdot 10^{61}$	$1.32641 \cdot 10^{61}$	$1.32498 \cdot 10^{61}$
305.7	$-3.93590 \cdot 10^{105}$	$-3.93835 \cdot 10^{105}$	$-3.66025 \cdot 10^{105}$	$-3.66071 \cdot 10^{105}$	$4.92432 \cdot 10^{105}$	$4.92664 \cdot 10^{105}$

Table 2. $C_\alpha(a)$ approximated with the methods from Section 2 and $\widetilde{C}_\alpha(a)$ obtained with Theorem 2 with 6 decimal digits given for $a \in \{1/10, 1/3, 2/3\}$.

The result follows immediately with (19) and $C_\alpha(a) = \gamma_\alpha(a) - \frac{\log^\alpha(a)}{a}$. □

In Table 2 we compare the approximation $C_\alpha(a)$ of the fractional Stieltjes constants obtained with the methods from Section 2 with the values $C_\alpha(a)$ obtained with the asymptotic formula from Theorem 2 for $a \in \{1/10, 1/3, 2/3\}$.

Coffey and Knessl [8] note that the asymptotic formula yields a good approximation for integral Stieltjes constants even for small values of α. We find that this also holds for fractional Stieltjes constants.

6. A Possible Bound

The bound for $C_a(\alpha)$ that we found in Section 3 holds for all $a \in (0, 1]$ and the plots in Figure 1 suggest that bounds for $C_a(\alpha)$ should be independent of a. The quality of the approximations obtained from the asymptotic formula from Theorem 2 raises the question whether it could lead to the formulation of a tight bound for $C_a(\alpha)$. In the following we find a bound for $\widetilde{C}_a(\alpha)$ that is independent of a and conjecture that this is a bound for $C_a(\alpha)$.

Corollary 1. *Let $0 < a \leq 1$ and $\alpha > 0$. Then*

$$|\widetilde{C}_a(\alpha)| \leq \frac{\log^\alpha(2)}{2} + 2\left|e^{-\frac{\alpha}{w(\alpha)} + \alpha \log w(\alpha)}\right|. \tag{20}$$

Proof. With $a \in (0, 1]$ we get

$$\left|\frac{\log^\alpha(1+a)}{2(1+a)} - \frac{\log^{\alpha+1}(1+a)}{\alpha+1}\right| \leq \log^\alpha(2)\left|\frac{1}{2(1+a)} - \frac{\log(1+a)}{\alpha+1}\right| \leq \frac{\log^\alpha(2)}{2} \tag{21}$$

As in the previous section we set $w(\alpha) = W_0\left(\frac{\alpha i}{2\pi}\right)$, where W_0 is the principal branch of the Lambert W function. Recall that we have $W_0(\beta) \cdot e^{W_0(\beta)} = \beta$. We have

$$\begin{aligned} \Re(-w(\alpha) + h(w(\alpha))) &= \Re\left(-w(\alpha) + 2\pi i(e^{w(\alpha)} - a) + \alpha \log w(\alpha)\right) \\ &= \Re\left(-w(\alpha) + 2\pi i e^{w(\alpha)} + \alpha \log w(\alpha)\right) \\ &= \Re\left(-w(\alpha) + 2\pi i \frac{\alpha i}{w(\alpha) 2\pi} + \alpha \log w(\alpha)\right) \\ &= \Re\left(-w(\alpha) - \frac{\alpha}{w(\alpha)} + \alpha \log w(\alpha)\right). \end{aligned}$$

As for $\beta \in \mathbb{R}$ we have $\Re(W_0(i\beta)) \geq 0$ (see [9]) we get

$$\left|\sqrt{\frac{2\alpha}{\pi(w(\alpha)+1)}}\right| \leq \left|2\sqrt{\frac{\alpha}{2\pi w(\alpha)}}\right| = \left|2\sqrt{-i\frac{\alpha i}{2\pi w(\alpha)}}\right| = \left|2\sqrt{-ie^{w(\alpha)}}\right| = \left|2e^{\frac{1}{2}w(\alpha)}\right|. \tag{22}$$

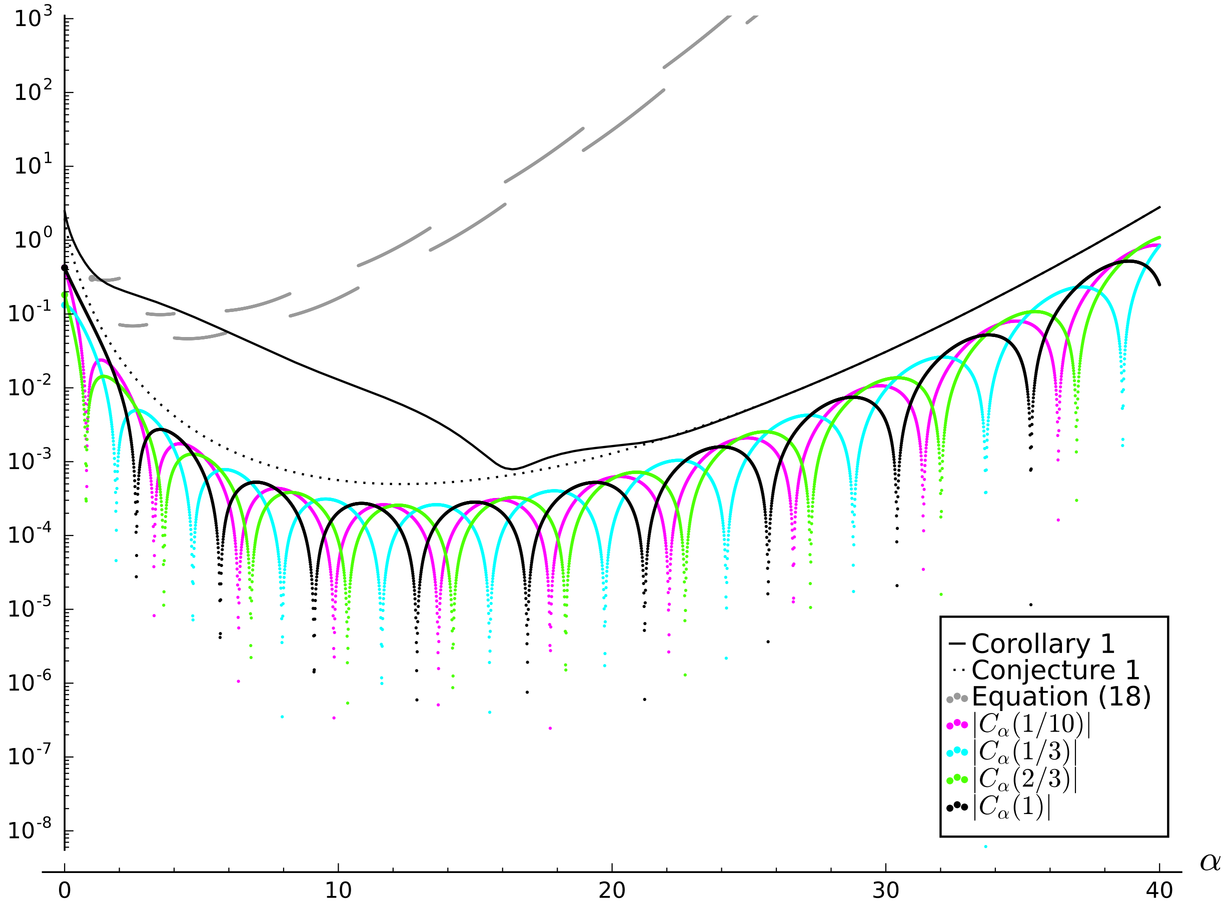

FIGURE 4. $|C_\alpha(a)|$ for $a \in \left\{\frac{1}{100}, \frac{1}{20}, \frac{1}{10}, \frac{1}{3}, \frac{1}{2}, \frac{2}{3}, \frac{9}{10}, 1\right\}$ and the bounds from (18), Corollary 1 and Conjecture 1.

Thus

$$|\widetilde{C}_a(\alpha)| \leq \frac{\log^\alpha(2)}{2} + 2\left|e^{\frac{1}{2}w(\alpha)}\right| \cdot \left|e^{-w(\alpha)-\frac{\alpha}{w(\alpha)}+\alpha\log w(\alpha)}\right| \leq \frac{\log^\alpha(2)}{2} + 2\left|e^{-\frac{\alpha}{w(\alpha)}+\alpha\log w(\alpha)}\right|$$

which concludes the proof. □

Since $\log^\alpha(2)$ approaches 0 as $\alpha \to \infty$ the bound (20) is certainly dominated by the second term for larger α Already for $\alpha = 50$ we have $\frac{\log^\alpha(2)}{2} < 10^{-8}$ while $2\left|e^{-\frac{\alpha}{w(\alpha)}+\alpha\log w(\alpha)}\right| > 500$. Numerical experiments suggest that the bound holds without the term $\frac{\log^\alpha(2)}{2}$ for $\widetilde{C}_\alpha(a)$ as well as $C_\alpha(a)$, compare Figures 4 and 3.

Conjecture 1. *Let $0 < a \leq 1$ and $\alpha > 0$ and set $w(\alpha) := W_0\left(\frac{\alpha i}{2\pi}\right)$, then $|C_\alpha(a)| \leq 2\left|e^{\alpha(\log w(\alpha) - 1/w(\alpha))}\right|$.*

We have verified this for $a \in \left\{\frac{1}{100}, \frac{1}{20}, \frac{1}{10}, \frac{1}{3}, \frac{1}{2}, \frac{2}{3}, 1\right\}$ and $\alpha \in \left\{\frac{i}{100} \mid i \in \{1, 2, 3, \ldots, 30000\}\right\} \subset (0, 300]$.

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