

Crandall's computation of the incomplete Gamma function and the Hurwitz Zeta function, with applications to Dirichlet L-series

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Abstract

This paper extends tools developed by Richard Crandall in [16] to provide robust, high-precision methods for computation of the incomplete Gamma function and the Lerch transcendent. We then apply these to the corresponding computation of the Hurwitz zeta function and so of Dirichlet L-series and character polylogarithms.

1 Introduction

In this article we continue the research in [5, 6, 7] and [16] by providing robust, high-precision methods for computation of the incomplete Gamma function and the Lerch transcendent. We subsequently apply these to the corresponding computation of the Hurwitz zeta function and of Dirichlet L-series.

1.1 Organization

The organization of the paper is as follows. In Section 2 we examine derivatives of the classical polylogarithm and zeta function. In Section 3 we reintroduce character polylogarithms (based on classical Dirichlet characters). In Section 4 we reprise work on the Lerch transcendent by Richard Crandall. In Section 5 we consider methods for evaluating the incomplete Gamma function, and in Section 6 we consider methods for evaluating the Hurwitz zeta function, relying on the methods of the two previous sections. Finally, in Section 7 we make some concluding remarks.

Our dear colleague Richard Crandall, with whom we have collaborated in previous papers in this line of research, passed away in December 2012. In this paper, we not only

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include some material from an invaluable but difficult-to-obtain paper by Crandall [16] (see Section 4), but we also follow, to some extent, Crandall’s style of exposition.

2 Underlying special function tools

We first review some requisite information on Dirichlet L-series and underlying special functions. In Section 4 we revisit the Lerch transcendent, which provides a more general platform for computation of Hurwitz zeta functions, and so also for Dirichlet L-series.

2.1 Polylogarithms and their derivatives with respect to order

We turn to the building blocks of our work. In regard to the needed polylogarithm values, [3, 6] gives formulas including the following. Here $H_n := 1 + \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{n}$ is the harmonic function, and the primed sum \sum' means to avoid the singularity $\zeta(1)$ when $n - m = 1$.

Proposition 1 (Formulas for the polylogarithm of any complex order). *When $s = n$ is a positive integer,*

$$\text{Li}_n(z) = \sum_{m=0}^{\infty'} \zeta(n-m) \frac{\log^m z}{m!} + \frac{\log^{n-1} z}{(n-1)!} (H_{n-1} - \log(-\log z)), \quad (1)$$

valid for $|\log z| < 2\pi$. For any complex order s not a positive integer,

$$\text{Li}_s(z) = \sum_{m \geq 0} \zeta(s-m) \frac{\log^m z}{m!} + \Gamma(1-s)(-\log z)^{s-1}. \quad (2)$$

(This formula is valid for $s = 0$.)

In formula (1), the condition $|\log z| < 2\pi$ precludes its use when $|z| < e^{-2\pi} \approx 0.0018674$. For such small $|z|$, however, it typically suffices to use the definition

$$\text{Li}_s(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^s}. \quad (3)$$

Note that $\text{Li}_0(z) = z/(1-z)$ and $\text{Li}_1(z) = -\log(1-z)$.

In fact, we have found that formula (3) is generally faster than (1) whenever $|z| < 1/4$, at least for precision levels in the range of 100 to 4000 digits. We illustrate this for Li_2 in Figure 1 and for Li_6 in Figure 2. The timings show the run time in microseconds required to compute the polyarithm (Li_2 or Li_6 , respectively) to 1000-digit precision (i.e., by using enough terms of (1) or (3), respectively, to achieve 1000-digit precision) as the modulus goes from 0 to 1, with blue showing superior performance of (1). The region records 10,000 trials of pseudorandom z , such that $-0.6 < \text{Re}(z) < 0.4$, $-0.5 < \text{Im}(z) < 0.5$.

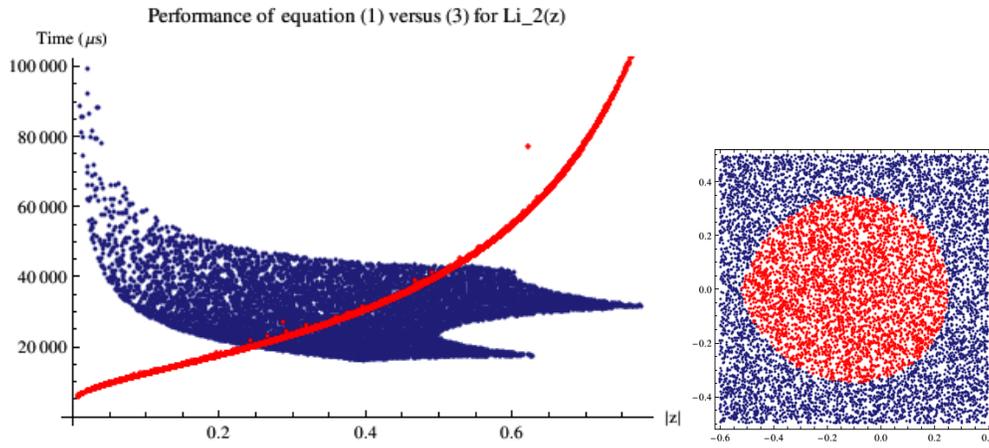


Figure 1: L: Timing (1) (blue) and (3) (red). R: blue region in which (1) performs better

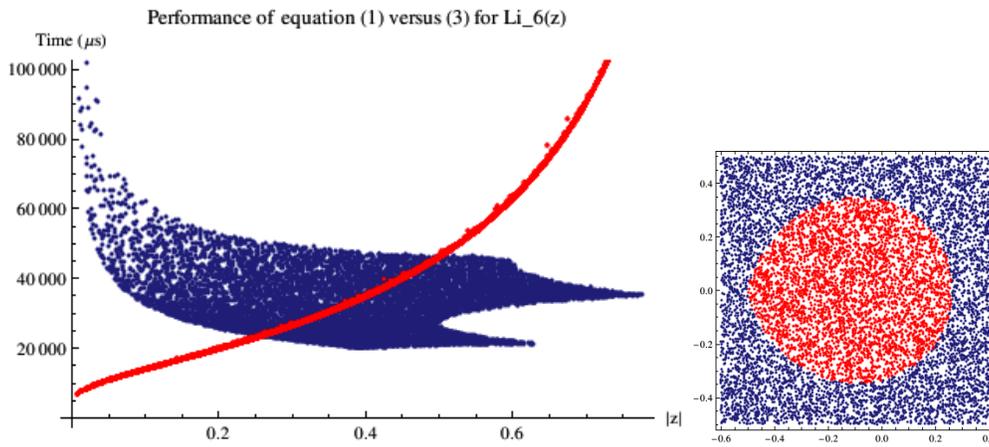


Figure 2: L: Timing (1) (blue) and (3) (red). R: blue region in which (1) performs better

2.2 Outer derivatives of general polylogarithms

We now present some formulas that permit one to calculate derivatives of polylogarithms $\text{Li}_k(z)$, with respect to the order k . We will refer to these derivatives as *outer derivatives*, and we will use the notation $\text{Li}_k^{(m)}(z)$ to denote the m th outer derivative.

In the following, $\mathcal{L} := \log(-\log z)$. The *Stieltjes constants* [16, 21, §7.1] γ_n , with $\gamma_0 = \gamma$ (Euler's constant) are defined as the coefficients in the classical expansion

$$\zeta(z) = \frac{1}{z-1} + \sum_{n=0}^{\infty} \frac{(-1)^n}{n} \gamma_n (z-1)^n.$$

We will employ some constants $c_{k,j}$ derived from the the Stieltjes constants as follows:

$$c_{k,j}(\mathcal{L}) = \frac{(-1)^j}{j!} \gamma_j - b_{k,j+1}(\mathcal{L}), \quad (4)$$

where the $b_{k,j}$ terms—corrected from [16, §7.1]—are given by

$$b_{k,j}(\mathcal{L}) := \sum_{\substack{p+t+q=j \\ p,t,q \geq 0}} \frac{\mathcal{L}^p}{p!} \frac{\Gamma^{(t)}(1)}{t!} (-1)^t f_{k,q}, \quad (5)$$

and $f_{k,q}$ is the coefficient of x^q in $\prod_{m=1}^k \frac{1}{1+x/m}$. The $f_{k,q}$ coefficients can be calculated via the recursion $f_{0,0} = 1, f_{0,q} = 0$ ($q > 0$), $f_{k,0} = 1$ ($k > 0$) and

$$f_{k,q} = \sum_{h=0}^q \frac{(-1)^h}{k^h} f_{k-1,q-h}. \quad (6)$$

Our formulas for outer derivatives are based on the following formula, obtained by carefully manipulating (2). For integer $k \geq 0$, for $|\log z| < 2\pi$ and for $\tau \in [0, 1)$,

$$\text{Li}_{k+1+\tau}(z) = \sum_{0 \leq n \neq k} \zeta(k+1+\tau-n) \frac{\log^n z}{n!} + \frac{\log^k z}{k!} \sum_{j=0}^{\infty} c_{k,j}(\mathcal{L}) \tau^j \quad (7)$$

(see [16, §9, eqn. (51)]). Here we employed the functional equation for the Gamma function to remove singularities at negative integers.

While (7) has little directly to recommend it computationally, it is highly effective for finding outer derivatives. To obtain, for example, the first derivative $\text{Li}_{k+1}^{(1)}(z)$, we differentiate (7) at zero, and so require the evaluation $c_{k,1}$.

Theorem 1 (Outer derivatives of polylogarithms at positive integer orders). *Fix $k = 0, 1, 2, \dots$ and $m = 1, 2, \dots$. For $|\log z| < 2\pi$ and $\mathcal{L} = \log(-\log z)$,*

$$\text{Li}_{k+1}^{(m)}(z) = \sum_{0 \leq n \neq k} \zeta^{(m)}(k+1-n) \frac{\log^n z}{n!} + m! c_{k,m}(\mathcal{L}) \frac{\log^k z}{k!}. \quad (8)$$

In particular,

$$\text{Li}_1^{(1)}(z) = \sum_{n=1}^{\infty} \zeta'(1-n) \frac{\log^n z}{n!} - \gamma_1 - \frac{1}{12} \pi^2 - \frac{1}{2} (\gamma + \log(-\log z))^2, \quad (9)$$

which, as before, is valid whenever $|\log z| < 2\pi$.

For $k = -1$, or, in other words, for $\text{Li}_0^{(m)}(z)$, things are simpler, as we may use (2):

Theorem 2 (Outer derivatives of polylogarithms at zero order). *With $\Gamma^{(t)}(1)$ and $\mathcal{L} = \log(-\log z)$ as above for arbitrary z , we have for m any positive integer*

$$\text{Li}_0^{(m)}(z) = \sum_{n \geq 0} \zeta^{(m)}(-n) \frac{\log^n z}{n!} - \sum_{t=0}^m (-1)^t \binom{m}{t} \Gamma^{(t)}(1) \frac{\mathcal{L}^{m-t}}{\log z}. \quad (10)$$

Note that by applying the simple computational technique of symmetric divided differences to (7), one can rapidly check (8), (9) or (10) to moderate precision (say 50 digits).

3 Character polylogarithms

We first consider a class of general real character L-series (see [12, 14] and [26, §27.8]). For $d \geq 3$ we employ the multiplicative characters $\chi_{\pm d}(n) := \left(\frac{\pm d}{n}\right)$ in terms of the generalized *Legendre-Jacobi symbol*, and for later use we set $\chi_1(n) := 1, \chi_{-2}(n) := (-1)^{n-1}$, so that $L_1 := \zeta$, while $L_{-2} := \eta$, the alternating zeta function. When we write d without a sign, it always denotes $|d|$.

3.1 Character L-series

We shall call upon the series given by the following, for integer $d \geq 3$:

$$L_{\pm d}(s) := \sum_{n>0} \frac{\chi_{\pm d}(n)}{n^s}, \quad (11)$$

In the following, $\zeta(s, \nu) := \sum_{n \geq 0} 1/(n + \nu)^s$ is the *Hurwitz zeta function* (see [21] and [24]), which satisfies $\zeta(s, 1) = \zeta(s)$. Also, for $m = 1, 2, \dots$ and $s \neq 1$, we have

$$L_{\pm d}^{(m)}(s) = \frac{1}{d^s} \sum_{k=1}^{d-1} \chi_{\pm d}(k) \sum_{j=0}^m \binom{m}{j} (-\log d)^j \zeta^{(m-j)}\left(s, \frac{k}{d}\right). \quad (12)$$

This provides access to numerical methods for derivatives of the Hurwitz zeta function for evaluation of quantities like $L_{\pm d}^{(m)}(s)$ with $s > 1$. Various mathematical packages, such as *Maple*, have a good implementation of $\zeta^{(m)}(s, \nu)$ with respect to arbitrary complex s .

We say such a character and the corresponding series is *principal* if $\chi(k) = 1$ for all k relatively prime to d . For all other characters $\sum_{k=1}^{d-1} \chi(k) = 0$, and we shall say the character is *balanced*. We say the character and series are *primitive* if it is not induced by character for a proper divisor of d . We will be particularly interested in cases when $d = P, 4P$ or $8P$, where P is a *product* of distinct odd primes, since only such d admit primitive characters.

It transpires [10, 14, 12] that a unique *primitive* series exists for 1 and each odd prime p , such as $L_{-3}, L_{+5}, L_{-7}, L_{-11}, L_{+13}, \dots$, with the sign determined by the remainder modulo 4, and at 4 and four times primes, while two occur at $8p$, e.g., $L_{\pm 24}$. We then obtain primitive sums for products of distinct odd primes P or $4P$, and again two at $8P$. That is, e.g., $L_{-4}, L_{+12}, L_{-20}, L_{+60}, L_{-84}$. In the primitive cases, $\chi_{\pm d}(n) := \left(\frac{\pm d}{n}\right)$, where $\left(\frac{\pm d}{n}\right)$ the generalized *Legendre-Jacobi symbol*.

Thence, L_{-2} is an example of an *imprimitive* series, in that it is reducible [26, §27.8] to L_1 via the relation $\eta(s) = \sum_{n=1}^{\infty} (-1)^{n-1}/n^s = (1 - 2^{1-s})\zeta(s)$. Note the imprimitive series $L_{+6}(s) = \sum_{n>0} (1/(6n+1)^s + 1/(6n+5)^s)$ has all positive coefficients, while $L_{-6}(s) = \sum_{n>0} (1/(6n+1)^s - 1/(6n+5)^s) = (1 - 1/2^s)L_{-3}(s)$ is imprimitive but balanced, as is $L_{-12}(s) = \sum_{n>0} (1/(12n+1)^s + 1/(12n+5)^s - 1/(12n+7)^s - 1/(12n+11)^s)$, which, being non-principal, has $\sum_{k=1}^{11} \chi_{-12}(k) = 0$.

Recall that the sign determines that $\chi_{\pm d}(d-1) = \pm 1$. For example, $\chi_{+5}(n) = 1$ for $n = 1, 4$, and $\chi_{+5}(n) = -1$ for $n = 2, 3$.

Remark 1 (An integral representation of the Hurwitz zeta function). A useful integral formula [26, (25.11.27)] is

$$\zeta(s, a) = \frac{a^{1-s}}{s-1} + \frac{1}{2}a^{-s} + \frac{1}{\Gamma(s)} \int_0^{\infty} \left(\frac{1}{e^x - 1} - \frac{1}{x} + \frac{1}{2} \right) \frac{x^{s-1}}{e^{ax}} dx, \quad (13)$$

valid for $\text{Re } s > -1, s \neq 1, \text{Re } a > 0$; an extension for $\text{Re } s > -(2n+1), s \neq 1, \text{Re } a > 0$ is given in [26, (25.11.28)]. From (13) we adduce for $d \geq 3$ that

$$\begin{aligned} L_{\pm d}(s) := & \frac{1}{d} \sum_{k=1}^{d-1} \chi_{\pm d}(k) \frac{k^{1-s} - 1}{s-1} + \frac{1}{2} \sum_{k=1}^{d-1} \frac{\chi_{\pm d}(k)}{k^s} \\ & + \int_0^{\infty} \left(\frac{x^{s-1}}{\Gamma(s)} \right) \left(\frac{1}{e^{dx} - 1} - \frac{1}{dx} + \frac{1}{2} \right) \sum_{k=1}^{d-1} \frac{\chi_{\pm d}(k)}{e^{kx}} dx. \end{aligned} \quad (14)$$

For the case L_{-3} we have

$$L_{-3}(s) = \frac{2^{1-s} - 1}{3(1-s)} + \frac{1}{2} \left(1 - \frac{1}{2^s} \right) + \frac{2}{\Gamma(s)} \int_0^{\infty} x^{s-1} e^{-3x/2} \left(\frac{1}{e^{3x} - 1} - \frac{2}{3x} + \frac{1}{2} \right) \sinh \left(\frac{x}{2} \right) dx. \quad (15)$$

For L_{+5} this simplifies to

$$L_{+5}(s) = \frac{1 - 2^{1-s} - 3^{1-s} + 4^{1-s}}{5(s-1)} + \frac{(1 - 2^{-s} - 3^{-s} + 4^{-s})}{2} \quad (16)$$

$$+ \frac{2}{\Gamma(s)} \int_0^\infty x^{s-1} e^{-5x/2} \left(\frac{1}{e^{5x} - 1} - \frac{1}{5x} + \frac{1}{2} \right) \left(\cosh\left(\frac{3x}{2}\right) - \cosh\left(\frac{x}{2}\right) \right) dx.$$

For all non-principal characters, the first-term singularity in (13) at $s = 1$ is removable, leaving an analytic function and so (14) can be used to numerically compute or confirm values of $L_{\pm d}^{(m)}(1)$. Explicitly for $m \geq 1$,

$$L_{\pm d}^{(m)}(1) := \sum_{k=2}^{d-1} \chi_{\pm d}(k) (-\log k)^m \left(\frac{1}{2k} - \frac{\log k}{d(m+1)} \right) \quad (17)$$

$$+ \int_0^\infty \left(\frac{x^{s-1}}{\Gamma(s)} \right)_{s=1}^{(m)} \left(\frac{1}{e^{dx} - 1} - \frac{1}{dx} + \frac{1}{2} \right) \sum_{k=1}^{d-1} \frac{\chi_{\pm d}(k)}{e^{kx}} dx$$

valid at least for $\operatorname{Re} s > -1$. ◇

Recall also that for $d > 4$, as Dirichlet showed, the class number formula for imaginary quadratic fields, $-\frac{\mu_{-d}(1)}{d}$, is $h(-d)$.

Each such primitive L -series obeys a simple functional equation [1]:

$$L_{\pm d}(s) = C(s) \left\{ \begin{array}{l} \sin(s\pi/2) \\ \cos(s\pi/2) \end{array} \right\} L_{\pm d}(1-s), \quad C(s) := 2^s \pi^{s-1} d^{-s+1/2} \Gamma(1-s). \quad (18)$$

Indeed, this is true exactly for primitive series [1]. Moreover, the primitive series can be summed at various integer values:

$$L_{\pm d}(1-2m) = \begin{cases} (-1)^m R(2m-1)!/(2d)^{2m-1} \\ 0 \end{cases}$$

$$L_{\pm d}(-2m) = \begin{cases} 0 \\ (-1)^m R'(2m)!/(2d)^{2m} \end{cases} \quad (19)$$

$$L_{+d}(2m) = R d^{-1/2} \pi^{2m}, \quad L_{-d}(2m-1) = R' d^{-1/2} \pi^{2m-1},$$

where m is a positive integer and R, R' are rational numbers which depend on m, d . For $d = 1$ these engage the Bernoulli numbers, while for $d = -4$ the Euler numbers appear. The precise formulas for R and R' are given in [14, Appendix 1]. Also, famously,

$$L_{+p}(1) = 2 \frac{h(p)}{\sqrt{p}} \log \epsilon_0, \quad (20)$$

where $h(p)$ is the class number¹ of the quadratic form with discriminant p and ϵ_0 is the fundamental unit in the real quadratic field $Q(\sqrt{p})$.

¹See http://en.wikipedia.org/wiki/List_of_number_fields_with_class_number_one.

3.2 Character polylogarithms

We now introduce our *character polylogarithms*, namely,

$$L_{\pm d}(s; z) := \sum_{n=1}^{\infty} \binom{\pm d}{n} \frac{z^n}{n^s} \quad (21)$$

$$L_{\pm d}^{(m)}(s; z) := \frac{\partial^m}{\partial s^m} L_{\pm d}(s; z). \quad (22)$$

These are well defined for all characters, but of primary interest for primitive ones.

While such objects have been used before, most of the computational tools we provide appear to be new or previously inaccessible. In the sequel, the reader will lose very little if he or she assumes all characters are primitive.

3.3 Balanced character polylogarithms and Lerch's formula

As discussed further in Section 4.3 the following parametric version of (2) holds:

$$\sum_{n=0}^{\infty} \frac{z^{(n+\nu)}}{(n+\nu)^s} = \Gamma(1-s)(-\log z)^{s-1} + \sum_{r=0}^{\infty} \zeta(s-r, \nu) \frac{(\log z)^r}{r!}. \quad (23)$$

Here $\zeta(s, \nu)$ is again the *Hurwitz zeta* function, $s \neq 1, 2, 3, \dots$, $\nu \neq 0, -1, -2, \dots$, and, as before, $|\log z| < 2\pi$ (see [17, vol. 1, p.29, eqn. (8)]). Then (2) is the case $\nu = 1$. Using (23) it is possible to substantially extend (8).

We obtain

$$\sum_{n=0}^{\infty} \frac{z^{dn+k+\varepsilon}}{(dn+k+\varepsilon)^s} = \frac{1}{d} \Gamma(1-s)(-\log z)^{s-1} + \sum_{r=0}^{\infty} \zeta\left(s-r, \frac{k+\varepsilon}{d}\right) \frac{d^{r-s}(\log z)^r}{r!}. \quad (24)$$

From this we obtain, for $k = 1, 2, \dots, d-1$, $s \neq 1, 2, 3, \dots$, and $0 < \varepsilon < 1$, that

$$\sum_{n=1}^{\infty} \binom{\pm d}{n} \frac{z^{(n+\varepsilon)}}{(n+\varepsilon)^s} = \sum_{r=0}^{\infty} \left(\frac{1}{d^{s-r}} \sum_{k=1}^{d-1} \binom{\pm d}{k} \zeta\left(s-r, \frac{k+\varepsilon}{d}\right) \right) \frac{(\log z)^r}{r!}, \quad (25)$$

since for balanced characters $\sum_{m=1}^d \binom{\pm d}{m} = 0$ for $d > 2$ and so any term independent of m vanishes.

We then have a tractable formula for differentiation wrt the order. For $m = 0, 1, 2, \dots$, we can write

$$\begin{aligned} L_{\pm d}^{(m)}(s; z) &:= \sum_{n=1}^{\infty} \binom{\pm d}{n} \frac{(\log n)^m}{n^s} z^n \\ &= \sum_{r=0}^{\infty} \frac{\partial^m}{\partial s^m} \left(\frac{1}{d^{s-r}} \sum_{k=1}^{d-1} \binom{\pm d}{k} \zeta\left(s-r, \frac{k}{d}\right) \right) \frac{(\log z)^r}{r!} \end{aligned} \quad (26)$$

We can now derive the character counterpart to (8) namely:

Theorem 3 (Balanced L-series summations for character polylogarithms [5]). *For balanced $d = -2, -3, -4, +5, \dots$ and all s (since the poles at $s = 1, 2, \dots$ cancel) we have*

$$L_{\pm d}^{(m)}(s; z) = \sum_{r=0}^{\infty} L_{\pm d}^{(m)}(s-r) \frac{(\log z)^r}{r!} \quad (27)$$

when $|\log z| < 2\pi/d$.

Now, however, unlike the case for ζ , this is also applicable at $s = 1, 2, 3, \dots$. It also leads to two attractive Fourier series

$$\sum_{n=1}^{\infty} \chi_{\pm d}(n) \frac{\cos n\theta}{n^s} = \sum_{r=0}^{\infty} L_{\pm d}^{(m)}(s-2r) \frac{(-1)^r \theta^{2r}}{(2r)!} \quad (28a)$$

$$\sum_{n=1}^{\infty} \chi_{\pm d}(n) \frac{\sin n\theta}{n^s} = \sum_{r=0}^{\infty} L_{\pm d}^{(m)}(s-2r+1) \frac{(-1)^r \theta^{2r-1}}{(2r-1)!} \quad (28b)$$

when $|\theta| < 2\pi/d$.

3.4 L-series derivatives at negative integers

To employ (27) for non-negative integer order s , we are left with the job of computing $L_{\pm d}^{(m)}(-n)$ at negative integers. This can be achieved from the requisite functional equation in (18) by the methods of [2].

We begin for primitive $d = 1, 2, \dots$, with (18), which we rewrite as:

$$\sqrt{d} L_{\pm d}(1-s) = \Psi_{\pm d}(s) L_{\pm d}(s), \quad \Psi_{\pm d}(s) := \left(\frac{d}{2\pi}\right)^s \left\{ \begin{array}{l} 2 \operatorname{Re} e^{i\pi s/2} \\ 2 \operatorname{Im} e^{i\pi s/2} \end{array} \right\} \Gamma(s). \quad (29)$$

Then for real s and $\kappa_d := -\log \frac{2\pi}{d} + \frac{1}{2}\pi i$,

$$\sqrt{d} L_{+d}(1-s) = (\operatorname{Re} 2e^{s\kappa_d}) \Gamma(s) L_{+d}(s), \quad (30a)$$

$$\sqrt{d} L_{-d}(1-s) = (\operatorname{Im} 2e^{s\kappa_d}) \Gamma(s) L_{-d}(s). \quad (30b)$$

Two applications of Leibnitz' formula for n -fold differentiation with respect to s leads to the following:

Theorem 4 (L-series derivatives at negative integers [5]). *Let $L_{\pm d}$ be a primitive non-principal L-series. For all integers $n \geq 1$,*

$$L_{+d}^{(m)}(1-2n) = \frac{(-1)^{m+n} d^{2n-1/2}}{2^{2n-1} \pi^{2n}} \sum_{k=0}^m \binom{m}{k} \sum_{j=0}^k \binom{k}{j} (\operatorname{Re} \kappa_d^j) \Gamma^{(k-j)}(2n) L_{+d}^{(m-k)}(2n) \quad (31a)$$

$$L_{+d}^{(m)}(2-2n) = \frac{(-1)^{m+n} d^{2n-3/2}}{2^{2n-2} \pi^{2n-1}} \sum_{k=0}^m \binom{m}{k} \sum_{j=0}^k \binom{k}{j} (\operatorname{Im} \kappa_d^j) \Gamma^{(k-j)}(2n-1) L_{+d}^{(m-k)}(2n-1) \quad (31b)$$

and

$$L_{-d}^{(m)}(1-2n) = \frac{(-1)^{m+n} d^{2n-1/2}}{2^{2n-1} \pi^{2n}} \sum_{k=0}^m \binom{m}{k} \sum_{j=0}^k \binom{k}{j} (\operatorname{Im} \kappa_d^j) \Gamma^{(k-j)}(2n) L_{-d}^{(m-k)}(2n) \quad (31c)$$

$$L_{-d}^{(m)}(2-2n) = \frac{(-1)^{m+n+1} d^{2n-3/2}}{2^{2n-2} \pi^{2n-1}} \sum_{k=0}^m \binom{m}{k} \sum_{j=0}^k \binom{k}{j} (\operatorname{Re} \kappa_d^j) \Gamma^{(k-j)}(2n-1) L_{-d}^{(m-k)}(2n-1), \quad (31d)$$

where $\kappa_d = -\log \frac{2\pi}{d} + \frac{1}{2}\pi i$.

Since j is a positive integer, $\operatorname{Re} \kappa_d^j$ and $\operatorname{Im} \kappa_d^j$ can be fully expanded. From the prior result and the known asymptotics, $\Gamma^{(m)}(n) \approx \log^m(n) \Gamma(n)$, one may deduce:

Corollary 1 (L-series derivative asymptotics). *Let $L_{\pm d}$ be a primitive non-principal L-series. For all integers $m \geq 0$, as $n \rightarrow +\infty$ we have*

$$\frac{L_{+d}^{(m)}(1-2n)}{(2n-1)!} \approx 2 \frac{(-1)^{m+n} d^{2n-1/2}}{(2\pi)^{2n}} \operatorname{Re} \left(\frac{\pi i}{2} + \log \left(\frac{(2n)d}{2\pi} \right) \right)^m \quad (32a)$$

$$\frac{L_{+d}^{(m)}(2-2n)}{(2n-2)!} \approx 2 \frac{(-1)^{m+n} d^{2n-3/2}}{(2\pi)^{2n-1}} \operatorname{Im} \left(\frac{\pi i}{2} + \log \left(\frac{(2n-1)d}{2\pi} \right) \right)^m \quad (32b)$$

and

$$\frac{L_{-d}^{(m)}(1-2n)}{(2n-1)!} \approx 2 \frac{(-1)^{m+n} d^{2n-1/2}}{(2\pi)^{2n}} \operatorname{Im} \left(\frac{\pi i}{2} + \log \left(\frac{(2n)d}{2\pi} \right) \right)^m \quad (32c)$$

$$\frac{L_{-d}^{(m)}(2-2n)}{(2n-2)!} \approx 2 \frac{(-1)^{m+n+1} d^{2n-3/2}}{(2\pi)^{2n-1}} \operatorname{Re} \left(\frac{\pi i}{2} + \log \left(\frac{(2n-1)d}{2\pi} \right) \right)^m. \quad (32d)$$

One may, if one wishes, use Stirling's approximation to remove the factorial. For modest n this asymptotic allows an excellent estimate of the size of derivative. For instance,

$$\frac{L_5^{(3)}(-98)}{98!} = -1.157053952 \cdot 10^{-8} \dots$$

while the asymptotic gives $-1.159214401 \cdot 10^{-8} \dots$. Similarly

$$\frac{L_{-3}^{(5)}(-38)}{38!} = 1.078874094 \cdot 10^{-10} \dots,$$

while the asymptotic gives $-1.092285447 \cdot 10^{-8} \dots$. These are the type of terms we need to compute below.

We note that taking n -th roots on each side of the asymptotics in Corollary 1 shows that the radius of convergence in Theorem 3 is as given. We also observe that $\left(\frac{\pi^2}{4} + \log^2\left(\frac{nd}{\pi}\right)\right)^{m/2}$ provides a useful upper bound for each real and imaginary part in Corollary 1. For example,

$$\sqrt{\left(\frac{\mathbf{L}_{-d}^{(m)}(1-2n)}{(2n-1)!}\right)^2 + \left(\frac{\mathbf{L}_{+d}^{(m)}(1-2n)}{(2n-1)!}\right)^2} \approx \frac{2}{\sqrt{d}} \left(\frac{\pi^2}{4} + \log^2\left(\frac{nd}{\pi}\right)\right)^{m/2} \left(\frac{d}{2\pi}\right)^{2n}.$$

In Sections 5 of this paper we detail convergent series methods for the incomplete Gamma function, and consequently in Section 6 for the Hurwitz zeta functions. To do so, we first must reprise a section from the manuscript [16] of Richard Crandall, which provides the basic methods for the Lerch transcendent. Crandall's manuscript appears in the collection [16] from Crandall's now defunct *Perfectly Scientific Inc. Press*, but is consequently very hard to find.

4 Representations of the Lerch transcendent

It turns out that all of special functions listed above can be cast in terms of just one of them, namely the Lerch transcendent, whose classical definition is (later we shall employ a modified transcendent we call Φ):

$$\Phi(z, s, a) := \sum_{n=0}^{\infty} \frac{z^n}{(n+a)^s}, \quad (33)$$

where under the constraints

$$|z| \leq 1, \quad a \notin \{0, -1, -2, \dots\}, \quad \operatorname{Re}(s) > 1, \quad (34)$$

Φ is absolutely convergent as a direct sum. Analytic continuation will eventually serve to relax constraints, but for the moment we shall stick to the absolute-convergence scenario.

The simplest instance of Lerch evaluation is the elementary sum

$$\Phi(z, 0, a) = \frac{1}{1-z}, \quad (35)$$

which when coupled with the formal relation

$$\Phi(z, s-1, a) = \left(a + z \frac{\partial}{\partial z}\right) \Phi(z, s, a) \quad (36)$$

yields all Lerch values at negative integer s as rational functions of z . However, for $z = 1$ the analytic continuation to nonpositive integer s simply gives a polynomial in the parameter a —that is, the operations of continuation and $z \rightarrow 1$ do not necessarily commute (see the discussion after relation (41)).

Another simple observation is that since the entire real line is a disjoint union of integer translates of the right-closed interval $(0, 1]$, $\operatorname{Re}(a)$ in (33) can always be relegated to said interval, as follows. One observes the elementary *translation property* for fixed positive integer m :

$$\Phi(z, s, a) = z^m \Phi(z, s, a + m) + \sum_{k=0}^{m-1} \frac{z^k}{(k+a)^s}. \quad (37)$$

Now a choice $m := \lceil \operatorname{Re}(a) \rceil - 1$ allows us instead to evaluate $\Phi(z, s, \bar{a})$ for some \bar{a} having $\operatorname{Re}(\bar{a}) \in (0, 1]$.

Various other simple but useful relations include the *doubling formula*

$$\Phi(z, s, a) = \frac{1}{2^s} \Phi\left(z^2, s, \frac{a}{2}\right) + \frac{z}{2^s} \Phi\left(z^2, s, \frac{1+a}{2}\right),$$

obtained by using even/odd indices in the sum (33). This in turn implies

$$\Phi(z, s, a) - \Phi(-z, s, a) = \frac{z}{2^s} \Phi\left(z^2, s, \frac{a+1}{2}\right), \quad (38)$$

a form of doubling relation that is actually quite useful for certain computations (see [16]).

Not so simple is the general *functional relation* discovered by Lerch [24, 22, 23]:

$$\frac{(2\pi)^s z^a}{\Gamma(s)} \Phi(z, 1-s, a) = e^{\frac{i\pi s}{2}} \Phi\left(e^{-2ia\pi}, s, \frac{\log z}{2\pi i}\right) + e^{2i\pi a - \frac{i\pi s}{2}} \Phi\left(e^{2ia\pi}, s, 1 - \frac{\log z}{2\pi i}\right), \quad (39)$$

valid over a wide range of complex parameters.

Remark 2. Reference [22] has an interesting development of alternative functional relations involving combinations of Lerch-like functions. For our present purposes, the primary advantage of this functional relation is in checking numerical schemes. Indeed, even though one may not know a closed form for say $\Phi(1, 5, 1/3)$, still the relation (39) should read $3.866 \dots + 1025.9 \dots i$ on both sides. In this way, a profound and beautiful theoretical result can be used in computations, to ensure self-consistency. \diamond

Conversely, one of our methods—the Riemann-splitting Algorithm 3—implies by way of its very development the above functional relation (39).

4.1 Bernoulli-series representation of Lerch Φ

Under the stated constraints (34), one has a valid integral representation:

$$\Phi(z, s, a) = \frac{1}{\Gamma(s)} \int_0^\infty \frac{t^{s-1} e^{-at}}{1 - ze^{-t}} dt, \quad (40)$$

for $\operatorname{Re}(a) > 0$. Our scheme is based on the observation that this integral can be cast in various, manifestly convergent, dual-series forms; moreover, a delicate branching chain based on parameter regions chooses the ideal series form, thereby providing essentially invariant convergence rate across the various functions in the introduction—again, assuming bounded parameters.

We cite two important, classical expansions, both absolutely convergent under the given criteria on t :

$$\begin{aligned}\frac{e^{xt}}{e^t - 1} &= \sum_{n \geq 0} B_n(x) \frac{t^{n-1}}{n!} \quad ; \quad |t| < 2\pi \\ \frac{2e^{xt}}{e^t + 1} &= \sum_{n \geq 0} E_n(x) \frac{t^n}{n!} \quad ; \quad |t| < \pi,\end{aligned}$$

where B_n, E_n are the Bernoulli, Euler polynomials, respectively. Incidentally the different criteria on $|t|$ here can be thought of in the following way: The Bernoulli-number series is essentially an expansion of $\operatorname{cosech}(t/2)$, while the Euler-number series is for $\operatorname{sech}(t/2)$. In the complex plane, the former has poles at $t = \pm 2m\pi$, while the latter has poles at $t = \pm m\pi$, and these poles constrain the radii of convergence.

To obtain what we call a Bernoulli master representation, we split the integral in (40) as $\int_0^\infty \rightarrow \int_0^\lambda + \int_\lambda^\infty$, where λ denotes a free parameter. Furthermore we invoke either Bernoulli- or Euler-polynomial expansions depending on the real part of the Lerch parameter z . This integral-splitting leads formally to such series as the following, where we assume $\operatorname{Re}(z) \in (1/2, 1]$, say:

$$\Phi(z, s, a) = \frac{1}{\Gamma(s)} \sum_{n=0}^{\infty} \frac{\Gamma(s, \lambda(n+a)) z^n}{(n+a)^s} + \frac{z^{-a}}{\Gamma(s)} \sum_{m=0}^{\infty} \frac{B_m(1-a)}{m!} \int_0^\lambda t^{s-1} (t - \log z)^{m-1} dt. \tag{41}$$

A similar construction involving Euler polynomials is straightforward, and applies best to say $\operatorname{Re}(z) \in [-1, -1/2)$. In this way a complete computational algorithm can be created for z on the closed unit disk. We exhibit this procedure as Algorithm 1.

Note that in the case of negative $\operatorname{Re}(z)$, the C_m in Algorithm 1 are all terminating hypergeometric functions, so evaluations for such as z negative real are especially easy to implement. Note also that when $z = 1$ and $s = -m = 0, -1, -2, \dots$, the first sum in (41) vanishes and the second has a cancelled Gamma-singularity, giving a closed-form analytic-continuation result

$$\Phi(1, -m, a) = -\frac{B_{m+1}(a)}{m+1},$$

said value being a Hurwitz ζ evaluation $\zeta(-m, a)$.

Algorithm 1 (Bernoulli-series algorithm for Lerch transcendent ϕ). *This algorithm computes the classical Lerch transcendent $\Phi(z, s, a)$ for z on the complex unit disk, $|z| \leq 1$, and real $a \in (0, 1]$.*

1) If $(|z| \leq 1/2)$ use parameter $\lambda := 0$, i.e. return the direct sum (33) which will be linearly convergent.

2) If $(s = -m \in (0, -1, -2, -3, \dots))$
 if $(z = 1)$ return

$$-\frac{B_{m+1}(a)}{m+1};$$

else return the rational function of z determined by (35, 36);

3) If $(\text{Re}(z) \geq 0)$ $p := -\log z$; else $p := -\log(-z)$;

4) $\lambda := 1 - p$;

5) Define coefficients C_m as follows:

If $(\text{Re}(z) \geq 0)$ {
 if $(z \neq 1 + 0i)$

$$C_m := B_m(1-a) \frac{\lambda^s p^{m-1}}{s} {}_2F_1 \left(-m+1, s; s+1; -\frac{\lambda}{p} \right);$$

else

$$C_m := B_m(1-a) \frac{\lambda^{m-1+s}}{m-1+s};$$

} else {

if $(z \neq -1 + 0i)$

$$C_m := \frac{1}{2} E_m(1-a) \frac{\lambda^s p^m}{s} {}_2F_1 \left(-m, s; s+1; -\frac{\lambda}{p} \right);$$

else

$$C_m := \frac{1}{2} E_m(1-a) \frac{\lambda^{m+s}}{m+s};$$

}

5) return Φ as

$$\frac{1}{\Gamma(s)} \sum_{n=0}^{\infty} \frac{\Gamma(s, \lambda n) z^n}{(n+a)^s} + \frac{e^{ap}}{\Gamma(s)} \sum_{m=0}^{\infty} C_m.$$

This concludes the algorithm.

□

4.2 Bernoulli multisectioning

In Algorithm 1 and various consequent algorithms, we require perhaps a great many Bernoulli numbers. Realizing that $B_1 = -1/2$ but the rest of B_{odd} vanish, we can contemplate the power series

$$\frac{x^2}{\cosh x - 1} = -2 + \sum_{n \geq 0} \frac{2n-1}{(2n)!} B_{2n} x^{2n}$$

as an expedient for extracting Bernoulli numbers, or, even more stably, the numbers $B_{2n}/(2n)!$, to required precision. One simply takes enough power-series terms of cosh and performs Newton inversion of that finite cosh series.

Remark 3 (Further “multisectioning”). A technique pioneered by J. Buhler for the Bernoulli numbers (see the original treatise [15], which by now has been followed by several enhancement papers and theses)—can reduce memory. In the more advanced setting, one calculates say all B_k with $k \bmod 8$ fixed, and does this separately for 4 values of k . The multisectioning technique is also discussed in the guise of “value recycling” in the calculation of large sets of $\zeta(2n)$ values [11], which values being required for many “rational zeta series.” \diamond

4.3 Erdélyi-series representation for Lerch Φ

In [18], expanding those given above for the polylogarithms and Hurwitz zeta, we find:

$$z^a \Phi(z, s, a) = \sum_{n \geq 0} \zeta(s - n, a) \frac{\log^n z}{n!} + \Gamma(1 - s)(-\log z)^{s-1}, \quad (42)$$

where appears the Hurwitz zeta function, itself an instance of Lerch, with direct sum (when convergent): $\zeta(s, a) := \sum_{k \geq 0} \frac{1}{(k+a)^s} = \Phi(1, s, a)$.

When s is a positive integer, adjustments must be made, being as the Erdélyi expansion’s Γ singularity is neatly cancelled by one of the Hurwitz- ζ summands. We have need for the *incomplete Gamma function* given by

$$\Gamma(s, z) := \int_z^\infty t^{s-1} e^{-t} dt, \quad (43)$$

and its analytic continuations [26, §8]. When s is not a positive integer, and for parameter $a \in (0, 1]$, $|\log z| < 2\pi$, one has a linearly convergent Erdélyi expansion. An overall procedure for applying this Erdélyi form is as follows:

Algorithm 2 (Erdélyi-series algorithm for Lerch transcendent Φ). *This algorithm computes the classical Lerch transcendent $\Phi(z, s, a)$ for any complex s , with $a \in (0, 1]$, and any complex z in the region $|\log z| < 2\pi$ (which z -region certainly contains the annulus $|z| \in (e^{-2\pi}, 1]$).*

- 1) If ($|z| \leq 1/2$) return the direct sum (33) which will be linearly convergent.
- 2) If ($s = -m \in (0, -1, -2, -3, \dots)$)
if ($z = 1$) return

$$-\frac{B_{m+1}(a)}{m+1},$$

else return the rational function of z determined by (35, 36);

3) If (s is not a positive integer) return Φ as

$$z^{-a} \left(\sum_{n \geq 0} \zeta(s-n, a) \frac{\log^n z}{n!} + \Gamma(1-s)(-\log z)^{s-1} \right).$$

4) Here, denote $s = k + 1$ for integer $k \geq 0$ and return Φ as

$$z^{-a} \left(\sum_{0 \leq n \neq k} \zeta(k+1-n, a) \frac{\log^n z}{n!} + \frac{\log^k z}{k!} \left(\psi^{(0)}(1+k) - \psi^{(0)}(a) - \log(-\log z) \right) \right),$$

where $\psi^{(0)}$ is the standard digamma function.

This concludes the algorithm. □

4.4 Riemann-splitting representation for Lerch variant $\bar{\Phi}$

It turns out that one can forge a “master equation” for computation of the analytic continuation of a certain Lerch variant, call it $\bar{\Phi}$:

$$\bar{\Phi}(z, s, a) := \sum_{n=0}^{\infty'} \frac{z^n}{((n+a)^2)^{s/2}}, \quad (44)$$

where $'$ on the sum indicates any denominator singularity is avoided. For $\text{Re}(a) > 0$ this form $\bar{\Phi}$ is equivalent to the classical definition (33) for Φ .

Our purpose in employing the square-then-half-power paradigm here is to allow transformation of integral representations such as this generalization of Riemann’s ζ -function decomposition:

$$\sum_{n \in \mathbb{Z}} \frac{z^n}{((n+a)^2)^{s/2}} = \frac{1}{\Gamma(s/2)} \int_0^\infty t^{s/2-1} \sum_{n \in \mathbb{Z}} z^n e^{-(n+a)^2 t} dt. \quad (45)$$

The celebrated *Riemann prescription* is to split such an integral via $\int_0^\infty \rightarrow \int_0^\lambda + \int_\lambda^\infty$, then apply theta-function identities (see also [10, §3.5]) in the integrand’s sum, eventually to yield a rapidly converging series with free parameter λ .

But how do we deal with the issue that $\bar{\Phi}$ is asking for a sum over nonnegative integer n , not $n \in \mathbb{Z}$? One way is to use the following “magical” expedient—a phenomenon discovered by Crandall at the start of this work in the late 1980s.² The idea is, a sum over integers on a specific half-line can be written

$$\sum_{S(n+a) > 0} f(n) = \frac{1}{2} \sum_{n \in \mathbb{Z}} f(n) + \frac{1}{2} \sum_{n \in \mathbb{Z}} f(n) S(n+a),$$

²It may well be that this expedient exists elsewhere in the literature; at any rate, this one simple trick opens up a whole world of computational analyticity.

where we define

$$S(z) := \text{sign}(\text{Re}(z))$$

with $\text{sign}(0) := 0$. Now, the key is that, for the sake of Riemann-splitting, we can write simply (for nonzero complex ρ): $S(\rho) = \frac{\rho}{(\rho^2)^{1/2}}$, and this allows the evaluation of the $\bar{\Phi}$ sum via *two* Riemann integrals.

Just as Riemann's original incomplete-Gamma series for ζ is one way to establish the functional equation, so, too, is the current method for $\bar{\Phi}$; that is, we not only get a computational algorithm following, or we can prove such as (39). We omit the tedious details, opting instead to display the incomplete-Gamma series in the next algorithm.

Algorithm 3 (Riemann-splitting algorithm for $\bar{\Phi}$ and its analytic continuation). *This algorithm computes $\bar{\Phi}(z, s, a)$ —being for a wide class of parameters equivalent to the classical Φ —for any complex s , any complex z , and a in the complex region $\{\text{Re}(z) \in [0, 1)\} \cup \{z = 1 + 0i\}$ (the translation relation (37) can be used for other a).*

- 1) If $(z = 0)$ return $1/a^s$; Optionally: If $(|z| \leq 1/2)$ return the direct sum (44) which will be linearly convergent.
- 2) If $(s = -m \in (0, -1, -2, -3, \dots))$
if $(z = 1)$ return

$$-\frac{B_{m+1}(a)}{m+1};$$

else return the rational function of z determined by (35, 36);

- 3) Choose a parameter λ , say $\lambda := \pi$ (but see the important discussion about the possibility of complex λ in [16] and below);
- 4) Return the analytic continuation of $\bar{\Phi}$ as:

$$\begin{aligned} \bar{\Phi}(z, s, a) &= -\frac{z^{-a}\lambda^{s/2}}{s\Gamma(s/2)}\delta_{a \in Z} + \frac{1}{s-1} \frac{\pi^{1/2}\lambda^{(s-1)/2}}{\Gamma(s/2)}\delta_{z=1} + \\ &\frac{1}{2} \sum'_{n \in Z} \frac{z^n}{(A^2)^{s/2}} \left(\frac{\Gamma(s/2, \lambda A^2)}{\Gamma(s/2)} + \frac{\Gamma((s+1)/2, \lambda A^2)}{\Gamma((s+1)/2)} S(A) \right) + \\ &\frac{\pi^{s-1/2}}{2z^a} \sum'_{u \in Z} \frac{e^{-2\pi i a u}}{(U^2)^{(1-s)/2}} \left(\frac{\Gamma\left((1-s)/2, \frac{\pi^2}{\lambda} U^2\right)}{\Gamma(s/2)} + i \frac{\Gamma\left(1-s/2, \frac{\pi^2}{\lambda} U^2\right)}{\Gamma((s+1)/2)} S(U) \right), \end{aligned} \quad (46)$$

where in the first summation, $A := n + a$ and in the second summation $U := u + \frac{\log z}{2\pi i}$.

This concludes the algorithm. □

As we shall see, for special cases of $\bar{\Phi}$, such as polylogarithms and zeta variants, the above incomplete-Gamma decomposition can be significantly simplified. We turn to discussion of the computation of the incomplete Gamma function as is required in Algorithm 3 and so in the sequel for Dirichlet L-series.

5 The incomplete Gamma function

We defer to [9, 19, 26] for basic information on the *incomplete Gamma function*, which is given, for appropriate line integrals, by

$$\Gamma(s, z) := \int_z^\infty t^{s-1} e^{-t} dt \quad (47)$$

and its analytic continuations, so that $\Gamma(s, 0) = \Gamma(s)$; see [26, Chapter 8]. As an aside, by [26, Eqn. (8.7.3)] we have

$$\frac{\Gamma(s, z)}{z^s} = \frac{\Gamma(s)}{z^s} - \sum_{j=0}^{\infty} \frac{(-1)^j z^j}{j!(s+j)}, \quad (48)$$

which can easily be symbolically differentiated with respect to s , using methods described in [6] for the derivation of $\Gamma(s)$.

Alternatively, we may apply the following result from Henrici [20]. Let $(\alpha)_n = \Gamma(\alpha + n)/\Gamma(\alpha)$, with $(\alpha)_0 = 1$, denote the rising factorial, and let $\beta(a, b) = \Gamma(a)\Gamma(b)/\Gamma(a+b)$. Define the generalized *Laguerre polynomial*, for $n = 0, 1, 2, \dots$, by

$$L_n^{(\alpha)}(-z) = \sum_{k=0}^n \frac{(\alpha + k)_k}{(n-k)! k!} z^k = \frac{(\alpha + 1)_n}{n!} {}_1F_1\left(\begin{matrix} -n \\ \alpha + 1 \end{matrix}; -z\right) \quad (49)$$

(see [26, (18.5.12)]).

Theorem 5 (Henrici's formula for the incomplete Gamma function). *The following formula holds away from all complex (z, s) from the zeroes of the Laguerre polynomials:*

$$\Gamma(s, z) = z^s e^{-z} \sum_{n=0}^{\infty} \frac{(1-s)_n}{(n+1)!} \frac{1}{L_{n+1}^{(-s)}(-z) L_n^{(-s)}(-z)} \quad (50)$$

$$= z^s e^{-z} \sum_{n=0}^{\infty} \frac{\beta(1-s, n+1)}{{}_1F_1(-n; 1-s; -z) {}_1F_1(-n-1; 1-s; -z)}. \quad (51)$$

In Theorem 5, we use $L_0^{(\alpha)}(-z) = 1$, $L_1^{(\alpha)}(-z) = 1 + \alpha + z$, while

$$L_n^{(\alpha)}(-z) = \frac{(z + \alpha + 2n - 1)}{n} L_{n-1}^{(\alpha)}(-z) - \frac{(\alpha + n - 1)}{n} L_{n-2}^{(\alpha)}(-z),$$

so we can write

$$L_n^{(-\alpha)}(-z) = \sum_{k=0}^n \binom{n-\alpha}{n-k} \frac{z^k}{k!}. \quad (52)$$

Thus, equation (50) is valid away from Laguerre polynomial zeros of the denominator. It is also worth recording

$$\Gamma(a, x) = x^a e^{-x} \sum_{n=0}^{\infty} \frac{L_n^{(a)}(x)}{n+1},$$

from [26, (8.7.6)], valid for $x > 0$ which while less useful computationally is an interesting partner to (50).

Remark 4 (Symbolic differentiation of $\Gamma(s, z)$ wrt to s). For $m = 1, 2, \dots$

$$\frac{\partial^m}{\partial s^m} L_n^{(s)}(x) = \sum_{k=0}^{n-1} \frac{\partial^{m-1}}{\partial s^{m-1}} \frac{L_k^{(s)}(x)}{k-n},$$

and for $|z| < 1$ we have [26, (18.12.13)] the ordinary generating function

$$(1-z)^{-\alpha-1} \exp\left(\frac{xz}{z-1}\right) = \sum_{n=0}^{\infty} L_n^{(\alpha)}(x) z^n, \quad (53)$$

so that

$$\sum_{n=0}^{\infty} \frac{\partial^m}{\partial \alpha^m} L_n^{(\alpha)}(x) z^n = (-\log(1-z))^m \sum_{n=0}^{\infty} L_n^{(\alpha)}(x) z^n. \quad (54)$$

From this we obtain a closed form

$$\frac{\partial^m}{\partial \alpha^m} L_n^{(\alpha)}(x) = \sum_{k=0}^m h_k L_{n-k}^{(\alpha)}(x), \quad (55)$$

where $h_k := \sum_{k=n_1 > n_2 > \dots > n_k > 0} \frac{1}{n_1 n_2 \dots n_k}$. Correspondingly, the derivative of the rising factorial is easily seen to be $(1-s)_n' = (\Psi(1-s) - \Psi(1+n-s))(1-s)_n$ so that

$$(1-s)_n^{(m)} = (-1)^m \sum_{k=0}^{m-1} \binom{m-1}{k} (\Psi^{(k)}(1+n-s) - \Psi^{(k)}(1-s))(1-s)_n^{(m-1-k)}. \quad (56)$$

Explicitly, in terms of *Stirling numbers of the first kind*, the derivatives are polynomials:

$$(x)_n^{(m)} = \sum_{k=0}^n (-1)^{n-k} s_1(n, k) (k-m+1)_m x^{k-m}. \quad (57)$$

Thence, using (57) and, say, (55) we see that (50) can be symbolically differentiated repeatedly with respect to s . When $s = -m$ is a negative integer, a little more care is needed to obtain the result. \diamond

In [9] effective symbolically computable sub-exponential error bounds valid for all complex z, s with z not negative and real, are give for $L_n^{(\alpha)}(-z)$. For example, with $s = 3/2, z = 100$, (50) summed to 500 terms give 391 digits agreement, and for $s = 3/2, z = 300$, (50) summed to 50 terms give 258 digits agreement (a similar relative error bound obtains). In addition, for fixed (α, z) we have the sub-exponential estimate:

$$L_{n+1}^{(-\alpha)}(-z) \sim \frac{e^{-z/2}}{2\sqrt{\pi}} \frac{e^{2\sqrt{nz}}}{z^{1/4-\alpha/2} n^{1/4+\alpha/2}} \left(1 + O\left(\frac{1}{n^{1/2}}\right)\right). \quad (58)$$

When $s = n$ is a positive integer then

$$\Gamma(n+1, z) = n! e^{-z} \sum_{k=0}^n \frac{z^k}{k!}, \quad (59)$$

giving the promised elementary closed form [26, (8.48)] and a fine computational check for (50) which is terminating in this case.

For fixed a and large z we recall the classical asymptotic expansion [26, (8.11.2)]:

$$\Gamma(a, z) = z^{a-1} e^{-z} \left(\sum_{k=0}^{n-1} \frac{(1-a)_k}{(-z)^k} + R_n(a, z) \right), \quad (60)$$

where $R_n(a, z) = O(z^{-n})$ for $|\arg z| < 3\pi/2 - \delta$.

6 The Hurwitz zeta function

First note that the *Bernoulli polynomials* can be expanded, see [26, §24], as follows:

$$B_{2m}(a) = (-1)^{m+1} \frac{2(2m)!}{(2\pi)^{2n}} \sum_{k=1}^{\infty} \frac{\cos(2\pi ka)}{k^{2m}}, \quad (61)$$

for $m \geq 1$, while for $m \geq 0$,

$$B_{2m+1}(a) = (-1)^{m+1} \frac{2(2m+1)!}{(2\pi)^{2m+1}} \sum_{k=1}^{\infty} \frac{\sin(2\pi ka)}{k^{2m+1}}. \quad (62)$$

Following [16] and Section 4.1, we can now present a formula for the Hurwitz zeta, based on the incomplete Gamma function (48):

Theorem 6 (Hurwitz zeta in terms of the incomplete Gamma function). *For $0 < a < 1, s > 1$ and free variable $0 < \lambda < 2\pi$, we can neatly write the Hurwitz zeta function of Section 3.1 as*

$$\Gamma(s) \zeta(s, a) = \sum_{n=0}^{\infty} \frac{\Gamma(s, \lambda(n+a))}{(n+a)^s} + \sum_{m=0}^{\infty} (-1)^m \frac{B_m(a) \lambda^{m+s-1}}{m! (m+s-1)}. \quad (63)$$

An even faster-converging formula can be derived by specializing and manipulating a formula of Crandall's [16, Alg. 3] for the *Lerch transcendent*:

Theorem 7 (Faster-converging formula for the Hurwitz zeta). *Let the notation $\sigma(x)$ denote $\text{sign}(x)$. Then for $0 < a < 1$ and λ a free variable in $(0, 2\pi)$ ($\lambda = \pi$ is an equitable choice), and for $s \neq 0, -1, -2, \dots$, we have*

$$\begin{aligned} \zeta(s, a) &= \frac{\sqrt{\pi} \lambda^{(s-1)/2}}{(s-1)\Gamma(s/2)} + \frac{1}{2} \sum_{n=-\infty}^{\infty} \left(\frac{\Gamma(\frac{s}{2}, \lambda(n+a)^2)}{\Gamma(s/2)} + \sigma(n+a) \frac{\Gamma(\frac{s+1}{2}, \lambda(n+a)^2)}{\Gamma((s+1)/2)} \right) \frac{1}{|n+a|^s} \\ &+ \pi^{s-1/2} \sum_{m=1}^{\infty} \frac{1}{m^{1-s}} \left(\frac{\Gamma(\frac{1-s}{2}, \frac{m^2 \pi^2}{\lambda})}{\Gamma(s/2)} \cos(2\pi m a) + \frac{\Gamma(1-\frac{s}{2}, \frac{m^2 \pi^2}{\lambda})}{\Gamma((s+1)/2)} \sin(2\pi m a) \right). \end{aligned} \quad (64)$$

Note that each sum decays exponentially, grace of (60). This is very efficient: summing to 30 terms with $\lambda = \pi$ yields 1000 digits of $\zeta(4, 2/3)$ or $\zeta(2, 2/3)$.

In a similar vein, by using (11) we may obtain explicit formulas for balanced $L_{\pm d}(s)$, which remove the singularity at $s = 1$.

Theorem 8 (Non-principal real L-series computation). *Let the notation $\sigma_{n,k}(d)$ denote $\text{sign}(n|d| + k)$. Then*

$$\begin{aligned} L_{\pm d}(s) &= \frac{1}{2} \sum_{n=-\infty}^{\infty} \sum_{k=1}^{|d|-1} \frac{\binom{\pm d}{k}}{|n|d| + k|^s} \left\{ \frac{\Gamma\left(\frac{s}{2}, \pi\left(n + \frac{k}{|d|}\right)^2\right)}{\Gamma\left(\frac{s}{2}\right)} + \sigma_{n,k}(d) \frac{\Gamma\left(\frac{s+1}{2}, \pi\left(n + \frac{k}{|d|}\right)^2\right)}{\Gamma\left(\frac{s+1}{2}\right)} \right\} \\ &+ \frac{1}{\sqrt{\pi}} \left(\frac{\pi}{|d|}\right)^s \sum_{m=1}^{\infty} \frac{\Gamma\left(\frac{2-s}{2}, \pi m^2\right)}{m^{1-s} \Gamma\left(\frac{s+1}{2}\right)} \sum_{k=1}^{|d|-1} \binom{\pm d}{k} \sin\left(\frac{2\pi km}{|d|}\right) \end{aligned} \quad (65)$$

for all non-principal characters.

For *primitive* non-principal characters, and only for those, an appeal to [5, Remark 2] shows that the Gauss sums above collapse and, after further rearrangement, for a free parameter, initially with $0 < \lambda \leq 2|d|$, we have:

Theorem 9 (Primitive real L-series computation). *For primitive non-principal characters with free parameter λ we have:*

$$L_{-d}(s) = \sum_{m=1}^{\infty} \frac{\Gamma\left(\frac{s+1}{2}, \frac{\pi}{|d|} m^2 \lambda\right)}{\Gamma\left(\frac{s+1}{2}\right)} \frac{\binom{-d}{m}}{m^s} + \left(\frac{\pi}{|d|}\right)^{s-1/2} \sum_{m=1}^{\infty} \frac{\Gamma\left(\frac{2-s}{2}, \frac{\pi}{|d|} m^2 / \lambda\right)}{\Gamma\left(\frac{s+1}{2}\right)} \frac{\binom{-d}{m}}{m^{1-s}} \quad (66)$$

and

$$L_{+d}(s) = \sum_{m=1}^{\infty} \frac{\Gamma\left(\frac{s}{2}, \frac{\pi}{|d|} m^2 \lambda\right)}{\Gamma\left(\frac{s}{2}\right)} \frac{\binom{+d}{m}}{m^s} + \left(\frac{\pi}{|d|}\right)^{s-1/2} \sum_{m=1}^{\infty} \frac{\Gamma\left(\frac{1-s}{2}, \frac{\pi}{|d|} m^2 / \lambda\right)}{\Gamma\left(\frac{s}{2}\right)} \frac{\binom{+d}{m}}{m^{1-s}}. \quad (67)$$

Proof. Indeed, as $\Gamma(a, z)$ is entire in a when z is non zero, these identities certainly hold for $\text{Re}(\lambda) > 0$. \square

Example 1 (Numerical illustration of Theorem 9 and Corollary 2). In Table 1 we illustrate (67) for $d = +5, +8, +24, +40$ and (66) for $-3, -15, -24, -40$, in each case with $s = 1/10, 1$ and 10. In each row, we list the correct digits produced with M terms, where M ranges from 10 to 40. The last column, labeled M_{1000} , is the number of terms M required to achieve at least 1000-digit accuracy in the results. For these experiments, we used $\lambda = 1$, as this choice appeared to be a nearly optimal value for all cases we have tried of d and s .

Note that convergence in these series is very good, with errors decreasing very rapidly with the number of terms M . Doubling the number of terms, say from $M = 20$ to $M = 40$, typically more than triples the number of correct digits in the result. The rate of convergence does not appear to depend much on the value of s . This is all consistent with the error estimate derived from the incomplete Gamma asymptotic, $\Gamma(a, z) \sim z^{a-1}e^{-z}$, implicit in (60) with $z := \pi M^2/|d|$. These methods are effective—if less needed—for larger s , so for $M = 250$, $L_{\pm 120}(201/2)$ is computed correctly to 861 places. \diamond

Remark 5. The formulas (66) and (67) actually are valid for all complex λ and become especially pretty when $\lambda = i$ since $\Gamma(a, -ip) = \overline{\Gamma(a, ip)}$ for $p > 0$. Moreover, setting $\lambda = 0$ or $+\infty$ yields the reflection formulas of (18) for $L_{\pm d}(s)$, in an unusual form. An application of the duplication formula for $\Gamma(s)$ recovers the usual forms. \diamond

Alternatively, setting $\lambda = 1$ we may write:

Corollary 2 (Primitive real L-series computation and reflection). *For primitive non-principal characters we have:*

$$\begin{aligned} \left(\frac{|d|}{\pi}\right)^{s/2} \Gamma\left(\frac{s+1}{2}\right) L_{-d}(s) &= \left(\frac{|d|}{\pi}\right)^{s/2} \sum_{m=1}^{\infty} \frac{\binom{-d}{m} \Gamma\left(\frac{s+1}{2}, \frac{\pi m^2}{|d|}\right)}{m^s} \\ &+ \left(\frac{|d|}{\pi}\right)^{(1-s)/2} \sum_{m=1}^{\infty} \frac{\binom{-d}{m} \Gamma\left(\frac{1+(1-s)}{2}, \frac{\pi m^2}{|d|}\right)}{m^{1-s}} \end{aligned} \quad (68)$$

and

$$\begin{aligned} \left(\frac{|d|}{\pi}\right)^{s/2} \Gamma\left(\frac{s}{2}\right) L_{+d}(s) &= \left(\frac{|d|}{\pi}\right)^{s/2} \sum_{m=1}^{\infty} \frac{\binom{+d}{m} \Gamma\left(\frac{s}{2}, \frac{\pi m^2}{|d|}\right)}{m^s} \\ &+ \left(\frac{|d|}{\pi}\right)^{(1-s)/2} \sum_{m=1}^{\infty} \frac{\binom{+d}{m} \Gamma\left(\frac{1-s}{2}, \frac{\pi m^2}{|d|}\right)}{m^{1-s}}. \end{aligned} \quad (69)$$

In particular,

$$\left(\frac{|d|}{\pi}\right)^{s/2} \Gamma\left(\frac{s+1}{2}\right) L_{-d}(s) = \left(\frac{|d|}{\pi}\right)^{(1-s)/2} \Gamma\left(\frac{2-s}{2}\right) L_{-d}(1-s), \quad (70)$$

$$\left(\frac{|d|}{\pi}\right)^{s/2} \Gamma\left(\frac{s}{2}\right) L_{+d}(s) = \left(\frac{|d|}{\pi}\right)^{(1-s)/2} \Gamma\left(\frac{1-s}{2}\right) L_{+d}(1-s). \quad (71)$$

Proof. Since the righthand side of both (68) and (69) is invariant under $s \mapsto 1-s$ we simultaneously obtain reflection formulas (70) and (71), as well as efficient computational methods in both cases. \square

Remark 6 (Incomplete Gamma values at nonnegative integers, half-integers and negative integers). In the special case that the first argument $\Gamma(a, z)$ is a nonnegative integer $a = n$, the following formula can be used for computation [26, §8.4.8]:

$$\Gamma(n, z) = (n-1)! e^{-z} \sum_{k=0}^{n-1} \frac{z^k}{k!}. \quad (72)$$

When $a = n + 1/2$, where n is nonnegative, the following formula can be used [26, §8.4.14]:

$$\Gamma(n + 1/2, z^2) = (1/2)_n \sqrt{\pi} \left(\operatorname{erfc}(z) + \frac{e^{-z^2}}{\sqrt{\pi}} \sum_{k=1}^n \frac{z^{2k-1}}{(1/2)_k} \right). \quad (73)$$

Here $(\alpha)_n = \Gamma(\alpha + n)/\Gamma(\alpha)$, $(\alpha)_0 = 1$ is the rising factorial as in Section 5 and

$$\operatorname{erfc}(z) := \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-t^2} dt = 1 - \operatorname{erf}(z),$$

is the *complementary error function* [26, (7.2.2)]. The case when the first argument is a negative integer may be handled by [26, §8.4.15]:

$$\Gamma(-n, z) = \frac{(-1)^n}{n!} \left(E_1(z) - e^{-z} \sum_{k=0}^{n-1} \frac{(-1)^k k!}{z^{k+1}} \right), \quad (74)$$

where

$$E_1(z) := \int_z^\infty \frac{e^{-t}}{t} dt = -\gamma - \log z + \sum_{n=1}^\infty \frac{z^n}{n \cdot n!}, \quad (75)$$

is the *exponential integral*. Finally,

$$\Gamma(a, z) = \frac{\Gamma(a+1, z) - z^a e^{-z}}{a} \quad (76)$$

allows one to recursively evaluate the incomplete Gamma function for other negative a . \diamond

To handle derivatives of $L_{\pm d}(s)$ at integers—so as to have access to Theorem 4 and results for character polylogarithms—one needs also derivative formulas for the incomplete Gamma function, as are available from (48) or (50).

7 Conclusion

In this paper, we have presented and further developed some techniques and formulas originally discovered by the late Richard Crandall, who sadly passed away in December 2012. He will be sorely missed in the experimental mathematics world, as well as in computational number theory and his native specialty of mathematical physics.

Polylogarithms, the Lerch transcendent function, and related functions are central to a great deal of 21st century mathematics and mathematical physics [4, 13, 25]. Thus new robust, efficient techniques to compute high-precision numerical values of these functions, which are required to apply tools such as the “PSLQ algorithm” [8] to discover new identities and relations among these functions, will increasingly be a key component of the mathematical toolbox for researchers in these fields. Developing a suite of such tools for a broad range of transcendental and special functions is the central objective of a new (2014 to 2016) Australian Research Council Discovery Project by the present authors in tandem with Richard Brent and several other colleagues.

We conclude by emphasizing once again that our research agenda is driven as much by the desire to improve tools for computer-assisted discovery as it is by the precise needs of the current project.

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| d | s | Correct digits achieved | | | | M_{1000} |
|-----|------|-------------------------|----------|----------|----------|------------|
| | | $M = 10$ | $M = 20$ | $M = 30$ | $M = 40$ | |
| +5 | 1/10 | 36 | 124 | 266 | 463 | 59 |
| | 1 | 35 | 123 | 265 | 462 | 59 |
| | 10 | 37 | 125 | 267 | 464 | 59 |
| +8 | 1/10 | 23 | 78 | 167 | 291 | 75 |
| | 1 | 22 | 78 | 167 | 290 | 75 |
| | 10 | 25 | 81 | 170 | 293 | 75 |
| +24 | 1/10 | 9 | 33 | 58 | 99 | 131 |
| | 1 | 8 | 32 | 57 | 98 | 131 |
| | 10 | 14 | 37 | 62 | 103 | 131 |
| +40 | 1/10 | 6 | 18 | 36 | 61 | 169 |
| | 1 | 5 | 17 | 35 | 60 | 169 |
| | 10 | 12 | 23 | 41 | 66 | 169 |
| -3 | 1/10 | 56 | 221 | 438 | 766 | 46 |
| | 1 | 56 | 221 | 438 | 766 | 46 |
| | 10 | 57 | 223 | 440 | 767 | 46 |
| -15 | 1/10 | 12 | 45 | 89 | 154 | 104 |
| | 1 | 12 | 45 | 89 | 154 | 104 |
| | 10 | 17 | 50 | 93 | 159 | 104 |
| -24 | 1/10 | 7 | 31 | 56 | 97 | 131 |
| | 1 | 7 | 31 | 56 | 97 | 131 |
| | 10 | 13 | 37 | 62 | 103 | 131 |
| -40 | 1/10 | 5 | 16 | 34 | 58 | 171 |
| | 1 | 5 | 16 | 34 | 59 | 171 |
| | 10 | 11 | 23 | 41 | 65 | 170 |

Table 1: Number of correct digits in (66) and (67) using M terms in the two infinite series, for different values of d and s . The last column is the value of M required to achieve at least 1000-digit accuracy.