## THE POLYLOGARITHM FUNCTION IN JULIA

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Abstract. The polylogarithm function is one of the constellation of important mathematical functions. It has a long history, and many connections to other special functions and series, and many applications, for instance in statistical physics. However, the practical aspects of its numerical evaluation have not received the type of comprehensive treatments lavished on its siblings. Only a handful of formal publications consider the evaluation of the function, and most focus on a specific domain and/or presume arbitrary precision arithmetic will be used. And very little of the literature contains any formal validation of numerical performance. In this paper we present an algorithm for calculating polylogarithms for both complex parameter and argument and evaluate it thoroughly in comparison to the arbitrary precision implementation in Mathematica. The implementation was created in a new scientific computing language Julia, which is ideal for the purpose, but also allows us to write the code in a simple, natural manner so as to make it easy to port the implementation to other such languages.

Key words. IEEE-754 Floating Point, Special functions

AMS subject classifications. 33E20, 33F05, 65B10

**1.** Introduction. The polylogarithm function is defined by the sum

(1.1) 
$$\operatorname{Li}_{s}(z) = \sum_{k=1}^{\infty} \frac{z^{k}}{k^{s}}$$

for |z| < 1 (or for  $|z| \le 1$  when  $\Re(s) \ge 2$ ), and by analytic continuation to the entire complex plane. For instance when  $\Re(s) > 0$  we can define it using the integral

(1.2) 
$$\operatorname{Li}_{s}(z) = \frac{1}{z} \int_{0}^{\infty} \frac{t^{s-1}}{e^{t}/z - 1} dt,$$

except for a pole at z = 1 for  $\Re(s) < 2$ . There are many other representations for the function, but these suffice for our understanding here. Figure 1.1 shows some examples for integer parameter s.

The polylogarithm is an interesting function. Zagier [24] describes just the dilogarithm (the instance with s = 2) as one of the simplest, and yet strangest of nonelementary functions. He states

"almost all the formulas relating to it, have something of the fantas-

tical in them, as if this function alone among all others possessed a sense of humor."

The polylogarithm has a long history; its early variants go back to 1696 with correspondance between Leibniz and the Bernoullis<sup>1</sup>. And it is an important function. It has direct relationships with the gamma function, Hurwitz and Riemann zeta functions and many others. An entire book has been written on it [13]. It's relationships to Fermi-Dirac integrals lead to physical applications, for instance, computations in statistical mechanics [12]. It also has many other applications including those in number theory and geometry [15].

Note, however, that the polylogarithm function is unrelated to *polylogarithmic complexity* as discussed in complexity theory.

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<sup>&</sup>lt;sup>1</sup>See Maximon [15] for a brief history.

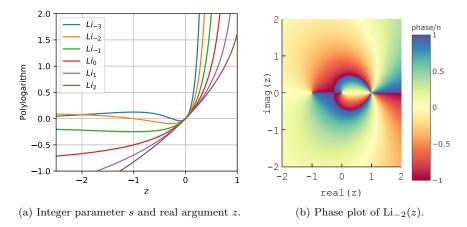


FIG. 1.1. Examples of the polylogarithm function.

The function gains its name [24] by comparison to the Taylor series of the ordinary logarithm

$$-\ln(1-z) = \sum_{n=1}^{\infty} \frac{z^n}{n}$$

leading to some authors (e.g., [15]) defining the polylogarithm to refer to the integer cases s = n, and using the term Jonquière's function or *fractional* polylogarithm for non-integer cases. We use the term polylogarithm to include all values of  $s \in \mathbb{C}$ .

There are many publications on the function, but only a handful on its numerical evaluation [10, 23, 7, 19, 8, 3, 4]. Zagier [24] precisely describes the situation

"It occurs not quite often enough, and in not quite an important enough way, to be included in the Valhalla of the great transcendental functions—the gamma function, Bessel and Legendre-functions, hypergeometric series, or Riemann's zeta function. And yet it occurs too often, and in far too varied contexts, to be dismissed as a mere curiosity."

It occurs not quite often enough to have always been given the consideration it deserves. In particular little work has been done on its numerical evaluation, and all of the existing works are incomplete, contain errors, or are specific to particular domains or sets of parameters, *e.g.*, *s* integer and real (see Section 3 for details). Notably, almost none of these present anything serious in the way of validation. And most existing implementations are (i) not open, and/or (ii) use arbitrary-precision arithmetic [17, 18, 20], in order to produce high-precision results for instance for examining zeros. Instead, we aim to provide a standard IEEE floating point [9] implementation of reasonable accuracy used for instance for computing zeta-distribution momentgenerating functions. Obtaining reasonable accuracy over the whole parameter space within the limits of 64 bit precision is still challenging. For instance, some stopping rules that are relatively straight forward in the deep tail of a series are less reliable early on in the sequence.

The implementation is provided in a relatively new programming language – Julia [5] – designed specifically for numerical computing. Julia is an ideal language for such tasks, providing both an adaptable and dynamic high-level language, but

also very good computational performance [11]. Note, however, that our code is open source<sup>2</sup> under the MIT licence and the intent is that the code be straight-forward enough to be adapted easily to any modern procedural language.

The algorithm is tuned to provide relative accuracy better than  $10^{-12}$  using standard IEEE double-precision floating point calculations. In over 30,000 tests it fails to attain this accuracy in only 88 cases, and the worst case accuracy is  $1.1 \times 10^{-11}$ . The typical accuracy is much better. The implementation's speed is comparable or substantially better than the alternatives for which we have data.

An additional goal of this work is to present a complete set of information for implementation of this function in other languages and settings, from the ground up, including many of the small technical pieces that are missing from earlier expositions.

2. Notation, Conventions and Standard Results. The standard notation for the polylogarithm is  $\text{Li}_s(z)$ , where we refer to s as the parameter, and z as the input argument. In the case where s is a real integer, it is often represented by n.

Note that the notation Li has also been used for the Eulerian logarithmic integral, which is not under consideration here.

**2.1. Standard Functions.** There is a common set of useful functions – Zagier's Valhalla – defined in most computational packages. Most are well-known, *e.g.*, see [1], but we define our notation here to be precise.

 $\Gamma(s) =$  the gamma function,

 $\psi(n)$  = the digamma function = the derivative of log-gamma,

 $\psi^{(m)}(n)$  = the polygamma function = the *m*th derivative of log-gamma,

$$\begin{aligned} \zeta(s) &= \text{the Riemann zeta function} = \sum_{n=0}^{\infty} 1/n^s, \text{ for } \Re(s) > 1, \\ \zeta(s,q) &= \text{the Hurwitz zeta function} = \sum_{n=0}^{\infty} 1/(n+q)^s, \text{ for } \Re(s) > 1, \Re(q) > 0, \\ \eta(s) &= \text{the Dirichlet eta function} = (1-2^{1-s})\zeta(s), \\ \beta(s) &= \text{the Dirichlet beta function} = 4^{-s} (\zeta(s,1/4) - \zeta(s,3/4)). \end{aligned}$$

These functions are provided by, or calculable directly from standard numerical packages such as the SpecialFunctions<sup>3</sup> package in Julia.

These have many useful relationships: e.g., one that is used here is [1, 6.4.2]

(2.1) 
$$\psi^{(n)}(1) = (-1)^{n+1} n! \zeta(n+1), \text{ for } n = 1, 2, \dots$$

**2.2.** Additional Functions and Sequences. There are a number of sequences and functions used in computing polylogarithms or as reference points for testing that are not as commonly implemented in standard numerical packages (*e.g.*, these are not provided by the SpecialFunctions package in Julia). In particular:

• The Stieltjes constants [14]  $\gamma_N$ , which we provide in our code from values from the OEIS [16]. Note that  $\gamma_0 = \gamma$ , which is also called the Euler-Mascheroni constant. The sequence is sometimes called the generalised Euler constants, but that this is confusing because there are other series called Euler numbers. Euler was prolific.

<sup>&</sup>lt;sup>2</sup>Source available at https://github.com/mroughan/Polylogarithms.jl.

<sup>&</sup>lt;sup>3</sup>https://juliamath.github.io/SpecialFunctions.jl/

• The harmonic numbers,  $\mathcal{H}_n = \sum_{k=1}^n 1/k$  (where  $\mathcal{H}_0 = 0$  by convention) and generalized harmonic numbers,  $\mathcal{H}_{n,r} = \sum_{k=1}^n 1/k^r$ . We calculate values for smaller n directly, while for larger we use the identity that

$$\mathcal{H}_n = \psi(n+1) + \gamma,$$

and we use a similar identity for generalised harmonic numbers.

• The Bernoulli numbers  $B_n$  and polynomials  $B_n(x)$ . The first 35 numbers are provided as exact rationals<sup>4</sup> based on [16, A027642], and larger values are derived as real numbers from the polynomials using  $B_n = B_n(0)$  because the integers in the rational representation come close to the bounds for 64 bit integers. Bernoulli polynomials are given exactly up to 5th order, otherwise calculated using the standard recursion, or for large n using the following identity [6],  $B_n(x) = -n\zeta(1-n, x)$ .

The advantage of expressing harmonic number and Bernoulli polynomials in terms of other special functions is that these special functions are given in many now standard numerical libraries, for instance, the **SpecialFunctions** module of Julia, but for small n it can be faster and more precise to calculate them directly.

**2.3. The Branch.** The polylogarithm function has a branch on the real axis for  $z \in [1, \infty)$ . The conventional behaviour around the branch is exemplified by particular values such as given in [7] for infinitesimally small  $\epsilon > 0$ 

(2.2) 
$$\operatorname{Li}_2(2) = \frac{\pi^2}{4} - i\pi \ln 2,$$

(2.3) 
$$\operatorname{Li}_2(2+i\epsilon) = \frac{\pi^2}{4} + i\pi \ln 2.$$

In general the discontinuity should take the form

(2.4) 
$$\operatorname{Disc} \operatorname{Li}_{s}(z) = 2\pi i \frac{(\ln z)^{s-1}}{\Gamma(s)},$$

the convention being [23, (3.1)] that

(2.5) 
$$\Im\left(\operatorname{Li}_{s}(z)\right) = -\pi \frac{(\ln z)^{s-1}}{\Gamma(s)},$$

(2.6) 
$$\Im \left( \operatorname{Li}_{s}(z+i\epsilon) \right) = +\pi \frac{(\ln z)^{s-1}}{\Gamma(s)},$$

and these terms go to zero for  $s = n \leq 0$ .

**3. Related Work.** It is surprising that there is relatively little written about computing standard polylogarithms, much of it in informal literature, rather than refereed publications. In rough chronological order:

- The pre-history of this work primarily concentrates only on di- and trilogarithms (s = 2 and 3), *e.g.*, see Jacobs and Lambert [10].
- Wood [23] presents the first somewhat complete set of series for calculating the polylogarithm function in various domains. Apart from frequent typographical mistakes, there are several major difficulties with the manuscript. Wood

<sup>&</sup>lt;sup>4</sup>Julia provides a Rational number type.

primarily presents series without any deep consideration of which should be applied. Wood also focusses on s real as do many other papers. The results often generalise, but special care was found to be needed for complex parameters.

- Crandall [7] provides an actual algorithm, specifying choice of domain for each piece. However, in this paper Crandall only considers s = n, integer and real. Crandall also provides only a few hints as to how the function is tested, but no numerical results. This is the first reference given in Python mpmath's implementation [17], and is presumably the basis of the code there.
- Vepstas [19] presents a new approach to solving problems of this type, but the algorithm uses arbitrary-precision arithmetic. We seek here to find a standard 64-bit floating-point implementation. Vepstas provides more details of tests of the function than any of the other publications. However, even here, the results are often unclear: for instance, images without scales are published.
- Crandall [8] presents a unified version of his earlier approach for general s (and other related functions), as well as the expression for the expansions near negative integer s, but in this work does not report a complete algorithm, and also suffers from some small mistakes.
- Bailey and Borwein [3, 4] use and refine Crandall's work for calculating polylogarithms and their derivatives. They discuss alternative approaches in different domains, but their main interest is in related functions and although they fill in some gaps of [8], they do not present a complete algorithm either.

Existing software is also limited in this domain. Many implementations are only valid for certain parameters (*e.g.*, integer and real s or even just a few values of s [21]).

Others [17, 18, 20] use arbitrary-precision arithmetic, for instance in order to produce high-precision results for computing zeros. Bailey and Borwein [2] argue cogently for the need to have high-precision calculations in many applications. However, a vast set of precedents show the value of standard floating-point implementations (for instance see the C/C++ mathematics library) of useful functions. We here seek to add the polylogarithm to the a list of commonly available functions. A simple instance in which this would be useful is the calculation of the moment generating and characteristic functions of the zeta distribution.

4. Components. As with many special functions we use series representations to calculate the polylogarithm. However, no single series converges over the entire domain and there are some places where special numerical care is needed even though the series technically converge. Thus, as in previous works we will present several components. These are largely consistent with those works, but some of the previous works are incomplete or have mistakes, and hence we will list all of the series used here in detail to eliminate any confusion.

We also use one identity to transform some parameter values into a more amenable range.

In the following section we will precisely define how these are combined into an algorithm.

**4.1. Direct Series.** Our first port of call is the definition (1.1). This definition can be used directly to calculate the polylogarithm for |z| < 1, and we shall refer to this approach to calculation as **Series 1**.

Although it is convergent for |z| < 1, the rate of convergence can be quite slow close to the boundary. Crandall [7] suggests use of this series for |z| < 1/2, which leads to an easy calculation of 1 bit of precision per term (asymptotically) in the series, based on the asymptotic dependence on the  $|z|^k$  term. Bailey and Borwein [4] suggest |z| < 1/4 based on experimental results, however we shall refine this the section below. However, note that much of the commentary presumes very-high precision will be required, and hence the sum must proceed deep into the tail of the series. We are concerned here with finite precision and when  $\Re(s) < 0$  the early part of the sequence is strongly impacted by the denominators of the sequence. If z is small, we may not need to proceed further into the tail, and so Crandall's comment about bits per term may not apply.

**4.2.** Alternative Series 2. The main alternative power series is about z = 1, where we find [8, (32)] and [23, (9.3)] and [4, (2)]

(4.1) 
$$\operatorname{Li}_{s}(z) = \Gamma(1-s)(-\ln z)^{s-1} + \sum_{k=0}^{\infty} \frac{\zeta(s-k)}{k!} (\ln z)^{k},$$

which converges for  $|\ln z| < 2\pi$  and s not a positive integer. We call this **Series 2**.

Convergence in the region  $|\ln z| < 2\pi$  arises from Riemann's functional equation [1, 23.2.6]

$$\zeta(s) = 2^{s} \pi^{s-1} \sin(\pi s/2) \Gamma(1-s) \zeta(1-s),$$

which, when substituted in the above series leads to

$$\begin{aligned} \operatorname{Li}_{s}(z) &= \Gamma(1-s)(-\ln z)^{s-1} \\ &+ 2^{s} \pi^{s-1} \sum_{k=0}^{\infty} \sin(\pi(s-k)/2) \zeta(1-s+k) \frac{\Gamma(1-s+k)}{\Gamma(1+k)} \left(\frac{\ln z}{2\pi}\right)^{k}, \end{aligned}$$

The terms  $\zeta(1-s+k)$  converges to 1 as  $k \to \infty$ , and the sine is bounded, and hence the tail of the sequence has much in common with that of Series 1, except that it is dominated by the term  $(\ln z/2\pi)^k$ . Figure 4.1 shows contours of  $\ln z/2\pi$  both at small and large scales.

This series has a much larger domain of convergence than Series 1, but there is a small region about the origin which is excluded and hence we cannot discount Series 1. Past approaches partition the space using Series 1 inside some radius around the origin, and Series 2 in a region around that with alternative radii being proposed by Crandall [7] (|z| = 1/2) and Bailey and Borwein [4] (|z| = 1/4).

However, it seems more natural (and is actually consistent with the detailed results in [4]) to make the dividing line between Series 1 and Series 2 slightly more complex: we will prefer Series 1 when  $2\pi |z| < |\ln z|$ . This leads to a more complex boundary, but results in a better tradeoff between the two approaches in some regions, particularly on the negative real axis where convergence of Series 2 is at its worst.

The regions are shown in Figure 4.2. Note that on the positive real axis we fall back to the advice of Bailey and Borwein in that our transition occurs at  $|z| \simeq 0.2323$  (near 1/4) and on the negative real axis we chose a threshold  $z \simeq 0.5113$  near that of Crandall (near 1/2). The shape of the region proposed for the choice matches very closely to the empirical results shown in Bailey and Borwein [4, Figure 1].

Many existing works presume that use of Series 2 will be restricted to the region  $\ln z/2\pi \leq 0.5$  in order that, asymptotically, we obtain 1 bit per term as for Series 1. Figures 4.1 and 4.2 together illustrate a seemingly unstated fact that despite being a very large region, the combined regions  $|z| \leq 0.5$  and  $|\ln z|/2\pi \leq 0.5$  still leave a small gap in the unit disc near the negative real axis (shaded yellow). This gap closes if we allow as small a change as  $|\ln z|/2\pi \leq 0.512$ , and so we can either allow a small

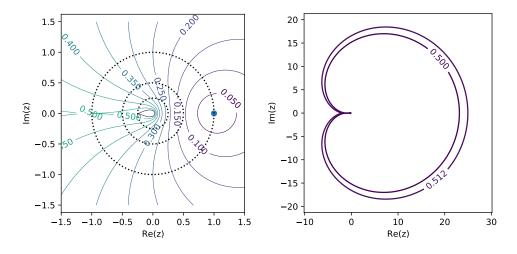


FIG. 4.1. Contours of constant magnitude for  $\ln z/2\pi$  (solid lines). The final tear-drop shaped contour near the origin corresponds to  $\ln z/2\pi = 0.55$ . Dotted lines show |z| = 0.25, 0.5 and 1.0 for comparison. The right figure illustrates the large regions of convergence outside the uni circle for given thresholds.

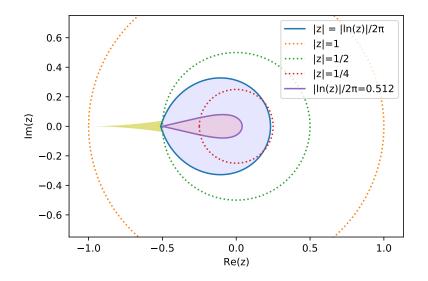


FIG. 4.2. Boundaries in the choice of Series 1 and 2. Series 1 is used in the shaded blue region. The yellow region indicates the region that is missed if we bound use of Series 2 by  $\ln z/2\pi < 0.5$ . The shaded red tear-drop region indicates the region excluded if we use Series 2 when  $\ln z/2\pi \le 0.512$ . As that this lies inside the region where Series 1 is used all of the unit disc is covered by either Series 1 or 2.

increase in the region allowed for Series 2, or use an alternative in this region. The duplication formula appears to work, but we have not proved that it converges for every point in this domain and so we prefer the former approach.

Detailed results of the tradeoffs are included in Section 6.1.

**4.3.** Alternative Series 3. For s = n > 0 (*i.e.*, a positive integer) we get the same summation, however, the terms  $\zeta(1)$  and  $\Gamma(1-s)$  both have poles. The poles 7

cancel, but if we naively calculate these, we run into numerical problems. Cancelling the two poles we get (as in [8, (33)])

(4.2) 
$$\operatorname{Li}_{n}(z) = \frac{(\ln z)^{n-1}}{(n-1)!} \left[ H_{n-1} - \mathcal{L} \right] + \sum_{\substack{k=0\\k \neq n-1}}^{\infty} \zeta(n-k) \frac{(\ln z)^{k}}{k!},$$

where  $\mathcal{L} = \ln(-\ln z)$ . This series could be used for cases where s = n but when s is near an integer then there are numerical difficulties in computing the difference of the two large terms. Hence for  $s = n + \tau$  for small  $\tau$ , we perform an expansion around s = n to get

(4.3) 
$$\operatorname{Li}_{n+\tau}(z) = \frac{(\ln z)^{n-1}}{(n-1)!} Q_{n-1}(\mathcal{L},\tau) + \sum_{\substack{k=0\\k\neq n-1}}^{\infty} \zeta(n+\tau-k) \frac{(\ln z)^k}{k!},$$

where the two problematic terms are grouped into  $Q_n(\mathcal{L}, \tau)$ , *i.e.*,

$$Q_n(\mathcal{L},\tau) = \zeta(1) + (-1)^n n! \Gamma(-n-\tau) (\ln z)^{\tau}.$$

Crandall [8, (51)] expands  $Q_n(\mathcal{L}, \tau)$  as a Taylor series about  $\tau = 0$  as

$$Q_n(\mathcal{L}, \tau) = \sum_{j=0}^{\infty} c_{n,j}(\mathcal{L}) \tau^j$$

and gives the  $c_{k,j}$  in [8, pp.35-36] recursively, but note that Crandall's manuscript has typographic errors; Bailey and Borwein [3, 4] give the correct formula. However, for  $|\tau| \ll 1$  we need only take a small number of terms, the first three of which can be written explicitly as

$$c_{n,0}(\mathcal{L}) = H_n - \mathcal{L},$$

$$c_{n,1}(\mathcal{L}) = -\gamma_1 - \frac{(\psi(n+1) - \mathcal{L})^2}{2} - \left(\frac{\pi^2}{6} - \frac{\psi^{(1)}(n+1)}{2}\right),$$

$$c_{n,2}(\mathcal{L}) = \frac{\gamma_2}{2} + \frac{(\psi(n+1) - \mathcal{L})^3}{6} + (\psi(n+1) - \mathcal{L})\left(\frac{\pi^2}{6} - \frac{\psi^{(1)}(n+1)}{2}\right) + \frac{\psi^{(2)}(n+1)}{6}.$$

Noting that from [1, 6.3.2] and (2.1) we get relationships such as

$$\psi^{(0)}(n) = \psi(n) = -\gamma + H_{n-1}$$
 and  $\psi^{(1)}(1) = \zeta(2) = \frac{\pi^2}{6}$ 

we see that  $c_{n,0}(\mathcal{L})$  and  $c_{0,1}(\mathcal{L})$  are consistent with the formulas given in [8, pp.36]. Wood [23, (9.4)] presents a similar expansion, but only the 1st term is the same. The 2nd term differs only in the signs of some terms and there are other typographic errors in the work.

Taking  $\tau = 0$  we use just the first term leading to a result consistent with (4.2). Taking a *j*th order approximatio we get

$$Q_n^{(j)}(\mathcal{L},\tau) = c_{n,0}(\mathcal{L}) + \tau c_{n,1}(\mathcal{L}) + \dots + \tau^j c_{n,j}(\mathcal{L}),$$

(4.4) 
$$\operatorname{Li}_{n+\tau}(z) \simeq \frac{(\ln z)^{n-1}}{(n-1)!} Q_{n-1}^{(j)}(\mathcal{L},\tau) + \sum_{\substack{k=0\\k\neq n-1}}^{\infty} \zeta(n+\tau-k) \frac{(\ln z)^k}{k!}.$$

We refer to (4.4) as **Series 3**. To determine how many terms are needed in Q and how small  $|\tau|$  need be before we swap to Series 3, we test the two series empirically near the point s = 1. Figure 4.3 shows the errors as a function of  $|\tau|$ . We see quite similar results for several other values of s = n that were tested. The figure indicates that around 5 terms are needed before the cross-over point between the two series lies below  $10^{-12}$  (our target precision) and that the threshold should be  $\tau < 10^{-3}$ .

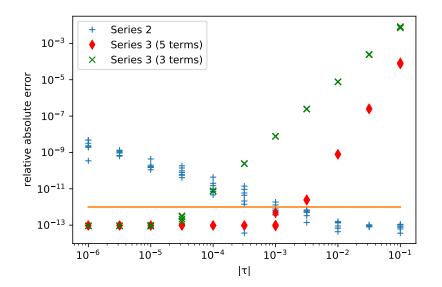


FIG. 4.3. A comparison of Series 2 and 3 near positive integer parameters, i.e.,  $s = n + \tau$ , for n > 0 (here n = 1 and z = -1/2). The number of terms in Series 3 is with respect to the approximation of  $Q_{n-1}(\mathcal{L},\tau)$  used in (4.3). Note that the cross-over point between Series 2 and Series 3 achieves the desired precision for 5 terms and a threshold around  $10^{-3}$ . The three term version of Series 3 is included because in that case the terms are known in closed form making calculation potentially faster with a loss of precision of about 1 order of magnitude.

**4.4. The Special Case At** z = 1. There are a number of special cases where the polylogarithm resolves to a more familiar function. The most obvious (the reason for which the function is named) is that  $\text{Li}_1(z) = -\ln(1-z)$ , but at the moment we do not use special cases in the calculations so that we can use these identies as test cases. However the following identity

(4.5) 
$$\operatorname{Li}_{s}(1) = \zeta(s), \text{ for } \Re(s) > 1,$$

is useful because at this allows Series 2 and Series 3 to be written without considering the special case in detail. Note that when  $\Re(s) \leq 1$  there is a pole at z = 1, so the function returns Inf.

in

**4.5. Duplication Identity.** The polylogarithm satisfies the duplication identity [12, (e)]

(4.6) 
$$\operatorname{Li}_{s}(z) + \operatorname{Li}_{s}(-z) = 2^{1-s} \operatorname{Li}_{s}(z^{2}).$$

Wood refers to this as the square formula [23, 14.1], and notes that in an alternative [23, 15.1] form

(4.7) 
$$\operatorname{Li}_{s}(z) = 2^{s-1} \left( \operatorname{Li}_{s}(\sqrt{z}) + \operatorname{Li}_{s}(-\sqrt{z}) \right],$$

it could be use recursively to put z into a domain where another algorithm can be brought to bear. However Wood recommends against this citing difficulties in implementing recursion in his contemporary Fortran as well as the increase in the number of polylogarithms to be calculated. Recursion is not difficult in many modern languages so this can be a useful technique noting that the increase in the number of polylogarithms is countered by faster convergence on the square root.

**4.6. Reciprocal Identity.** The polylogarithm also satisfies another identity often called Jonquière's Identity, which leads to a reciprocal relationship:

(4.8) 
$$\operatorname{Li}_{s}(z) + (-1)^{s} \operatorname{Li}_{s}(1/z) \\ = \frac{(2\pi i)^{s}}{\Gamma(s)} \zeta \left( 1 - s, \frac{1}{2} + \frac{\ln(-z)}{2\pi i} \right) - 2\pi i \Theta(z) \frac{(\ln z)^{s-1}}{\Gamma(s)},$$

where  $\Theta(z)$  is Crandall's domain-dependent step function

(4.9) 
$$\Theta(z) = \begin{cases} 1 & \text{if } \Im(z) < 0 \text{ or } z \in [1, \infty), \\ 0 & \text{otherwise.} \end{cases}$$

The function  $\Theta(z)$  is intended to provide the conventional behaviour on and around the branch.

Wood [23] and others suggest use of this for large |z|. We tested the reciprocal computation but we found this approach to be numerically unstable for *s* with a large, negative imaginary component<sup>5</sup> and thus prefer not to use it here. This choice also reduces the dependence of our code on the Hurwitz zeta function, which is perhaps the least commonly implemented function (of those used here) in standard scientific packages.

Note that if s takes negative integer values we hit poles of the Gamma functions. In these cases we use the relation [23, (10.3)]

(4.10) 
$$\operatorname{Li}_{-n}(z) + (-1)^{n} \operatorname{Li}_{-n}(1/z) = 0,$$

but we shall use this relationship primarily for validation in what follows.

## 5. Algorithm.

**5.1. Dependencies.** The calculations require a number of other mathematical constants, sequences and functions as described in Section 2. Many of these (the gamma, digamma, polygamma, and Riemann, Hurwitz and Dirichlet zeta functions) are provided by Julia's SpecialFunctions package (v0.10.3) designed around the

<sup>&</sup>lt;sup>5</sup>Wood and others primarily consider the calculation of the polylogarithm with real arguments.

**Algorithm 1** The polylogarithm algorithm  $Li_s(z)$  with inputs  $s, z \in \mathbb{C}$ .

 $\begin{array}{l} T_1 \leftarrow 0.512 \\ T_2 \leftarrow 10^{-3} \\ \mu \leftarrow \ln(z) \\ t \leftarrow |\mu|/2\pi \\ \text{if } 2\pi |z| \leq |\mu| \text{ then} \\ \text{Use Series 1 [defined in (1.1)];} \\ \text{else if } t \leq T_1 \text{ AND } s \text{ is further than } T_2 \text{ from a positive, real integer then} \\ \text{Use Series 2 [defined in (4.1)]} \\ \text{else if } t \leq T_1 \text{ then} \\ \text{Use Series 3 [defined in (4.4) with } j = 4] \\ \text{else} \\ \text{Recurse on the Duplication Identity (4.7)} \\ \text{end if} \end{array}$ 

**OpenSpecFun**<sup>6</sup> and **OpenLibm**<sup>7</sup> libraries. The implementation of the polygamma is restricted to integer orders m but that is all we require. The Euler-Mascheroni constant  $\gamma$  and  $\pi$  are provided as part of **Base.MathConstants** as **Irrational** type constants, which is a type that supports both floating point and functional (arbitrary precision) definition.

Other required constants, sequences and functions are defined as part of this package using standard values and algorithms as indicated in Section 2. The implementations of these components are comparatively straight forward.

**5.2. Domain breakup.** The algorithm selects various approaches in different domains. The completed algorithm is given via the pseudo-code described in Algorithm 1, which describes the breakup of the input domain in detail. The main breaks occur to use Series 3 near positive integer values of s and to separate the domains where Series 2 and Series 3 have the best convergence.

There are special cases of the function for certain values (for instance  $\text{Li}_1(z) = -\ln(1-z)$ ) but we do not use these at present because these identities are useful in testing series convergence. These might be used more in future versions.

**5.3.** Stopping Criteria. Determining at which point to stop each sequence to attain a given accuracy with minimal cost is not completely trivial. For instance, Series 1 has terms like  $z^k/k^s$ . For large k we can approximate these as  $\sim z^k$  and hence the remainder term is that of the geometric series, and hence for real, positive z it should be almost trivial to determine a cut-off at which we terminate the series, which seems to work well for |z| near 0.5. However, for small z the series drops so fast we don't reach this asymptotic domain. Luckily, a practical compromise is to terminate the sequence when the relative value of a summation term drops below 1/2 of the desired precision bound, *i.e.*, at the first m such that

$$\frac{z^m/k^m}{\sum_{k=1}^m z^k/k^s} \le 0.5a$$

where for the majority of the work here we use  $a = 10^{-12}$ . We must be a little careful for very small z and  $\Re(s) < 0$  to terminate the sequence only after it begins

 $<sup>^{6}</sup>$ OpenSpecFun uses AMOS and Faddeeva to provide Bessel, Airy and error functions.

 $<sup>^7 {\</sup>tt OpenLibm}$  uses the standard C libm, which includes, for instance the gamma function suite.

to decrease at  $k = \lceil \Re(s) / \ln |z| \rceil$ .

The bound will may be somewhat conservative for imaginary or negative z where the sequence oscillates and thus may contain cancelling terms.

We will show the relative merits of this cut-off in the following sections.

Series 2 appears much more complicated, but has essentially the same characterisics with the exception that its tail is dominated by powers of  $\ln z$ . However, it is somewhat more oscillatory and we have found that testing the relative size of the last two terms in the tail are both  $\leq 0.5a$ , is more reliable, but once again, it is somewhat conservative due to the oscillatory nature of the sequence.

The tail of the summation in Series 3 is almost identical to that in Series 2 and so we use the same termination criteria.

6. Tests. The goal we set here is to attain a relative absolute error  $\leq 10^{-12}$ . This value was chosen to be challenging but realistic. More importantly, if we set the goal to be machine precision, we would not be able to see by how much the approach exceeds the goal and hence is being potentially wasteful of computation.

The majority of tests performed here were conducted by creating benchmark data using Mathematica's arbitrary precision Polylog function, to high precision. Note that, in reading this data into double-precision floating point variables in Julia there is an inevitable loss of accuracy to machine precision, and so there is a lower bound on the degree to which we can test the accuracy of our code, *i.e.*, errors around  $10^{-15}$  should not be over-interpreted.

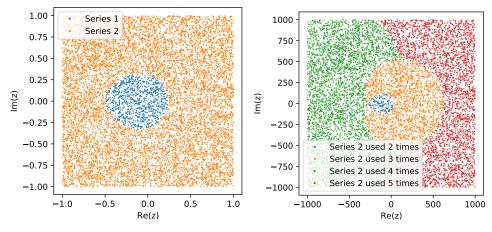
In addition to the tests reported below, a large number of additional tests (nearly 1000) were created using special values, common identities between the polylogarithm function and other standard functions, and relationships between polylogarithms, *e.g.*, (4.10).

**6.1. Testing of** |z| **domains.** The breakup of the z domain is illustrated in Figure 6.1. The left figure shows the boundary (explained in Section 4.2) between use of Series 1 and 2 on a large set of random points. It is natural to question how well this breakup works.

A set of test points z were created on the unit disc, spread in even radii circles about the origin, and we performed this test for around three different values of s and errors in Series 1 and 2 compared.

Figure 6.2 shows the results: both the relative absolute errors and number of iterations required by the two series as functions of |z| and arg z. Noteworthy features include the trade-off in number of iterations in the two series (lower-left) which crossesover between 0.25 and 0.5, with the larger values being along the negative real axis (bottom right figure).

Figure 6.1 (b) illustrates the regions in which the recursive duplication identity is used, and to what depth. Of note, the recursion is not a straight-forward matter of breaking the calculation up into a balanced binary tree to a given depth. The positive square-root term in the recursion quickly drops into the domain where we use Series 2. It is the negative square-root term that bounces around before hitting this region. The recursion tree is illustrated Figure 6.3 in a typical case of 2 levels of recursion, where Series 2 would be evaluated 3 times rather than 4 as one might guess.



(a) The boundary between Series 1 and Series 2. (b) The duplication identity at work.

FIG. 6.1. Illustration of the alternative approaches used as a function of z.

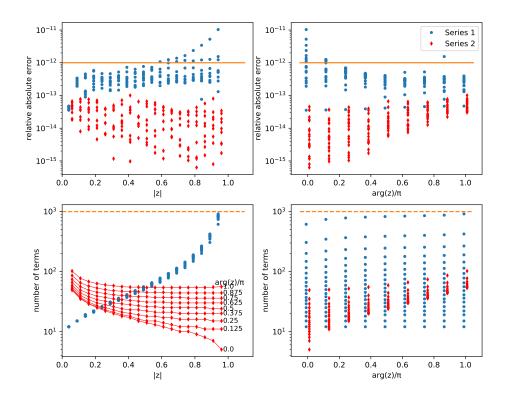


FIG. 6.2. A comparison of Series 1 and 2 for z on the unit circle (with s = -2). The top two plots show relative accuracy showing that the two approaches meet the accuracy requirements within the domains in which we calculate them. The stopping rule for Series 2 is perhaps a little conservative. The two lower plots show number of terms calculated in the series showing exactly the trade-off described in Section 4.2, namely, that the cut-off between them lies between approximately 1/4 and 1/2, and that while the number of terms in Series 1 is somewhat independent of  $\arg(z)$ , Series 2 performs better for positive real values of z, and worst for negative real values.

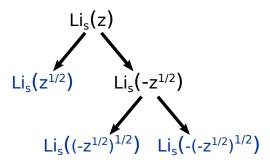


FIG. 6.3. A typical recursion using the duplication identity twice, but evaluating Series 2 only 3 times (blue terms), not 4.

**6.2.** Accuracy. We assessed overall accuracy using three sets of 10,000 uniformly at-random values of s and z with z chosen over 2x2, 16x16 and 2000x2000 rectangles centred on the origin of the complex plane, and with s chosen in the 16x16 rectangle. The data used to perform tests is included with our open source code. The package also contains code to regenerate all test figures included here.

We present three sets of tests over different sized ranges of z in order to test the polylogarithm function (i) in the typical region around the unit circle, (ii) for a larger domain including some recursion, and (iii) for a very large range of z to stress the algorithms, particularly the recursion. Histograms of the performance of the algorithm are shown in Figure 6.4. Only 88 cases out of 30,000 tests fell outside the desired accuracy of a relative error no more than  $10^{-12}$ , and the worst case was  $1.1 \times 10^{-11}$ . Achieving a higher degree of accuracy is possible, but then the majority of points are calculated too accurately (and hence are wasteful of computations).

It is interesting to understand where the errors occur. The vast majority occur for large z, in the range where 3 or 4 levels of recursion were required. Moreover, they occur for s with a large, real component as shown in Figure 6.5.

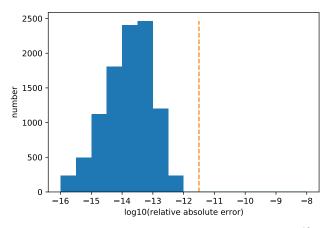
**6.3.** Computational Speed. Table 1 reports the average computation times on the three random datasets used above on an Intel i9-10900K CPU running in Julia v1.4.2 with v0.10.3 of the SpecialFunctions package, using a single core, running under Linux Mint 19.3.

The main impact on performance occurs when recursion is needed for large z values, which requires multiple evaluations of earlier series.

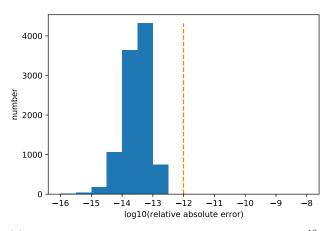
The table also shows Mathematica<sup>8</sup> computation times. The Julia code is at least ten times as fast, which reflects Julia's desire to provide very fast computations. However, we do not argue that this is an entirely valid comparison. It is problematic comparing computation times between programming languages as their internal measurement facilities may use different concepts and underlying libraries, and therefore comparisons are not "apples-to-apples" comparisons. Nevertheless, the speeds we are attaining seem creditable for a function of this type.

A second comparison arises in the results presented in [4], where times for computations of the order of 20,000-40,000  $\mu$ s are reported, though once again note that we cannot simplistically compare these results as they were computed to 1000 digits of precision. However, presuming 1 bit of accuracy per summation term, *i.e.*, that the computation time is somewhat proportional to the required accuracy, these times

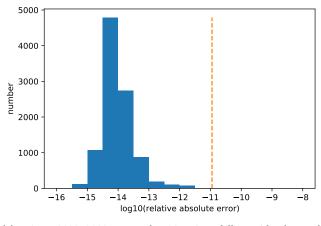
<sup>&</sup>lt;sup>8</sup>Calculations for this component are made to the same precision goal as our code.



(a) z in a 2x2 rectangle; 2 points fall outside the goal  $10^{-12}.$ 



(b) z in a 16x16 rectangle; 0 points fall outside the goal  $10^{-12}$ .



(c) z in a 2000x2000 rectangle; 86 points fall outside the goal  $10^{-12}$ .

FIG. 6.4. Histograms of  $\log_{10}$  of the relative, absolute errors. The dashed lines in each plot indicate the maximum error. In total, 88 points out of 30,000 fell outside of the desired accuracy goal.

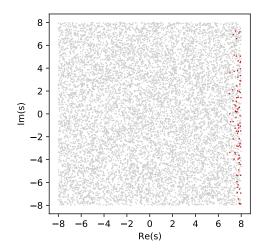


FIG. 6.5. A scatter plot of the random values of s used for testing. Red points indicate those with a relative error larger than  $10^{-12}$ .

Dataset	Julia	Mathematica	$\zeta(z)$
$\Re(z), \Im(z) \in [-1, 1]$	30.3	1606.0	1.0
$\Re(z), \Im(z) \in [-8, 8]$	41.3	1790.0	1.0
$\Re(z), \Im(z) \in [-1000, 1000]$	143.2	1890.0	0.8
TABLE 1			

Computation times for the polylogaarithm and zeta functions. All times are given in  $\mu s$  and are averages over 10,000 computations.

would scale to around 240-480  $\mu$ s to obtain 12 digits. The comparison is still flawed because Bailey and Borwein [4] don't report details of the system used to perform their computations, but the Julia implementation seems to compare favourably.

As another comparison point we also report the time to compute Julia's  $\zeta$  function over the same range of inputs. The polylogarithm calculation is an order of magnitude slower, which is quite reasonable given that the more common computation strategy (Series 2) requires evaluation of a series of  $\zeta$  functions. However, the result should allow readers to benchmark the expected performance they would receive against performance of zeta function calculations in existing libraries.

The current code has room for improvement. The code was written to be simple and clear and does not exploit Julia's language-dependent tricks to improve performance. Nor does it use numerical techniques such as Kahan summation.

The slowest computations involve the recursion. Developing a more stable reciprocal method would obviate this, and bring these times back towards those on other domains. However, an interesting alternative would be to combine the terms in the two components: Series 2 could then reuse some of the component calculations, notably the zeta function calculations.

We leave these improvements as future work.

7. Conclusion. This paper describes a complete algorithm for computing numerical values of the polylogarithm for complex arguments using standard double-precision floating-point calculations.

There are many possibilities for improvements. Most obviously, the current code has been written for simplicity and clarity and could be optimised in many ways. Simple improvements include more extensive use of look-up tables and series termination thresholds that cope better with oscillation. Moreover series are added in the most direct way as they are calculated (generally from largest to smallest) which isn't necessarily optimal, not to mention that Kahan summation or Shank's transformation might be used to speed up convergence of summations.

There are also additional sequences that could be applied. In particular, asymptotic forms valid for  $|z| \gg 1$ , though our experiments with these showed little promise. There are many extensions to be made in the future.

- Extending the toolkit to produce some of the standard related functions such as Fermi-Dirac integrals.
- Mass production of calculations: Julia's default approach to calculating multiple values of a function is to broadcast the inputs, which is ideal for parallelisation, but in calculating polylogarithms for multiple values of z but the same s, we can potentially reuse many of the terms in the calculation, thus saving a large amount of computations.
- Calculation of incomplete polylogarithm functions.
- Calculation of Neilsen generalised polylogarithm functions [10].
- Calculation of multiple polylogarithms [22].

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