The Computation of Polylogarithms

David C. Wood

ABSTRACT

The polylogarithm function, $\mathrm{Li}_p(z)$, is defined, and a number of algorithms are derived for its computation, valid in different ranges of its real parameter p and complex argument z. These are sufficient to evaluate it numerically, with reasonable efficiency, in all cases.

1. Definition

The polylogarithm may be defined as the function

$$\mathrm{Li}_p(z) = \frac{z}{\Gamma(p)} \int_0^\infty \frac{t^{p-1}}{e^t - z}\,dt, \quad \text{for } p > 0 \,. \tag{1.1}$$

In the following, p will represent the real parameter, and z the complex argument. In the important case where the parameter is an integer, it will be represented by n (or -n when negative).

It is often convenient to write the argument as e^w (or sometimes $-e^w$); for example

$$\mathrm{Li}_p(e^w) = \frac{1}{\Gamma(p)} \int_0^\infty \frac{t^{p-1}}{e^{t-w} - 1}\,dt \,. \tag{1.2}$$

In this case, w is normally restricted to the range $|\mathrm{Im}(w)| \le \pi$.

2. Introduction

Special cases of this function, particularly the dilogarithm (§ 7), have been studied at least since the time of Euler, usually with small integer parameters ($n = 2, 3, \cdots$). Lewin ([1]) gives a detailed account of this and related functions for this case.

Truesdell ([2]) covers most of the properties of the function for real parameters.

Some work has been done on this function with a complex parameters ([3]). This is not considered here, although most of the formulae hold with real p relaced by $p + iq$.

It arises in physics, often in the form of the Fermi–Dirac or Bose–Einstein functions, usually with parameters of the form $n + ½$ (§ 18).

It is a special case of Lerch's function (§ 19).

It has appeared under many names; that used here is due to Lewin.

All other notation is that used by Abramowitz and Stegun ([4]), except where stated otherwise.

3. General Behaviour

Because of the singularity in the integrand of Eqn (1.2) at $t = w$, the integral is singular at $w = 0$ (and $w = -2\pi i$ etc.), where it becomes infinite for $p \le 1$, and it is multi-valued. The principal branch is chosen to be that for which $\mathrm{Li}_p(e^u)$ is real for real $u < 0$, and which is continuous except on the positive real axis, where a cut is made from $w = 0$ to infinity, such that $-\pi < \arg(-w) \le \pi$.

It follows that the function is complex for real arguments $u > 0$, $x = e^u > 1$. The imaginary part is

$$\mathrm{Im}[\mathrm{Li}_p(e^u)] = -\frac{\pi u^{p-1}}{\Gamma(p)}\ , \tag{3.1}$$

so

$$\mathrm{Im}[\mathrm{Li}_{-n}(e^u)] = 0, \quad \text{for } n = 0,\ 1,\ 2,\ \cdots\ .$$

4. Derivatives

From Eqn (1.2),

$$\frac{d}{dw}\mathrm{Li}_p(e^w) = \mathrm{Li}_{p-1}(e^w), \quad \frac{d^m}{dw^m}\mathrm{Li}_p(e^w) = \mathrm{Li}_{p-m}(e^w)\ ; \tag{4.1}$$

or

$$z\frac{d}{dz}\mathrm{Li}_p(z) = \mathrm{Li}_{p-1}(z), \quad \left(z\frac{d}{dz}\right)^m \mathrm{Li}_p(z) = \mathrm{Li}_{p-m}(z)\ . \tag{4.2}$$

5. Special Values of the Argument

Obviously,

$$\mathrm{Li}_p(0) = 0\ . \tag{5.1}$$

For $z = -1$ and $z = -i$, the polylogarithm reduces to the Riemann zeta function and related functions ([4] § 23.2):

$$\mathrm{Li}_p(1) = \zeta(p), \quad \text{for } p > 1\ , \tag{5.2}$$

$$\mathrm{Li}_p(-1) = -\eta(p)\ , \tag{5.3}$$

and

$$\mathrm{Li}_p(-i) = 2^{-p}\,\eta(p) - i\,\beta(p)\ ; \tag{5.4}$$

where

$$\zeta(p) = \frac{1}{\Gamma(p)}\int_0^\infty \frac{t^{p-1}}{e^t - 1}dt = \sum_{k=1}^\infty \frac{1}{k^p}\ ,$$

$$\eta(p) = \frac{1}{\Gamma(p)}\int_0^\infty \frac{t^{p-1}}{e^t + 1}dt = -\sum_{k=1}^\infty \frac{(-1)^k}{k^p} = (1 - 2^{1-p})\,\zeta(p), \quad \eta(1) = \ln(2)\ ,$$

and

$$\beta(p) = \frac{1}{\Gamma(p)}\int_0^\infty \frac{t^{p-1}}{e^t + e^{-t}}dt = \sum_{k=0}^\infty \frac{(-1)^k}{(2k+1)^p}\ .$$

Another related function will be required later:

$$\lambda(p) = \frac{1}{\Gamma(p)}\int_0^\infty \frac{t^{p-1}}{e^t - e^{-t}}dt = \sum_{k=0}^\infty \frac{1}{(2k+1)^p} = (1 - 2^{-p})\,\zeta(p)\ .$$

6. Special Values of the Parameter

From Eqn (1.1),

$$\mathrm{Li}_1(z) = -\ln(1 - z) \,. \tag{6.1}$$

Hence, by Eqn (4.2),

$$\mathrm{Li}_0(z) = \frac{z}{1 - z}\,,\ \ \mathrm{Li}_{-1}(z) = \frac{z}{(1 - z)^2}\,,\ \ \mathrm{Li}_{-2}(z) = \frac{z(z + 1)}{(1 - z)^3}\,,\ \ \cdots \,. \tag{6.2}$$

In general, $\mathrm{Li}_n(z)$ is easy to compute for integer $n \le 1$:

$$\mathrm{Li}_{-n}(z) = \frac{1}{(1 - z)^{n+1}} \sum_{k=1}^{n} a_{n,k}\, z^k, \quad \text{for } n > 0\,, \tag{6.3}$$

or

$$\mathrm{Li}_{-n}(z) = \sum_{k=1}^{n+1} \frac{b_{n,k}}{(1 - z)^k}, \quad \text{for } n > 0\,, \tag{6.4}$$

where the coefficients can be obtained by the recurrence equations:

$$a_{n,k} = (n + 1 - k)\, a_{n-1,k-1} + k\, a_{n-1,k}$$

and

$$b_{n,k} = (k - 1)\, b_{n-1,k-1} - k\, b_{n-1,k} \,.$$

The first few of these coefficients are tabulated below.

	$a_{n,k}$						$b_{n,k}$							
n k	1	2	3	4	5	6	0	1	2	3	4	5	6	7
0	1						1	1						
1	1							–1	1					
2	1	1						1	–3	2				
3	1	4	1					–1	7	–12	6			
4	1	11	11	1				1	–15	50	–60	24		
5	1	26	66	26	1			–1	31	–180	390	–360	120	
6	1	57	302	302	57	1		1	–63	602	–2100	3360	–2520	720

The case $n = 0$, which is somewhat anomalous in both representations, is included.

The b coefficients can be expressed as

$$b_{n,k} = (-1)^{n+k+1}(k - 1)!\ T^{(k)}_{n+1}\,,$$

where $T^{(k)}_n$ is the Stirling number of the second kind ([4] § 24.1.4), defined by

$$(e^t - 1)^k = k! \sum_{j=k}^{\infty} T^{(k)}_j \frac{t^j}{j!}\,.$$

(This notation is not standard. The script S recommended in [4], even when available, may not be easily distinguishable from italic, which is reserved for the Stirling numbers of the first kind.)

For negative real arguments, $|\mathrm{Li}_{-n}(-x)| \le |\eta(-n)| \approx 2n!/\pi^{n+1}$, but the sum of the a coefficients is $n!$, so the algorithm suffers from cancellation errors for large n; see § 13.

A minor practical difficulty is that an array of about n elements is required for these coefficients, which is a limitation in Fortran where the size of the array must be a constant. However, cancellation or overflow will occur before this becomes a real problem, so other methods must be used anyway.

7. The Dilogarithm

The case $\mathrm{Li}_2(z)$, the dilogarithm ([4] § 27.7),

$$\mathrm{Li}_2(z) = -\int_0^z \frac{\ln(1-t)}{t}\,dt\ , \tag{7.1}$$

is of particular importance, since it arises in many integrals that cannot be expressed in terms of elementary functions. For this reason, it is included in many computer algebra systems, such as Maple ([5]), where it takes the form $\mathrm{dilog}(z) = \mathrm{Li}_2(1-z)$.

The name of the function comes from the fact that it is derived from the logarithm in much the same way as the logarithm is derived from simple rational functions.

It has many special properties, as well as those of the general polylogarithm. In particular,

$$\mathrm{Li}_2(z) + \mathrm{Li}_2(1-z) = \frac{\pi^2}{6} - \ln(z)\ln(1-z)\ ; \tag{7.2}$$

and

$$\mathrm{Li}_2(z) + \mathrm{Li}_2(1/z) = -\frac{\pi^2}{6} - \tfrac{1}{2}\ln(-z)^2\ , \tag{7.3}$$

which is a special case of Eqn (10.1–2). These equations, together with the group of transformations

$$x,\ \ \frac{1}{x},\ \ 1-x,\ \ \frac{1}{1-x},\ \ \frac{x-1}{x},\ \text{ and } \frac{x}{x-1}\ ,$$

allow any real argument to be reduced to $|x| \le \tfrac{1}{2}$, so $\mathrm{Li}_2(x)$ can be computed efficiently using Eqn (8.1). The three remaining cases are

$$\mathrm{Li}_2(x) - \mathrm{Li}_2\left(\frac{1}{1-x}\right) = -\frac{\pi^2}{6} + \tfrac{1}{2}\ln(1-x)\ln\left(\frac{1-x}{x^2}\right)\ ,$$

$$\mathrm{Li}_2(x) - \mathrm{Li}_2\left(\frac{x-1}{x}\right) = \frac{\pi^2}{6} + \tfrac{1}{2}\ln(x)\ln\left(\frac{x}{(1-x)^2}\right)\ ,$$

and

$$\mathrm{Li}_2(x) + \mathrm{Li}_2\left(\frac{x}{x-1}\right) = -\tfrac{1}{2}\ln(1-x)^2\ .$$

The trilogarithm, $\mathrm{Li}_3(z)$, etc. satisfy related equations of increasing complexity, but they are not generally useful for computation.

8. Power Series in z

Writing Eqn (1.1) as

$$\mathrm{Li}_p(z) = \frac{z}{\Gamma(p)}\int_0^\infty \frac{e^{-t}\,t^{p-1}}{1-ze^{-t}}\,dt\ ,$$

the integrand can be expanded by the binomial theorem and integrated term by term, giving

$$\mathrm{Li}_p(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^p}\ ,\ \ \text{for } |z| < 1\ . \tag{8.1}$$

The inequality is strict only for $p \le 0$, or $p \le 1$ when $z = 1$, so Eqn (5.2–4) follow in those ranges.

The remainder after a finite number of terms is given by

$$\mathrm{Li}_p(z) = \sum_{k=1}^{m} \frac{z^k}{k^p} + \frac{z^{m+1}}{\Gamma(p)}\int_0^\infty \frac{e^{-mt}\,t^{p-1}}{e^t - z}\,dt\ , \tag{8.2}$$

by integration by parts.

For integer parameters n, this series in works well for $|z| \ll 1$. The powers are simpler to compute for small n, but the series converges faster for larger n.

The case $Li_{n+½}(z)$ is of practical importance. Computing $k^{n+½}$ as $k^n\sqrt{k}$ is reasonably fast; or, if the maximum number of terms required is known in advance, a pre-computed table of square roots can be used.

For real parameters p this algorithm is much slower, since the powers must be computed by $k^p = e^{p\ln(k)}$. Again, if the number of terms is known, a considerable saving can be obtained by using a pre-computed array of ln(k).

In principle, only the powers of primes need be computed directly (using a table of their logarithms), the powers of composite numbers being obtained from those of their factors. However, the additional complication of this algorithm costs more time than it saves, though it is very advantageous in computing the zeta function (§ 23).

9. Power Series in w

By Taylor’s theorem, using Eqn (4.1),

$$Li_p(e^{c+w}) = \sum_{k=0}^{\infty} Li_{p-k}(e^c)\frac{w^k}{k!}, \text{ for } |w| < |c| . \tag{9.1}$$

In particular,

$$Li_p(-e^{w}) = -\sum_{k=0}^{\infty} \eta(p-k)\frac{w^k}{k!}, \text{ for } |w| < \pi . \tag{9.2}$$

To obtain the corresponding series for $Li_p(e^w)$, consider the Mellin transform of $Li_p(e^{-u})$ with respect to u ([6]):

$$M_p(q) = \frac{1}{\Gamma(p)}\int_0^{\infty}\int_0^{\infty}\frac{t^{p-1}u^{q-1}}{e^{t+u}-1}dt\, du .$$

Note the symmetry of the integrand.

The change of variable $t = rs$, $u = r(1-s)$ allows the integrals to be separated:

$$M_p(q) = \frac{1}{\Gamma(p)}\int_0^1 s^{q-1}(1-s)^{p-1}ds \int_0^{\infty}\frac{r^{p+q+1}}{e^r-1}dr$$

$$= \Gamma(q)\,\zeta(p+q) ;$$

and the original function is recovered through the inverse Mellin transform:

$$Li_p(e^{-u}) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}\Gamma(q)\,\zeta(p+q)u^{-q}\, dq .$$

where c is a constant to the right of the poles of the integrand.

The path of integration may be converted into a closed contour, and the poles of are those of $\Gamma(q)$ at $q = 0, -1, -2, \cdots$, and $\zeta(p+q)$ at $q = 1 - p$. Summing the residues gives

$$Li_p(e^{w}) = \sum_{k=0}^{\infty}\zeta(p-k)\frac{w^k}{k!} + \Gamma(1-p)(-w)^{p-1}, \text{ for } |w| < 2\pi, \ p \neq 1, 2, 3, \cdots . \tag{9.3}$$

Integer Parameters

If the parameter is a positive integer, n, both the term in $k = n - 1$ and the gamma function become infinite, although their sum does not. This gives rise to computational difficulties when p is very close to a positive integer. The sum of the two large terms can be expanded in powers of ε, where $p = n + \varepsilon$, $|\varepsilon| \ll 1$:

$$\mathrm{Li}_{n+\varepsilon}(e^{\omega}) = \sum_{\substack{k=0 \\ k \neq n-1}}^{\infty} \zeta(n+\varepsilon-k)\frac{\omega^k}{k!} + Q\frac{\omega^{n-1}}{(n-1)!}\,, \tag{9.4}$$

where

$$\begin{aligned} Q &= \zeta(1+\varepsilon) + \Gamma(1-n-\varepsilon)(-\omega)^{n+\varepsilon-1} \\ &= \gamma + \psi(n) - \ln(-\omega) + \left\{\gamma_1 - \frac{[\psi(n) - \ln(-\omega)]^2}{2} + \frac{\pi^2}{6} + \frac{\psi'(n)}{2}\right\}\varepsilon \\ &\quad + \left\{\gamma_2 + \frac{[\psi(n) - \ln(-\omega)]^3}{6} + \left[\frac{\pi^2}{6} + \frac{\psi'(n)}{2}\right][\psi(n) - \ln(-\omega)] + \frac{\psi''(n)}{6}\right\}\varepsilon^2 + O(\varepsilon^3)\,. \end{aligned}$$

Here γ_n is the generalized Euler constant ([4] § 23.2.5):

$$\gamma_n = \lim_{m\to\infty}\left\{\sum_{k=1}^{m}\frac{\ln(k)^n}{k} - \frac{\ln(m)^{n+1}}{n+1}\right\},\quad \gamma = \gamma_0\,;$$

$\psi(n)$ is the digamma function, the logarithmic derivative of the gamma function ([4] § 6.3):

$$\psi(p) = \frac{d}{dp}\ln(\Gamma(p)),\quad \psi(n) = H_{n-1} - \gamma\,,$$

where H_n is the harmonic number

$$H_n = \sum_{k=1}^{n}\frac{1}{k}\,;$$

and $\psi^{(m)}(n)$ is the polygamma function ([4] § 6.4):

$$\psi^{(m)}(p) = \frac{d^m}{dp^m}\psi(p),\quad \psi^{(m)}(n) = (-1)^m\, m!\left\{\sum_{k=1}^{n-1}k^{-(m+1)} - \zeta(m+1)\right\}.$$

For positive integer parameters, the limit as $\varepsilon \to 0$ gives

$$\mathrm{Li}_n(e^{\omega}) = \sum_{\substack{k=0 \\ k\neq n-1}}^{\infty}\zeta(n-k)\frac{\omega^k}{k!} + [H_{n-1} - \ln(-\omega)]\frac{\omega^{n-1}}{(n-1)!},\quad \text{for } |\omega| < 2\pi,\quad n = 1, 2, 3, \cdots\,. \tag{9.5}$$

An Optimization

The Riemann zeta function for negative arguments must be computed using ([4] § 23.2.6)

$$\zeta(p) = 2\,(2\pi)^{p-1}\sin(\tfrac{1}{2}\pi p)\,\Gamma(1-p)\,\zeta(1-p)\,.$$

Hence the computation of Eqn (9.3) can be made more efficient by re-writing it as

$$\begin{aligned} \mathrm{Li}_p(e^{\omega}) = \sum_{k=0}^{m}\zeta(p-k)\frac{\omega^k}{k!} \\ &+ 2\,(2\pi)^{p-1}\sum_{k=m+1}^{\infty}\sin(\tfrac{1}{2}\pi[p-k])\,\Gamma(1-p+k)\,\zeta(1-p+k)\frac{(\omega/2\pi)^k}{k!} \\ &+ \Gamma(1-p)\,(-\omega)^{p-1}\,, \end{aligned} \tag{9.6}$$

where $m = \lfloor p \rfloor$. For $p < 0$, the first sum disappears.

This not only saves the computation of many separate sines and gamma functions, as each can be obtained from the previous one:

$$\sin(\tfrac{1}{2}\pi[p-1]) = -\cos(\tfrac{1}{2}\pi p), \quad \cos(\tfrac{1}{2}\pi[p-1]) = \sin(\tfrac{1}{2}\pi p) ,$$

and

$$\Gamma(p+1) = p\,\Gamma(p) ;$$

but also simplifies the test for convergence, since the oscillatory factor is separated from the zeta function.

The same optimization can also be applied to Eqn (9.4–5). For integer parameters, half the terms in the second sum are zero, the sines in the remaining terms reduce to –1, and the gamma function becomes a factorial:

$$\mathrm{Li}_n(e^w) = \sum_{k=0}^{n-2} \zeta(n-k)\frac{w^k}{k!} + [H_{n-1} - \ln(-w)]\frac{w^{n-1}}{(n-1)!} - \frac{w^n}{2n!} \qquad (9.7)$$

$$- \frac{w^{n+1}}{2\pi^2}\sum_{j=0}^{\infty} \zeta(2j+2)\frac{(2j+1)!}{(2j+n+1)!}[-(w/2\pi)^2]^j .$$

Similarly, when $p = n + \tfrac{1}{2}$, the sines reduce to $-1/\sqrt{2}$. The gamma functions could again be simplified to factorials:

$$\Gamma(n+\tfrac{1}{2}) = (2\pi)^{\frac{1}{2}}\, 2^{\frac{1}{2}-2n}\frac{(2n-1)!}{(n-1)!} .$$

However, in both these cases, it is more efficient to use pre-computed tables of the zeta and gamma functions.

The eta series, Eqn (9.2), can be treated like the zeta series, using

$$\eta(p) = -2\pi^{p-1}\sin(\tfrac{1}{2}\pi p)\,\Gamma(1-p)\,\lambda(1-p) .$$

In this case there is no problem with integer parameters.

Convergence

The circles of convergence of these series, and of Eqn (18.2), are determined by the distance from the singularity at $w = 0$ (or, in the case of Eqn (9.3–5), from those at $w = -2\pi i$).

In terms of z, the regions of convergence are more complicated. For Eqn (9.2), the boundary crosses the negative real axis at $z = -e^{-\pi}$, and the imaginary axis at $z = -ie^{-\sqrt{3}\pi/2}$; it touches the positive real axis, from both sides, at $z = 1$. For (9.3–5), for the region corresponding to $|\mathrm{Im}(w)| \le \pi$, it crosses the positive real axis at $z = e^{-2\pi}$, the imaginary axis at $z = -ie^{-\sqrt{15}\pi/2}$, and meets the negative real axis at $z = -e^{-\sqrt{3}\pi}$. The region for the eta series is wholly contained in that for the zeta series, and it is faster only in a small area around $z = -1$. However, it is sometimes useful, particularly for computing $\mathrm{Li}_p(x)$ for real $x < 0$, where the zeta series requires the use of complex arithmetic.

In principle, Eqn (9.1) provides a method of computing $\mathrm{Li}_p(e^w)$ for $|w| \ge 2\pi$, but it is obviously very inefficient, and better algorithms are given below. It is still useful for checking.

10. Reciprocal Formulae

Terms involving zeta functions of odd arguments can be eliminated between the series for $\mathrm{Li}_n(e^{\omega})$ and $\mathrm{Li}_n(e^{-\omega})$ in Eqn (9.5). Then, because $\zeta(-2k) = 0$,

$$\mathrm{Li}_n(e^{\omega}) + (-1)^n \mathrm{Li}_n(e^{-\omega}) = 2\sum_{k=0}^{\lfloor n/2 \rfloor} \zeta(2k)\frac{\omega^{n-2k}}{(n-2k)!} - i\pi\frac{\omega^{n-1}}{(n-1)!} \tag{10.1}$$

$$= -\sum_{j=0}^{n} B_j \frac{(2\pi i)^j}{j!}\frac{\omega^{n-j}}{(n-j)!}$$

$$= -\frac{2\pi i}{n!} B_n\left(\frac{\omega}{2\pi i}\right),$$

and from Eqn (9.2),

$$\mathrm{Li}_n(-e^{\omega}) + (-1)^n \mathrm{Li}_n(-e^{-\omega}) = -2\sum_{k=0}^{\lfloor n/2 \rfloor} \eta(2k)\frac{\omega^{n-2k}}{(n-2k)!} \tag{10.2}$$

$$= \sum_{j=0}^{n} (1 - 2^{1-j})B_j \frac{(2\pi i)^j}{j!}\frac{\omega^{n-j}}{(n-j)!}.$$

The Bernoulli polynomials and numbers ([4] § 23.1) are defined by

$$\frac{te^{xt}}{e^t - 1} = \sum_{k=0}^{\infty} B_k(x)\frac{t^k}{k!}, \quad B_k = B_k(0);$$

where

$$B_0 = 1, \quad B_1 = -\frac{1}{2}, \quad B_{2k} = (-1)^{k+1}\frac{2\,(2k)!}{(2\pi)^{2k}}\zeta(2k), \quad \text{and } B_{2k+1} = 0, \quad \text{for } k = 1, 2, 3, \cdots.$$

Computationally, it is more convenient to use tables of zeta and eta functions.

These formulae are conveniently used in conjunction with Eqn (8.1) for arguments $|z| > 1$. The two forms are useful when the argument is real, to avoid complex arithmetic.

For $n < 0$, the sums on the right are zero, so

$$\mathrm{Li}_{-n}(z) + (-1)^n \mathrm{Li}_{-n}(1/z) = 0, \quad \text{for } n = 1, 2, 3, \cdots. \tag{10.3}$$

Real Parameters

For real parameters, an equation related to Eqn (10.1) is:

$$\mathrm{Li}_p(e^{\omega}) + e^{i\pi p}\mathrm{Li}_p(e^{-\omega}) = \frac{e^{i\pi p/2}(2\pi)^p}{\Gamma(p)}\zeta\left(1 - p, \ \frac{\omega}{2\pi i}\right), \tag{10.4}$$

where

$$\zeta(p, \alpha) = \sum_{k=0}^{\infty}\frac{1}{(k+\alpha)^p}, \quad \text{for } p > 1$$

$$= 2(2\pi)^{p-1}\Gamma(1-p)\sum_{k=1}^{\infty} k^{p-1}\sin(2\pi k\alpha + \tfrac{1}{2}\pi p), \quad \text{for } p < 1$$

is the generalized zeta function of Hurwitz ([7] § 13.11, [8] § 1.10). The first form is just half of Eqn (13.1), and the second can be obtained from Eqn (8.1) for $|z| = 1$ (where it is least useful). Neither seems helpful computationally.

11. Asymptotic Formulae

Consider

$$\mathrm{Li}_p(-e^{w}) = -\frac{1}{\Gamma(p)}\int_0^{\infty}\frac{t^{p-1}}{e^{t-w}+1}dt\ ,$$

where $w = u + iv$. The denominator of the integrand is close to one for $t \ll u$, and very large for $t \gg u$, which suggests splitting the range of integration at $t = u$, giving

$$\mathrm{Li}_p(-e^{w}) = -\frac{1}{\Gamma(p)}\left\{\int_0^{u} t^{p-1}dt + \int_0^{u}\frac{t^{p-1}}{e^{w-t}+1}dt + \int_u^{\infty}\frac{t^{p-1}}{e^{t-w}+1}dt\right\} .$$

Putting $s = w - t$ in the second integral and $s = t - w$ in the third gives

$$\mathrm{Li}_p(-e^{w}) = -\frac{w^p}{\Gamma(p+1)} + \frac{1}{\Gamma(p)}\int_0^{\infty}\frac{(w-s)^{p-1}-(w+s)^{p-1}}{e^s+1}ds + \frac{1}{\Gamma(p)}\int_u^{\infty}\frac{(w-s)^{p-1}}{e^s+1}ds\ .$$

Reverting to $t = s - w$ in the last integral gives $(-1)^{p-1}\,\mathrm{Li}_p(-e^{-w})$, so

$$\mathrm{Li}_p(-e^{w}) + (-1)^p\,\mathrm{Li}_p(-e^{-w}) = -\frac{w^p}{\Gamma(p+1)} + \frac{1}{\Gamma(p)}\int_0^{\infty}\frac{(w-s)^{p-1}-(s-w)^{p-1}}{e^s+1}ds\ .$$

If p is a positive integer, expanding the terms in the numerator of the integrand and integrating term by term gives Eqn (10.2). Otherwise, the binomial theorem holds only for $s < |u|$, but for $u \gg 1$ the integrand is so small beyond this point that the error incurred is $O(e^{-w})$. The second term on the left is of the same order, so it may be dropped, giving

$$\mathrm{Li}_p(-e^{w}) \sim -2\sum_{k=0}^{\infty}\eta(2k)\frac{w^{p-2k}}{\Gamma(p-2k+1)} + O(e^{-w}),\ \text{ for } \mathrm{Re}(w) \gg 1\ . \tag{11.1}$$

Similarly, with a little extra care over the singularity,

$$\mathrm{Li}_p(e^{w}) \sim 2\sum_{k=0}^{\infty}\zeta(2k)\frac{w^{p-2k}}{\Gamma(p-2k+1)} - i\pi\frac{w^{p-1}}{\Gamma(p)} + O(e^{-w}),\ \text{ for } \mathrm{Re}(w) \gg 1\ , \tag{11.2}$$

Again, the two forms are useful for real arguments. In each case the leading term is

$$\mathrm{Li}_p(-e^{w}) \sim -\frac{w^p}{\Gamma(p+1)}\ . \tag{11.3}$$

12. Contour Integral

Eqn (1.2) may be extended to negative values of p by the standard technique of writing it as a contour integral ([7] § 12.22):

$$\mathrm{Li}_p(e^{w}) = -\frac{\Gamma(1-p)}{2\pi i}\int_{\infty}^{(0+)}\frac{(-t)^{p-1}}{e^{t-w}-1}dt\ , \tag{12.1}$$

where the contour starts at infinity on the positive real axis, circles the origin anticlockwise, and returns to infinity.

13. Series for Negative Parameter

The contour in Eqn (12.1) can be modified so that it encloses the poles of the integrand, at $t = w - 2k\pi i$, and the integral can be evaluated as the sum of the residues:

$$\mathrm{Li}_p(e^{w}) = \Gamma(1-p)\sum_{k=-\infty}^{\infty}(2k\pi i - w)^{p-1},\ \text{ for } p < 0\ . \tag{13.1}$$

Expanding $(1 - w/2kpi)^{p-1}$ by the binomial theorem gives an alternative derivation of Eqn (9.3). (It actually gives the form of Eqn (9.6) more directly.)

This series can be summed using the Euler–Maclaurin formula ([4] § 23.1.30):

$$\mathrm{Li}_p(e^w) = G(1-p)\left\{ \sum_{k=l+1}^{m-1} (2kpi - w)^{p-1} \right. \tag{13.2}$$
$$+ \frac{i}{2pp}\left[(2mpi - w)^p - (2lpi - w)^p\right]$$
$$+ \frac{1}{2}\left[(2mpi - w)^{p-1} + (2lpi - w)^{p-1}\right]$$
$$\left. - i\sum_{j=1}^{¥} \frac{z(2j)}{p}\,\frac{G(p)}{G(p-2j+1)}\left[(2mpi - w)^{p-2j} - (2lpi - w)^{p-2j}\right] \right\} .$$

As in Eqn (10.1–2), the coefficients are more concisely expressed as Bernoulli numbers, but the form above is computationally more convenient.

The values of l and m can be chosen to make the first and last terms in the first sum approximately equal in magnitude, and to minimize the total amount of computation required. The second sum is easier to compute than the first, since each new term can be generated from the previous one, but it is only an asymptotic series, so sufficient terms in the first sum are needed before the second can give the required accuracy.

For integer parameters $n \ll 0$, this algorithm is preferable to the rational expressions, Eqn (6.2–4), since it is not subject to cancellation.

14. Square Formula

From Eqn (1.1),

$$\mathrm{Li}_p(z) + \mathrm{Li}_p(-z) = 2^{1-p}\mathrm{Li}_p(z^2) . \tag{14.1}$$

This provides a way of computing $\mathrm{Li}_p(x)$ for negative real x in terms of functions of positive arguments.

To a limited extent, successive application also does the opposite:

$$\mathrm{Li}_p(z) = -\sum_{k=0}^{m-1} 2^{k(1-p)}\mathrm{Li}_p(-z^{2^k}) + 2^{m(1-p)}\mathrm{Li}_p(z^{2^m}) , \tag{14.2}$$

which converges for $|z| < 1$, and

$$\mathrm{Li}_p(z) = \sum_{k=1}^{m} 2^{k(p-1)}\mathrm{Li}_p(-z^{2^{-k}}) + 2^{m(p-1)}\mathrm{Li}_p(z^{2^{-m}}) . \tag{14.3}$$

The first of these has been proposed ([9], [10]), but generally these formulae are not useful for computation.

15. m^{th}-Root Formula

Eqn (14.1) may be re-written as

$$\mathrm{Li}_p(z) = 2^{p-1}[\mathrm{Li}_p(\sqrt{z}) + \mathrm{Li}_p(-\sqrt{z})] . \tag{15.1}$$

This provides a method of expressing functions of large arguments, $|z| \gg 1$, (or indeed $|z| \ll 1$, though this is unlikely to be useful) in terms of those with $|z|$ closer to one. This can be applied recursively until $|z|$ is small enough (or large enough) for Eqn (9.3–5) to be used; for example,

$$\mathrm{Li}_p(z) = 4^{p-1}[\mathrm{Li}_p(\sqrt[4]{z}) + \mathrm{Li}_p(-\sqrt[4]{z}) + \mathrm{Li}_p(i\sqrt[4]{z}) + \mathrm{Li}_p(-i\sqrt[4]{z})] .$$

In practice, this is not a useful algorithm, partly because of the difficulty of implementing recursion in Fortran, but more importantly because of the inefficiency of computing many polylogarithms separately.

In fact, Eqn (15.1) is a special case of a more general property. Consider the factorization

$$(a^m - 1) = \prod_{k=0}^{m-1} (\omega^k a - 1), \quad \text{where } \omega = e^{2\pi i/m} .$$

Applying this to the denominator of

$$\mathrm{Li}_p(e^{\omega}) = \frac{m^p}{\Gamma(p)} \int_0^{\infty} \frac{t^{p-1}}{e^{mt-\omega} - 1} dt$$

and expanding in partial fractions gives

$$\mathrm{Li}_p(e^{\omega}) = m^{p-1} \sum_{k=0}^{m-1} \mathrm{Li}_p\left(e^{(\omega + 2k\pi i)/m}\right) , \tag{15.2}$$

where the sum is over the m complex m^{th} roots of the argument.

Combining this with the zeta series, Eqn (9.3), and interchanging the order of summation, the zeta functions need be computed only once each, so the algorithm is reasonably efficient:

$$\mathrm{Li}_p(e^{\omega}) = m^{p-1} \left\{ \sum_{k=0}^{\infty} \frac{\zeta(p-k)}{k!} \sum_{j=l}^{l+m-1} \left[\frac{\omega + 2j\pi i}{m}\right]^k + \Gamma(1-p) \sum_{j=l}^{l+m-1} \left[-\frac{\omega + 2j\pi i}{m}\right]^{p-1} \right\} . \tag{15.3}$$

Because of the periodicity of the exponential function in Eqn (15.2), l can be chosen to reduce the imaginary parts of the expressions $(\omega + 2j\pi i)/m$ to the range $\pm\pi$.

For all $k > 0$, each term in the inner sum can easily be obtained from the corresponding term for $k - 1$. This computation requires two arrays of m elements. However, since Eqn (11.1–2) can be used for very large arguments, these arrays need be of only moderate size.

The region of convergence of this algorithm is the intersection of the circles of convergence of the functions in the sum, so all the arguments must lie within the circle of convergence of the zeta series, Eqn (9.3–5). A sufficient condition for this is $|\mathrm{Re}(\omega)/m - i\pi| < 2\pi$, or $|\mathrm{Re}(\omega)| < m\sqrt{3}\pi$.

For a given ω, the requirement is $m > |\mathrm{Re}(\omega)|/\sqrt{3}\pi$, but computationally the choice of m is not critical; larger values give faster convergence of the outer sum, at the cost of more terms in the inner.

The same process can be applied using Eqn (9.4–7), although there is probably no reason to use it for integer parameters.

16. Debye Functions

Changing the variable in Eqn (1.2) to $s = t - \omega$ and expanding the numerator by the binomial theorem gives

$$\mathrm{Li}_n(e^{\omega}) = \sum_{k=0}^{n-1} Z_{n-k}(-\omega) \frac{\omega^k}{k!}, \quad \text{for } n > 0 , \tag{16.1}$$

where

$$Z_p(z) = \frac{1}{\Gamma(p)} \int_z^{\infty} \frac{t^{p-1}}{e^t - 1} dt, \quad Z_1(z) = -\ln(1 - e^{-z}), \quad Z_p(0) = \zeta(p) ,$$

is the ‘incomplete zeta function’ ([2] § 4), or Debye function ([4] § 27.1). This function is interesting in its own right, but not always easy to compute. One method is

$$Z_n(z) = \sum_{k=0}^{n-1} \mathrm{Li}_{n-k}(e^{-z}) \frac{z^k}{k!}, \quad \text{for } n > 0 . \tag{16.2}$$

The symmetry with Eqn (16.1) is remarkable, but not helpful here.

(This function has no generally accepted name; that used here is from [2].)

17. Real Arguments

For real argument x, it is convenient to ignore the imaginary part of the function for $x > 1$, which is in any case elementary (Eqn (3.1)), and deal only with the real part. Many of the formulae appear in two forms, convenient for positive and negative real arguments. Otherwise, most of the algorithms are essentially unchanged, though obviously real arithmetic is faster than complex.

Eqn (13.1) is fundamentally complex, but a significant optimization can still be made. For a positive real arguments, e^u, the double-sided sum can be ‘folded’, with the term in $k = 0$ taken out:

$$\begin{aligned} \mathrm{Li}_p(e^u) &= \Gamma(1-p)\left\{(-u)^{p-1} + \sum_{k=1}^{\infty}\left[(2k\pi i - u)^{p-1} + (-2k\pi i - u)^{p-1}\right]\right\} . \qquad (17.1) \\ &= \Gamma(1-p)\left\{(-u)^{p-1} + 2\sum_{k=1}^{\infty} \rho_k^{p-1}\cos([p-1]\theta_k)\right\} , \end{aligned}$$

where $\rho_k\cos(\theta_k) = -u$ and $\rho_k\sin(\theta_k) = 2k\pi$. The summand is $2\,\mathrm{Re}[(2k\pi i - u)^{p-1}]$.

Negative arguments, $-e^u = e^{u-i\pi}$, can be treated similarly, the even multiples of πi becoming odd multiples:

$$\begin{aligned} \mathrm{Li}_p(-e^u) &= \Gamma(1-p)\sum_{k=0}^{\infty}\left[([2k+1]\pi i - u)^{p-1} + (-[2k+1]\pi i - u)^{p-1}\right] . \qquad (17.2) \\ &= 2\Gamma(1-p)\sum_{k=0}^{\infty} \rho_k^{p-1}\cos([p-1]\theta_k) , \end{aligned}$$

where $\rho_k\cos(\theta_k) = -u$ and $\rho_k\sin(\theta_k) = (2k+1)\pi$.

The Euler–Maclaurin series, Eqn (13.2), can be treated in the same way, with $l + m = 0$ for positive arguments, and $l + m + 1 = 0$ for negative.

Eqn (15.3) is again complex. For real arguments, symmetry roughly halves the number of different terms that need to be calculated in the inner sum, but the computation of the zeta functions cannot be reduced, so the advantage is not great.

18. Related Functions

Inverse Tangent Integrals

For pure imaginary arguments, $z = iy = ie^v$,

$$\mathrm{Li}_p(-iy) = 2^{-p}\,\mathrm{Li}_p(-y^2) - i\,\mathrm{Ti}_p(y) , \qquad (18.1)$$

where $\mathrm{Ti}_p(y)$ is the inverse tangent integral ([1] Ch. VII § 1.2). Its properties follow directly from those of the polylogarithm, or can be derived in very similar ways. They are simply listed here.

From Eqn (5.4):

$$\mathrm{Ti}_p(-1) = -\beta(p) .$$

From Eqn (6.1–2):

$$\mathrm{Ti}_1(y) = \tan^{-1}(y),\quad \mathrm{Ti}_0(y) = \frac{y}{1+y^2},\quad \mathrm{Ti}_{-1}(y) = \frac{y(1-y^2)}{(1+y^2)^2},\quad \cdots .$$

The name of the function derives from:

$$\mathrm{Ti}_2(y) = \int_0^y \frac{\tan^{-1}(t)}{t}\,dt .$$

From Eqn (8.1):

$$\mathrm{Ti}_p(y) = \sum_{k=0}^{\infty} \frac{(-1)^k\, y^{2k+1}}{(2k+1)^p},\quad \text{for } |y| < 1 .$$

From Eqn (9.1):

$$\mathrm{Ti}_p(-e^{v}) = -\sum_{k=1}^{\infty} b(p-k)\frac{v^k}{k!}, \quad \text{for } |v| < \frac{p}{2} . \tag{18.2}$$

The technique of Eqn (9.6) can be applied, using ([8] § 1.12)

$$b(p) = (½p)^{p-1}\cos(½pp)\,G(1-p)\,b(1-p) .$$

As in Eqn (10.1–2), because $b(-2k-1) = 0$:

$$\mathrm{Ti}_n(e^{v}) - (-1)^n\ \mathrm{Ti}_n(e^{-v}) = 2\sum_{k=1}^{\lceil n/2\rceil} b(2k-1)\,\frac{v^{n-2k+1}}{(n-2k+1)!} .$$

As in Eqn (11.1–2):

$$\mathrm{Ti}_p(e^{v}) \sim 2\sum_{k=1}^{\infty} b(2k-1)\,\frac{v^{p-2k+1}}{G(p-2k+2)} + O(e^{-v}) .$$

From Eqn (13.1):

$$\mathrm{Ti}_p(e^{v}) = -½i\,G(1-p)\sum_{k=-\infty}^{\infty} (-1)^k\,([k-½]pi - v)^{p-1} .$$

Legendre's Chi Function

Legendre's chi function ([1] Ch. VII § 1.1, [11]) is

$$\begin{aligned} c_p(z) &= ½[\mathrm{Li}_p(z) - \mathrm{Li}_p(-z)] \\ &= \mathrm{Li}_p(z) - 2^{-p}\,\mathrm{Li}_p(z^2) \\ &= i\,\mathrm{Ti}_p(iz) . \end{aligned} \tag{18.3}$$

Again, the properties of this function follow directly from those of the polylogarithm.

As in Eqn (5.2–4):

$$c_p(-1) = -l(p) .$$

From Eqn (6.1–2):

$$c_1(z) = \tanh^{-1}(z), \quad c_0(z) = \frac{z}{1-z^2}, \quad c_{-1}(z) = \frac{z(1+z^2)}{(1-z^2)^2}, \quad \cdots .$$

From Eqn (8.1):

$$c_p(z) = \sum_{k=0}^{\infty} \frac{z^{2k+1}}{(2k+1)^p}, \quad \text{for } |z| < 1 .$$

From Eqn (9.3) and Eqn (9.5):

$$c_p(e^{w}) = \sum_{k=0}^{\infty} l(p-k)\frac{w^k}{k!} + ½G(1-p)(-w)^{p-1}, \quad \text{for } |w| < p, \quad p \neq 1, 2, 3, \cdots ,$$

and

$$c_n(e^{w}) = \sum_{\substack{k=0 \\ k \neq n-1}}^{\infty} l(n-k)\frac{w^k}{k!} + ½[H_{n-1} - \ln(-½w)]\frac{w^{n-1}}{(n-1)!}, \quad \text{for } |w| < p, \quad n = 1, 2, 3 \cdots .$$

These can be optimized, as in Eqn (9.6–7), using

$$l(p) = -p^{p-1}\sin(½pp)\,G(1-p)\,h(1-p) .$$

From Eqn (10.1):

$$\chi_n(e^{\omega}) + (-1)^n \chi(e^{-\omega}) = 2\sum_{k=0}^{\lfloor n/2\rfloor} \lambda(2k)\frac{\omega^{n-2k}}{(n-2k)!} - i\,\frac{\pi}{2}\,\frac{\omega^{n-1}}{(n-1)!} .$$

From Eqn (11.2):

$$\chi_p(e^{\omega}) \sim 2\sum_{k=0}^{\infty} \lambda(2k)\frac{\omega^{p-2k}}{\Gamma(p-2k+1)} - i\,\frac{\pi}{2}\,\frac{\omega^{p-1}}{\Gamma(p)} + O(e^{-\omega}) .$$

From Eqn (13.1):

$$\chi_p(e^{\omega}) = \tfrac{1}{2}\Gamma(1-p)\sum_{k=-\infty}^{\infty} (-1)^k (k\pi i - \omega)^{p-1}, \quad \text{for } p < 1 .$$

Clausen’s Integral and Related Functions

Polylogarithms with pure imaginary $\omega = i\theta$ give a family of functions including Clausen’s integral ([1] Ch. VII § 1.4, [4] § 27.8):

$$\mathrm{Li}_p(e^{-i\theta}) = \mathrm{Ci}_p(\theta) - i\,\mathrm{Si}_p(\theta) . \qquad (18.4)$$

Some of their properties are summarized below.

$$\mathrm{Ci}_p(-\theta) = \mathrm{Ci}_p(\theta) , \qquad \mathrm{Si}_p(-\theta) = -\mathrm{Si}_p(\theta) ;$$

$$\mathrm{Ci}_p(\pi-\theta) = \mathrm{Ci}_p(\pi+\theta) , \qquad \mathrm{Si}_p(\pi-\theta) = -\mathrm{Si}_p(\pi+\theta) .$$

From Eqn (4.1):

$$\frac{d}{d\theta}\mathrm{Si}_p(\theta) = \mathrm{Ci}_{p+1}(\theta) , \qquad \frac{d}{d\theta}\mathrm{Ci}_p(\theta) = -\mathrm{Si}_{p+1}(\theta) .$$

From Eqn (5.2–4):

$$\mathrm{Ci}_p(0) = \zeta(p), \ \text{for } p > 1 , \qquad \mathrm{Si}_p(0) = 0, \ \text{for } p > 1 ;$$

$$\mathrm{Ci}_p(-\pi/3) = \tfrac{1}{2}(1 - 3^{1-p})\eta(p) ;$$

$$\mathrm{Ci}_p(-\pi/2) = -2^{-p}\,\eta(p) , \qquad \mathrm{Si}_p(-\pi/2) = -\beta(p) ;$$

$$\mathrm{Ci}_p(-2\pi/3) = -\tfrac{1}{2}(1 - 3^{1-p})\zeta(p) ;$$

$$\mathrm{Ci}_p(-\pi) = -\eta(p) , \qquad \mathrm{Si}_p(-\pi) = 0 .$$

From Eqn (6.1–2):

$$\mathrm{Ci}_1(\theta) = -\ln[2\,|\sin(\tfrac{1}{2}\theta)|] , \qquad \mathrm{Si}_1(\theta) = \tfrac{1}{2}(\mathrm{sign}(\theta)\pi - \theta), \ \text{for } |\theta| < 2\pi ;$$

$$\mathrm{Ci}_0(\theta) = -\tfrac{1}{2} , \qquad \mathrm{Si}_0(\theta) = \tfrac{1}{2}\cot(\tfrac{1}{2}\theta) ;$$

$$\mathrm{Ci}_{-1}(\theta) = -\tfrac{1}{4}\csc(\tfrac{1}{2}\theta)^2 , \qquad \mathrm{Si}_{-1}(\theta) = 0 .$$

Clausen’s integral itself is

$$\mathrm{Si}_2(\theta) = -\int_0^{\theta} \ln[2\sin(\tfrac{1}{2}\phi)]\,d\phi .$$

From Eqn (8.1):

$$\mathrm{Ci}_p(\theta) = \sum_{k=1}^{\infty}\frac{\cos(k\theta)}{k^p}, \ \text{for } \begin{cases} p > 1, \ \theta = 2m\pi \\ p > 0, \ \text{otherwise} \end{cases} \qquad \mathrm{Si}_p(\theta) = \sum_{k=1}^{\infty}\frac{\sin(k\theta)}{k^p}, \ \text{for } p > 0 .$$

There are too many variants of the equations deriving from Eqn (9.1–5) to list here, for real and integer (odd and even) parameters, and with or without the optimization of Eqn (9.6–7). The eta series, Eqn (9.2), is faster than the zeta series, Eqn (9.3), for $|\theta| > 2\pi/3$ (or $|\theta - \pi| < \pi/3$). It may even be worth using the beta series, Eqn (18.2), for $|\theta|$ close to $\pi/2$.

For integer parameters, Eqn (10.1) gives the closed forms

$$Ci_{2n}(\theta) = \sum_{k=0}^{n} \zeta(2k)\frac{(-\theta^2)^{n-k}}{(2n-2k)!} - \frac{\pi}{2}\frac{|\theta|(-\theta^2)^{n-1}}{(2n-1)!}, \quad \text{for } |\theta| < 2\pi ,$$

and

$$Si_{2n+1}(\theta) = \theta\left\{\sum_{k=0}^{n} \zeta(2k)\frac{(-\theta^2)^{n-k}}{(2n-2k+1)!} - \frac{\pi}{2}\frac{|\theta|(-\theta^2)^{n-1}}{(2n)!}\right\}, \quad \text{for } |\theta| < 2\pi ;$$

in particular,

$$Ci_{-2n}(\theta) = Si_{-2n+1}(\theta) = 0, \quad \text{for } n = 1, 2, 3, \cdots .$$

Eqn (10.2) gives similar expressions:

$$Ci_{2n}(\theta+\pi) = -\sum_{k=0}^{n} \eta(2k)\frac{(-\theta^2)^{n-k}}{(2n-2k)!}, \quad \text{for } |\theta| < \pi ,$$

and

$$Si_{2n+1}(\theta+\pi) = -\theta\sum_{k=0}^{n} \eta(2k)\frac{(-\theta^2)^{n-k}}{(2n-2k+1)!}, \quad \text{for } |\theta| < \pi .$$

From Eqn (15.2),

$$Ci_p(m\theta) = m^{n-1}\sum_{k=0}^{m-1} Ci_p(\theta + 2\pi k/m) , \qquad Si_p(m\theta) = m^{n-1}\sum_{k=0}^{m-1} Si_p(\theta + 2\pi k/m) .$$

(This notation is not standard. Lewin uses $Cl_{2n}(\theta) = Si_{2n}(\theta)$ and $Cl_{2n+1}(\theta) = Ci_{2n+1}(\theta)$, so Clausen’s integral is $Cl_2(\theta)$; and $Gl_{2n}(\theta) = Ci_{2n}(\theta)$ and $Gl_{2n+1}(\theta) = Si_{2n+1}(\theta)$ for the polynomial forms. However, these names cannot be extended to real parameters.)

The Fermi–Dirac and Bose–Einstein Functions

The Fermi–Dirac ([12]) and Bose–Einstein functions ([6], [9]) are

$$F_p(w) = \int_0^\infty \frac{t^p}{e^{t-w}+1}\,dt = -\Gamma(p+1)\,Li_{p+1}(-e^{w})$$

and

$$G_p(w) = \int_0^\infty \frac{t^p}{e^{t-w}-1}\,dt = \Gamma(p+1)\,Li_{p+1}(e^{w})$$

respectively. Note that many of the equations above are given in terms of $Li_p(-e^{w})$, so this may sometimes be a more natural representation.

19. Generalizations

Lerch’s Function

Lerch’s function, $\Phi(z, p, a)$ ([8] § 1.11), bears the same relation to the Hurwitz zeta function, $\zeta(p, a)$, as $Li_p(z)$ does to the Riemann zeta function, $\zeta(p)$. Many properties of the polylogarithm follow. In terms of this function, $Li_p(z) = z\,\Phi(z, p, 1)$ and $\chi_p(z) = 2^{-p} z\,\Phi(z^2, p, ½)$.

$$F(z,\ p,\ a) = \frac{1}{\Gamma(p)}\int_0^\infty \frac{e^{(1-a)t}t^{p-1}}{e^t - z}dt$$

$$= \sum_{k=0}^{\infty} \frac{z^p}{(k+a)^p}\ .$$

Nielsen's Generalized Polylogarithms

Another generalization is due to Nielsen ([13]):

$$S_{m,n}(z) = \frac{(-1)^{m+n}}{(m-1)!\,n!}\int_0^1 \frac{\ln(t)^{m+1}\ln(1-zt)^n}{t}dt$$

$$= \sum_{k=0}^{\infty} \frac{(-1)^k S_{n+k}^{(n)}}{(n+k)!}\frac{z^{n+k}}{(n+k)^m},\ \text{ for } |z| < 1\ ,$$

where $S_k^{(n)}$ is the Stirling number of the first kind ([4] § 24.1.3), defined by

$$\ln(1+t)^n = n!\sum_{k=n}^{\infty} S_k^{(n)}\frac{t^k}{k!}\ .$$

Hence $Li_n(z) = S_{n-1,1}(z)$.

It is not clear how this can be generalized to real parameters.

The Debye function (§ 16) can also be expressed as $Z_n(z) = \zeta(n) - S_{1,n-1}(1 - e^{-z})$.

20. Summary

The following table lists the ranges over which the various algorithms are valid. The parameter is represented by n when an integer, and p when real, and the argument is $z = e^{\omega}$.

Parameter	Argument		Algorithm	Equation
—	$z = 0$	$\omega = -\infty$	0	(5.1)
$p < 1$	$z = 1$	$\omega = 0$	$\zeta(p)$	(5.2)
—	$z = -1$	$\omega = -i\pi$	$-\eta(p)$	(5.3)
—	$z = -i$	$\omega = -i\pi/2$	$2^{-p}\eta(p) - i\beta(p)$	(5.4)
$n \le 0$	—	—	Rational	(6.2–4)
$n = 1$	—	—	$-\ln(1 - z) = -\ln(1 - e^{\omega})$	(6.1)
$n = 2$	—	—	Dilogarithm transformations	(7.2–3)
$p < 0$	—	—	'Complex' series	(13.1–2)
—	$\lvert z\rvert < 1$	$Re(\omega) < 0$	Power series in z	(8.1)
$n \ne 0$	$\lvert z\rvert > 1$	$Re(\omega) > 0$	Reciprocal formulae	(10.1–2)
$n < 0$	—	—	Reciprocal formula	(10.3)
p	$\lvert z\rvert \gg 1$	$Re(\omega) \gg 1$	Asymptotic formulae	(11.1–2)
p	$\lvert\ln(z)\rvert < 2\pi$	$\lvert\omega\rvert < 2\pi$	ζ series	(9.3/6)
$n + \varepsilon$	$\lvert\ln(z)\rvert < 2\pi$	$\lvert\omega\rvert < 2\pi$	ζ series	(9.4)
$n > 0$	$\lvert\ln(z)\rvert < 2\pi$	$\lvert\omega\rvert < 2\pi$	ζ series	(9.5/7)
—	$\lvert\ln(-z)\rvert < \pi$	$\lvert\omega - i\pi\rvert < \pi$	η series	(9.2)
—	$\lvert\ln(-iz)\rvert < \pi/2$	$\lvert\omega - i\pi/2\rvert < \pi/2$	β series	(18.1–2)
—	$\lvert z\rvert < \sim e^{m\pi}$	$Re(\omega) < \sim m\pi$	m^{th}-root formula	(15.2–3)
$n > 0$	—	—	Debye functions	(16.1)

For integer parameters $n > 1$, (8.1) can be used for small $|z|$, (10.1–2) for large, and (9.5/7) for intermediate values (or (9.2) for negative real arguments). For $n \le 1$, where these series converge more slowly, (6.1–4) are available, or (13.2) if cancellation is a problem.

Similarly, for real parameters p, (8.1) can be used for small arguments, but there is a gap between (9.3/6), for intermediate values, and (11.1–2), which work only for very large arguments. Here (15.3) can be used. Again, for $p < 0$, where the convergence of these series becomes slow, another algorithm, (13.2), is available.

21. Zeros, Maxima, and Minima

The numerator in Eqn (6.2–3) is a polynomial of degree n, so $\mathrm{Li}_{-n}(z)$ has n zeros for $n > 0$. It is easy to show that they are all real, and, excluding $z = 0$, negative. From Eqn (10.3), they occur in reciprocal pairs; that is, if x is a zero, so is $1/x$. Hence $\mathrm{Li}_{-2n}(-1) = 0$, which also follows from Eqn (5.3).

Taking the first two terms of the power series, Eqn (8.1), shows that, for sufficiently large p, $\mathrm{Li}_{-p}(x)$ has a zero near -2^{-p}. This is actually an upper bound; -2^{n} is a lower bound for the zeros of $\mathrm{Li}_{-n}(x)$

For $p \gg 0$, even a single term of Eqn (17.2) gives a good estimate of the zeros of $\mathrm{Li}_{-p}(-e^{u})$; for example, $\mathrm{Li}_{-(4n+1)}(-e^{-p}) \approx 0$.

$\mathrm{Li}_{-p}(z)$ has $\lceil p \rceil$ zeros. $\mathrm{Li}_{p}(z)$ has no zeros, other than $z = 0$, for $p \neq 0$.

Since the derivative is as easy to compute as the function, by Eqn (4.2), the Newton–Raphson algorithm can be used to compute zeros accurately.

Again by Eqn (4.2), maxima and minima with respect to z are easily computed.

22. Limits

From Eqn (1.1),

$$\lim_{|z| \to 0} \mathrm{Li}_p(z) = \lim_{p \to \infty} \mathrm{Li}_p(z) = z\,.$$

From Eqn (11.3),

$$\lim_{\mathrm{Re}(w) \to \infty} \mathrm{Li}_p(e^{w}) = -\frac{w^p}{\Gamma(p+1)}, \quad \text{for } p \neq -1,\ -2,\ -3,\ \cdots\,.$$

From Eqn (10.3),

$$\lim_{\mathrm{Re}(w) \to \infty} \mathrm{Li}_{-n}(e^{w}) = -(-1)^n\, e^{-w}, \quad \text{for } n = 1,\ 2,\ 3\ \cdots\,.$$

From Eqn (9.3),

$$\lim_{|w| \to 0} \mathrm{Li}_p(e^{w}) = \Gamma(1-p)(-w)^p, \quad \text{for } p < 1\,.$$

23. Implementation

The algorithms have been implemented in Fortran 77 ([14]), because no other available language supports complex arithmetic, which is essential in this problem. ‘Complex*16’ (double-precision complex) arithmetic is used throughout. This is not a standard feature of Fortran, but is very widely available.

There are at least four versions of most of the functions: for real and integer (and sometimes half-integer) parameter, and real (sometimes positive and negative) and complex argument.

The many constants involved, such as tables of zeta and eta functions of integer (and half-integer) arguments, as well as multiples of π, ln(2), etc., have all been computed to high precision (greater than required for IEEE 64-bit floating-point arithmetic ([15])) using the computer algebra systems Maple and Mathematica ([16]), or the arbitrary-precision calculator bc ([17]).

The Euler–Maclaurin formula is used to compute the Riemann zeta function ([18] Ch. IX § 1) for positive arguments:

$$\zeta(p) = \sum_{k=1}^{m-1} \frac{1}{k^p} + \frac{1}{(p-1)m^{p-1}} + \frac{1}{2m^p} + \frac{1}{\Gamma(p)} \sum_{k=1}^{\infty} \frac{B_{2k}\Gamma(p+2k-1)}{(2k)!\,m^{p+2k-1}}, \quad \text{for } p \neq 0\,,$$

the powers of composite numbers being derived from those of their prime factors ([19]), using a table of ln(k). A table of

$$\frac{B_{2k}}{(2k)!m^{2k-1}}$$

is used for the second sum. For negative arguments,

$$z(p) = 2\,(2p)^{p-1}\sin(\tfrac{1}{2}pp)\,G(1-p)\,z(1-p)\ , \quad \text{for } p < 0\ .$$

The division between these formulae is actually taken at a small negative value of p, to avoid the occurrence of z(1) in the second.

The eta function is normally computed as $h(p) = (1 - e^{(1-p)\ln(2)})z(p)$, but for arguments near one, where zeta becomes infinite, it can be expanded as a power series, starting

$$h(1+e) = \ln(2) + [g\ln(2) - \tfrac{1}{2}\ln(2)^2\,]e - [g_1\ln(2) + \tfrac{1}{2}g\ln(2)^2 - \ln(2)^3\,/6]e^2 + O(e^3)\ .$$

The form of the coefficients is not important here; they can be found, in analytical or numerical form, using Maple.

Pre-computed tables are used for the zeta, eta, beta, and lambda functions of integer and half-integer arguments, from zero to the point where the functions become indistinguishable from one in machine arithmetic, and for G(n + ½), over the whole range in which it is representable.

24. Optimization

Many optimizations have already been mentioned, particularly the use of pre-computed tables of powers, zeta functions, etc. when the parameter is an integer, n (or n + ½).

In this case, if the number of terms required in the series is known, as a function of the parameter and argument, then nested multiplication can be used, and a loop of the form

```
repeat
   k := k + 1;
   power := power*z;
   term := power*coeft[k];
   sum := sum + term
until |term| < e;
```

can be replaced by

```
for k := max downto 1 do
   sum := sum*z + coeft[k];
```

The saving is usually so great that only a crude upper bound is sufficient; however, this method is probably not feasible except for particular values of the parameter, such as the dilogarithm.

25. Mass Production

If many values of $Li_{n+p}(z)$ are required for a range of integers n but fixed p and z, a great deal of computation can be saved in most of the algorithms by re-using terms from one value of n for the next. For example, in Eqn (8.1),

$$\frac{z^k}{k^p} = \frac{z^k}{k^{p-1}} \cdot \frac{1}{k}\ ;$$

in Eqn (9.3) etc.,

$$z(p-k)\frac{w^k}{k!} = z(p-k)\frac{w^{k-1}}{(k-1)!} \cdot \frac{w}{k}\ ;$$

and in Eqn (13.1),

$$(2kpi - w)^{p-1} = (2kpi - w)^{p-2} \cdot (2k\,pi - w)\ .$$

There are several situations where such sequences are required, for example Eqn (9.1) and Eqn (16.2).

26. References

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