Unified algorithms for polylogarithm, L-series, and zeta variants

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In memory of gentle colleague Jerry Keiper
1953-1995

Abstract: We describe a general computational scheme for evaluation of a wide class of number-theoretical functions. We avoid asymptotic expansions in favor of manifestly convergent series that lend themselves naturally to rigorous error bounds. By employing three fundamental series algorithms we achieve a unified strategy to compute the various functions via parameter selection. This work amounts to a compendium of methods to establish extreme-precision results as typify modern experimental mathematics. A fortuitous byproduct of this unified approach is automatic analytic continuation over complex parameters. Another byproduct is a host of converging series for various fundamental constants.

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1 Motivation

This work began two decades ago, when the present author collaborated with J. Keiper—then of Wolfram Research—on optimal ways to calculate polylogarithmic entities, especially in view of wide parameter-range and analytic-continuation requirements as serious computational-software users would, and should expect.[2]

By "Unified" in this work's title, we refer to the notion that a few strong algorithms can cover a great many different kinds of function evaluations. Which algorithm to choose then depends upon such issues as memory, desired speed, and simplicity of coding. We shall be able thus to provide a unified picture of how to calculate these entities together with their relevant analytic continuations:

- Lerch transcendent $\Phi(z,s,a) := \sum_{n=0}^{\infty} \frac{z^n}{(n+a)^s}$.
- Riemann zeta function $\zeta(s) := \sum_{n=1}^{\infty} \frac{1}{n^s}$.
- Hurwitz zeta function $\zeta(s,a) := \sum_{n=0}^{\infty} \frac{1}{(n+a)^s}$.
- Periodic zeta function $E(s,x) := \sum_{n=1}^{\infty} \frac{e^{2\pi i n x}}{n^s}$.
- Polylogarithm function $\mathrm{Li}_s(z) := \sum_{n=1}^{\infty} \frac{z^n}{n^s}$.
- Polygamma functions $\psi_n(z) := \frac{d^{n+1}}{dz^{n+1}} \log \Gamma(z)$.
- Clausen function $\mathrm{Cl}_s(\theta) := \sum_{n=1}^{\infty} \frac{\sin(n\theta)}{n^s}$.
- MTW zeta functions $\mathcal{W}(s_1,\ldots,s_n) := \sum_{m_j \ge 1} \frac{1}{m_1^{s_1}} \cdots \frac{1}{m_{k-1}^{s_{k-1}}} \frac{1}{(m_1+\cdots+m_k)^{s_k}}$.
- Multiple-zeta values $\overline{\zeta}(s_1,\ldots,s_n) := \sum_{k_1>k_2>\cdots>k_n} \frac{1}{k_1^{s_1}} \cdots \frac{1}{k_n^{s_n}}$.
- Epstein zeta functions (for matrix A) $Z_A(s;c,d) := \sum'_{n\in Z^D} \frac{e^{2\pi i c\cdot An}}{|An-d|^s}$.
- Various fundamental constants, such as Euler γ.

[2]Over these years I have been asked often by various researchers about such computational schemes, and thought it time now to write down the basics. Various ideas herein were carefully tested and implemented by Keiper, resulting in widely used *Mathematica* functions. (Any mistakes in exposition herein are not Jerry's.) Keiper was always fascinated by the Riemann zeta function, working on clever sidelines—such as the recursion scheme in Section 3.6—up until his untimely death. A superbly thoughtful obituary by S. Wolfram in Jerry's honor can be found at `http://www.stephenwolfram.com/publications/other-pubs/95-keiper.html`.

Often in computer systems, some or all of the above are calculated via Euler–Maclaurin expansions, which are of asymptotic character. As an alternative, we describe here how to use only convergent series. Just one reason for invoking series is that, typically, rigorous error bounds are accessible. We ultimately present three core algorithms for computation of the Lerch transcendent Φ—most everything else stems from that mighty function (the moniker "transcendent" is appropriate in the present context).

1.1 Acknowledgements and disclaimer

Over a long-term research project one hopes to enjoy substantial collegial support. The present author is happily indebted to pioneers in computation of functions: D. Bailey, D. Borwein, J. Borwein, P. Borwein, M. W. Coffey, P. Flajolet, A. Odlyzko, D. Platt, S. Plouffe, M. Rubinstein, J. Shallit, L. Vepstas. The pioneering work by R. Brent [16, 17] on fast evaluation is gratefully acknowledged. I. J. Zucker, expert in lattice sums, has over the years provided fascinating computational challenges. S. Wolfram has always provided encouragement for special-function investigation; he has suggested over the decades various of the lucrative pathways this work has followed. Virtually all of this research has involved intensive use of *Mathematica*; accordingly, the author thanks colleagues T. Gray, M. Trott, E. Weisstein, and Wolfram Research in general for all of the courtesy and aid over the years.

A disclaimer is in order here: Many of the ideas are already in the literature. To keep this paper at reasonable size, I endeavored to reference the key sources and discussions, so this work is not bibliographically perfect. Just my statement of a result should not be construed as implying it is an original thought. Importantly, my longtime colleague J. Buhler has conveyed many original thoughts now incorporated into this work.

2 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—the Lerch transcendent whose classical definition is (later we shall employ a modified transcendent we call $\overline{\Phi}$)

$$\Phi(z, s, a) := \sum_{n=0}^{\infty} \frac{z^n}{(n+a)^s}, \tag{1}$$

where under the constraints

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

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

$$\Phi(z, 0, a) \;=\; \frac{1}{1-z}, \tag{3}$$

which when coupled with the formal relation

$$\Phi(z, s-1, a) \;=\; \left(a + z\frac{\partial}{\partial z}\right) \Phi(z, s, a) \tag{4}$$

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 $z \to 1$ do not necessarily commute (see the discussion after relation (9)).

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

$$\Phi(z, s, a) \;=\; z^m \,\Phi(z, s, a+m) \;+\; \sum_{k=0}^{m-1} \frac{z^k}{(k+a)^s}\,. \tag{5}$$

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

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 (1). This in turn implies

$$\Phi(z, s, a) \;-\; \Phi(-z, s, a) \;=\; \frac{z}{2^{s-1}}\,\Phi\left(z^2, s, \frac{a+1}{2}\right), \tag{6}$$

a form of doubling relation that is actually quite useful for certain computations (see Section 8).

Not so simple is the general functional relation discovered by Lerch [43] [40] [41]

$$\frac{(2\pi)^s z^a}{\Gamma(s)}\,\Phi(z, 1-s, a) \;=\; e^{\frac{i\pi s}{2}}\,\Phi\left(e^{-2ia\pi}, s, \frac{\log z}{2\pi i}\right) \;+\; e^{2i\pi a - \frac{i\pi s}{2}}\,\Phi\left(e^{2ia\pi}, s, 1 - \frac{\log z}{2\pi i}\right), \tag{7}$$

valid over a wide range of complex parameters. Reference [40] 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 (7) should read $3.866\cdots + 1025.9\ldots i$ on both sides. In this way, a profound and beautiful theoretical result can be used in computations, to ensure self-consistency.

Conversely, one of our methods—the Riemann-splitting algorithm—implies by way of its very development the above functional relation.

2.1 Bernoulli-series representation of Lerch Φ

Under the stated constraints (2) one has a valid integral representation (with also $\Re(a) > 0$):

$$\Phi(z,s,a) = \frac{1}{\Gamma(s)} \int_0^\infty \frac{t^{s-1}e^{-at}}{1-ze^{-t}}\, dt. \tag{8}$$

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:

$$\frac{e^{xt}}{e^t-1} = \sum_{n\geq 0} B_n(x)\frac{t^{n-1}}{n!} \quad ; \ |t| < 2\pi$$

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

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 $\mathrm{cosech}(t/2)$, while the Euler-number series is for $\mathrm{sech}(t/2)$. 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 (8) as $\int_0^\infty \ \to \ \int_0^\lambda \ + \ \int_\lambda^\infty$, 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 $\Re(z) \in (1/2, 1]$, say:

$$\Phi(z,s,a) \ = \ \frac{1}{\Gamma(s)} \sum_{n=0}^{\infty} \frac{\Gamma(s, \lambda(n+a))\, z^n}{(n+a)^s} \ + \ \frac{z^{-a}}{\Gamma(s)} \sum_{m=0}^{\infty} \frac{B_m(1-a)}{m!} \int_0^\lambda t^{s-1}(t-\log z)^{m-1}\, dt. \tag{9}$$

A similar construction involving Euler polynomials is straightforward, and applies best to say $\Re(z) \in [-1, -1/2)$. 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 $\Re(z)$, the C_m in Algorithm 1 are all terminating hypergeometrics, so evaluations for such as z negative real are especially easy to implement.

Note also that when $z = 1$ and $s = -m = 0, -1, -2, \ldots$, the first sum in (9) 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, $|z| \le 1$, and real $a \in (0, 1]$.

1) If($|z| \le 1/2$) use parameter $\lambda := 0$, i.e. return the direct sum (1) 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 (3, 4);
3) If($\Re(z) \ge 0$) $p := -\log z$; else $p := -\log(-z)$;
4) $\lambda := 1 - p$;
5) Define coefficients C_m as follows:
 If($\Re(z) \ge 0$) {
   if($z \ne 1 + 0i$)

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

 else

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

 } else {
   if($z \ne -1 + 0i$)

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

 else

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

}
5) return Φ as

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

2.2 Bernoulli multisectioning

In Algorithm 1 and various algorithms to follow, 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. Further "multisectioning"—a technique pioneered by J. Buhler for the Bernoulli numbers (see the original treatise [20], which by now has been followed by several enhancement papers)—can reduce memory. In the more advanced setting, one calculates say all B_k with k mod 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 [12], which values being required for many "rational zeta series."

Other special numbers appear in zeta-variant studies. For example the Nörlund numbers $B_n^{(n)}$, defined via generating function

$$\frac{t}{(1+t)\log(1+t)} \;=\; \sum_{n\geq 0} \frac{B_n^{(n)}}{n!} t^n \tag{10}$$

have entered naturally into studies on the Stieltjes constants [24, arXiv:1106.5146], a subject we discuss later in Section 7.1. Importantly, the Nörlund numbers *also* can be extracted via fast methods; one only need perform Newton inversion on the Taylor series for $\log(1+t)$.

2.3 Erdélyi-series representation for Lerch Φ

When s is not a positive integer, and for parameter $a \in (0,1]$, $|\log z| < 2\pi$, one has the linearly convergent Erdélyi expansion [6]

$$z^a \Phi(z,s,a) \;=\; \sum_{n\geq 0} \zeta(s-n,a) \frac{\log^n z}{n!} \;+\; \Gamma(1-s)(-\log z)^{s-1}, \tag{11}$$

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. 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($|z| \le 1/2$) return the direct sum (1) 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 (3, 4);
3) If(s is not a positive integer) return Φ as

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

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

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

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

2.4 Riemann-splitting representation for Lerch variant $\overline{\Phi}$

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

$$\overline{\Phi}(z, s, a) \;:=\; {\sum_{n=0}^{\infty}}' \frac{z^n}{((n+a)^2)^{s/2}}, \tag{12}$$

where $'$ on the sum indicates any denominator singularity is avoided. For $\Re(a) > 0$ this form $\overline{\Phi}$ is equivalent to the classical definition (1) 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:

$$\sum_{n\in Z}\frac{z^n}{((n+a)^2)^{s/2}} \;=\; \frac{1}{\Gamma(s/2)}\int_0^{\infty} t^{s/2-1}\sum_{n\in Z} z^n e^{-(n+a)^2}\,dt. \tag{13}$$

The celebrated Riemann prescription is to split such an integral via $\int_0^\infty \to \int_0^\lambda + \int_\lambda^\infty$, then apply theta-function identities 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 $\overline{\Phi}$ is asking for a sum over nonnegative integer n, not $n \in Z$? One way is to use the following "magical" expedient—a phenomenon discovered by the present author at the start of this work in the late 1980s.[3] The idea is, a sum over integers on a specific half-line can be written

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

where we define

$$S(z) \;:=\; sign(\Re(z))$$

with $sign(0) := 0$. 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 $\overline{\Phi}$ 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 $\overline{\Phi}$; that is, we not only get a computational algorithm following, or we can prove such as (7). We omit the tedious details, opting instead to display the incomplete-gamma series in the next algorithm.

[3] It 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.

Algorithm 3 Riemann-splitting algorithm for $\overline{\Phi}$ and its analytic continuation.

This algorithm computes $\overline{\Phi}(z, s, a)$—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 $\{\Re(z) \in [0, 1)\} \cup \{z = 1 + 0i\}$ (the translation relation (5) can be used for other a).

1) If($z == 0$) return $1/a^s$; Optionally: If($|z| \leq 1/2$) return the direct sum (12) 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 (3, 4);
3) Choose a parameter λ, say $\lambda := \pi$ (but see the important discussion about the possibility of complex λ in Section 3);
4) Return the analytic continuation of $\overline{\Phi}$ as (note that for special cases of $\overline{\Phi}$, such as polylogarithms and zeta variants, the following incomplete-gamma decomposition can be significantly simplified):

$$\begin{aligned}\overline{\Phi}(z, s, a) \quad = \quad & -\frac{z^{-a}\lambda^{s/2}}{s\Gamma(s/2)}\,\delta_{a\in Z} \;+\; \frac{1}{s-1}\frac{\pi^{1/2}\lambda^{(s-1)/2}}{\Gamma(s/2)}\,\delta_{z=1} \;+ \\ & \frac{1}{2}\sum_{n\in Z}{}^{'}\frac{z^n}{(A^2)^{s/2}}\left(\frac{\Gamma(s/2, \lambda A^2)}{\Gamma(s/2)} + \frac{\Gamma((s+1)/2, \lambda A^2)}{\Gamma((s+1)/2)}\,S(A)\right) + \\ \frac{\pi^{s-1/2}}{2z^a}\sum_{u\in Z}{}^{'}\frac{e^{-2\pi i a u}}{(U^2)^{(1-s)/2}} & \left(\frac{\Gamma\left((1-s)/2, \frac{\pi^2}{\lambda}U^2\right)}{\Gamma(s/2)} + i\,\frac{\Gamma\left(1-s/2, \frac{\pi^2}{\lambda}U^2\right)}{\Gamma((s+1)/2)}\,S(U)\right),\end{aligned} \tag{14}$$

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

3 Riemann zeta function

Being as the Riemann ζ-function is defined for its literal-convergence region $\Re(s) > 1$ as

$$\zeta(s) \;:=\; \sum_{n \geq 1} \frac{1}{n^s} \;=\; \Phi(1, s, 1) \;=\; \overline{\Phi}(1, s, 1),$$

the whole procedure behind Algorithms 1, 3 can be simplified. One may choose free parameter λ, and at the end of the algorithms one may return $\zeta(s)$ according to a Bernoulli series (requiring $|\lambda| < 2\pi$)

$$\zeta(s) \;=\; \frac{1}{\Gamma(s)} \sum_{n=1}^{\infty} \frac{\Gamma(s, \lambda n)}{n^s} \;+ \frac{1}{\Gamma(s)} \sum_{m \geq 0} \frac{B_m}{m!} \frac{\lambda^{m+s-1}}{m+s-1}, \tag{15}$$

or in the case of Riemann splitting we have for general parameter λ

$$\zeta(s) \;=\; -\frac{\lambda^{s/2}}{s\Gamma(s/2)} \;+\; \frac{1}{s-1} \frac{\pi^{1/2} \lambda^{(s-1)/2}}{\Gamma(s/2)} \;+ \tag{16}$$
$$\frac{1}{\Gamma(s/2)} \sum_{n=1}^{\infty} \left(\frac{\Gamma(s/2, \lambda n^2)}{n^s} \;+\; \pi^{s-1/2} \frac{\Gamma((1-s)/2, n^2 \pi^2/\lambda)}{n^{1-s}} \right).$$

We can conveniently set $\lambda := \pi$ to obtain

$$\Gamma(s/2)\, \zeta(s) \;=\; \frac{\pi^{s/2}}{s(s-1)} \;+\; \sum_{n=1}^{\infty} \left(\frac{\Gamma(s/2, \pi n^2)}{n^s} \;+\; \pi^{s-1/2} \frac{\Gamma((1-s)/2, \pi n^2)}{n^{1-s}} \right). \tag{17}$$

This is essentially Riemann's classical prescription, and as we have intimated, leads to both the functional equation for ζ and a rapidly-convergent computational algorithm.

3.1 Riemann–Siegel formula and Dirichlet L-functions

The representation (16) is similar to the celebrated Riemann–Siegel expansion for $\zeta(s)$, in that the both incomplete-gamma summations have terms that decay significantly for large index n. We refer the reader to separate treatments of Riemann–Siegel expansions; practical exposition for the Riemann–Siegel construct is found in [26, 12]. There is also a modern treatment of Riemann–Siegel ideas by J. Reyna [48], such that the techniques can now also be invoked off the critical line.

Incidentally, a major application of efficient high-precision ζ evaluations is *analytic* counting of prime numbers [42, 26]. Evidently the prime count $\pi(10^{23})$ has been resolved in this way, namely

$$\pi\left(10^{23}\right) \;=\; 1925320391606803968923,$$

a recent result of D. J. Platt [45].

The analogy of Riemann–Siegel formulae with (16) can be rendered sharper if free parameter λ is allowed to have complex values—perhaps even s-dependent values. This promising idea is the focus of ongoing research [25]. In the Lerch connection specifically, see [2] and references therein. An excellent work of M. Rubinstein [49, Sections 3.3, 3.4] analyzes Riemann-splitting formulae similar to (16) above—along with the aforementioned complex freedom for free parameters; moreover, Rubinstein gives analogous formulae for Dirichlet L-function computations.

3.2 Riemann-zeta derivatives

In many of our computational formulae we require values of the Riemann zeta function—or its derivatives—at nonpositive integers. First, we know as in Section 2.1 that

$$\zeta(-m) \;=\; (-1)^m \frac{B_{m+1}}{m+1}$$

for $m = 0, 1, 2, \ldots$. From the functional equation

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

we can extract derivatives

$$\zeta^{(1)}(0) \;=\; -\frac{1}{2}\log 2\pi, \quad \zeta^{(2)}(0) \;=\; \gamma_1 + \frac{\gamma^2}{2} - \frac{\pi^2}{24} - \frac{1}{2}(\log 2 + \log \pi)^2,$$

where γ_1 is a Stieltjes constant, and so on. For even $m = 2, 4, 6, \ldots$

$$\zeta^{(1)}(-m) := \frac{d}{ds}\zeta(s)|_{s=-m} \;=\; \frac{(-1)^{m/2} m!}{2^{m+1}\pi^m}\zeta(m+1),$$

for example

$$\zeta^{(1)}(-4) = \frac{3}{4}\frac{\zeta(5)}{\pi^4}.$$

For odd $m = 1, 3, 5 \ldots$, on the other hand,

$$\zeta^{(1)}(-m) \;=\; \zeta(-m)\left(\gamma \;+\; \log 2\pi \;-H_m - \frac{\zeta^{(1)}(m+1)}{\zeta(m+1)}\right),$$

for example

$$\zeta^{(1)}(-5) \;=\; \frac{15}{4\pi^6}\zeta^{(1)}(6) \;+\; \frac{137}{15120} \;-\; \frac{\gamma}{252} \;-\; \frac{1}{252}\log 2\pi.$$

Such machinations can be extended for higher derivatives, leading us to a

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Principle: For an Erdélyi sum of the general form (for any integer s):

$$\sum_{m\ge 0}{}' \zeta^{(d)}(s-m)\, T_m,$$

where coefficient T_m has no ζ-component, all computations can refer to a set of derivatives $\{\zeta^{(d)}(s) \; : \; s = 2,3,4,\dots\}$. That is, no ζ values or derivatives are required for any integer argument < 2.

This principle shows that in some instances one really can avoid numerical differentiation. But there is more to be said: Even if one is also unwilling to adopt derivatives $\zeta^{(d)}(s = 2,3,4,\dots)$ as "fundamental constants," there is a way to generate such derivatives with still another series strategy. Let us describe the scenario for first derivatives. Take (15) with parameter $\lambda := 1$, multiply through by $\Gamma(s)$, then differentiate to obtain, for $\Re(s) > 1$,

$$\zeta^{(1)}(s) \;=\; -\frac{\Gamma^{(1)}(s)}{\Gamma(s)}\zeta(s) + \frac{1}{\Gamma(s)}\sum_{n=1}^{\infty}\frac{\Gamma^{(1)}(s,n)-\Gamma(s,n)\log n}{n^s} - \frac{1}{\Gamma(s)}\sum_{m\ge 0}\frac{B_m}{m!}\frac{1}{(m+s-1)^2}. \tag{18}$$

It is relevant to point out here that there exist very simple and efficient schemes for evaluating ζ derivatives to moderate precision (see Section 7.6).

3.3 Gamma- and incomplete-gamma calculus

3.4 Γ and its derivatives

One of the best ways to calculate $\Gamma(s)$ itself is first to presume $\Re(s) > 0$ and use the Spouge formula with free real parameter $a > 0$:

$$\Gamma(1+z) \;=\; (z+a)^{z+1/2}e^{-z-a}\sqrt{2\pi}\left(c_0 + \sum_{k=1}^{\lceil a\rceil-1}\frac{c_k(a)}{z+k} + E(z,a)\right),$$

where $c_0(a) := 1$ and the rest of the c coefficients are defined

$$c_k(a) \;:=\; \frac{1}{\sqrt{2\pi}}\frac{(-1)^{k-1}}{(k-1)!}(a-k)^{k-1/2}e^{-k+a}.$$

Remarkably, the relative-error term enjoys a very convenient bound [46]

$$|E(z,a)| \;<\; \frac{1}{\sqrt{a}(2\pi)^{a+1/2}},$$

so it is quite clear how to choose the free parameter a to achieve required precision.

Some useful constants include the Taylor coefficients for Γ itself, from

$$\Gamma(1+x) \;=\; \sum_{n\ge 0} \Gamma^{(n)}(1)\,\frac{x^n}{n!},$$

which form is absolutely convergent for $|x|<1$, the constants exemplified by:

$$\Gamma^{(0)}(1) \;=\; \Gamma(1)=1,$$
$$\Gamma^{(1)}(1) \;=\; -\gamma,$$
$$\Gamma^{(2)}(1) \;=\; \gamma^2-\gamma+\frac{\pi^2}{6},$$
$$\Gamma^{(3)}(1) \;=\; -2\gamma^3+9\gamma^2-(\pi^2+6)\,\gamma+\frac{3}{2}\pi^2-4\zeta(3),$$

and so on. Such recondite forms can be deduced from relations involving polygamma functions, to which functions we shall later speak. We shall need these gamma-expansion constants in our work on general polylogarithm derivatives.

For limited argument ranges, there are other series of interest. One has two representation formulae (see [5, 12])

$$\log\Gamma(z) \;=\; -\log z \;+\; (z-1)(1-\gamma) \;+\; \sum_{n>1}\frac{\zeta(n)-1}{n}(1-z)^n, \tag{19}$$

$$\log\Gamma(x) \;=\; -\frac{1}{2}\,\log\frac{\sin(\pi x)}{\pi}+\frac{1}{2}\,(1-2x)\,(\gamma+\log 2\pi) \;+\; \frac{1}{\pi}\sum_{n\ge 1}\frac{\log n}{n}\sin(2\pi n x), \tag{20}$$

the first representation valid for $|z-1|<2$, and the second for real $x\in(0,1)$. Interestingly, since the trigonometric sum in (20) is essentially a Clausen outer-derivative form, we can thus cast $\log\Gamma$, for suitable arguments, into a convergent series involving zeta derivatives. (See the remarks following representation (58) for more on this notion.)

3.5 Incomplete gamma and its outer derivatives

The incomplete gamma function $\Gamma(s,x)$ and its derivatives $\Gamma^{(d)}(s,x) := (\partial/\partial s)^d\,\Gamma(s,x)$ play a major role in our computational schemes. Defining

$$\Gamma(s,x) \;:=\; \int_x^\infty t^{s-1}e^{-t}\,dt, \tag{21}$$

there are standard recursion schemes connecting $\Gamma(s,x)$ and $\Gamma(s+1,x)$.

One representation of incomplete gamma is the ascending series

$$\Gamma(s,x) \;=\; \Gamma(s)\left(1 \;-\; x^s\, e^{-x}\sum_{k\ge 0}\frac{x^k}{\Gamma(s+k+1)}\right), \tag{22}$$

valid at least for $\Re(s) > 0$. Because we shall often need $\Gamma(0,x)$ in our developments, a special series applies, in the "exponential-integral" form

$$\Gamma(0,x) \;=\; -\gamma - \log x \;-\; \sum_{k\ge 1}(-1)^k\frac{x^k}{k!\,k}. \tag{23}$$

Then there is the general continued fraction

$$\Gamma(s,x) \;=\; \cfrac{x^s e^{-x}}{x+\cfrac{1-s}{1+\cfrac{1}{x+\cfrac{2-s}{1+\cfrac{2}{x+\cdots}}}}} \tag{24}$$

which now *is* valid for $s = 0$. The natural asymptotic expansion for general s is

$$\Gamma(s,x) \;\sim\; x^{s-1}e^{-x}\left(1-\frac{1-s}{x}+\frac{(1-s)(2-s)}{x^2}\;-\cdots\right),$$

with error bounds not too hard to establish. Given the ascending series, continued fraction, and asymptotic forms, one may evaluate $\Gamma(s,x)$ to relative precision of D digits in $O(D^{1+\epsilon})$ operations. However, recall that one of our goals is to avoid asymptotics. We argue next that a manifestly converging (Laguerre) series can be used even for large $|x|$.

A remarkable, globally convergent (*not* merely asymptotic) expansion does exist for $\Gamma(s,x)$, namely

$$\Gamma(s,x) \;=\; x^s e^{-x}\sum_{n\ge 0}\frac{(1-s)_n}{(n+1)!}\frac{1}{L_n^{(-s)}(-x)L_{n+1}^{(-s)}(-x)}, \tag{25}$$

where $L_n^{(-s)}$ here is an associated Laguerre polynomial. In fact, given that such forms as (25) are symbolically differentiable, we always have means to calculate any derivatives $\Gamma^{(d)}(s,x)$ *using a convergent series involving only elementary summands.*

We should observe that in various of our computational algorithms herein we need *sets* of values such as $\{\Gamma(0,n) \;:\; n = 1,2,3,\ldots\}$. It may be of value that the difference of two successive set members is

$$\Gamma(0,n+1)-\Gamma(0,n) \;:=\frac{e^{-n}}{n}\sum_{k\ge 0}\frac{(-1)^k}{n^k}\mu_k$$

where the $\mu_k := \int_0^1 y^k e^{-y}\, dy$ are elementary constants. This suggests the possibility of evaluating the given set of $\Gamma(0, n)$ values via recursion.

As for derivatives of incomplete gamma, here is a beautiful relation for calculating s-derivatives of the Laguerre entities $L_n^{(s)}(x)$, namely

$$\frac{\partial}{\partial s} L_n^{(s)}(x) \ = \ \sum_{m=0}^{n-1} \frac{L_m^{(s)}(x)}{n-m}.$$

The very existence of this identity establishes that every derivative of every order for any incomplete gamma at integer s can be given a converging series—one only has to symbolically differentiate (25).

In a 2008 work [9], effective (rigorous, with explicit big-O constants) are established for Laguerre polynomials. In fact,

$$L_n^{(-a)}(-z) \ \sim \ \frac{e^{-z/2}}{2\sqrt{\pi}} \frac{e^{2\sqrt{mz}}}{z^{1/4-a/2}\ m^{1/4+a/2}} \left(1 + O\left(\frac{1}{m^{1/2}}\right)\right), \tag{26}$$

which is certainly enough to infer a complexity bound for computing (25) to some prescribed number of digits.

We can in the present context think of the fundamental derivatives as the set

$$\{\Gamma^{(d)}(0, x) \ : \ d = 0, 1, 2, 3 \ldots\}.$$

This is because of another valuable recurrence, obtainable directly from the integral definition (21) via integration by parts:

$$\Gamma^{(d)}(s, x) \ = \ \int_x^\infty t^{s-1} \ \log^d t\, e^{-t} \ dt$$

$$= \ x^{s-1} \log^d x\, e^{-x} + (s-1)\Gamma^{(d)}(s-1, x) + d\, \Gamma^{(d-1)}(s-1, x).$$

So we are allowed reductions of any derivative $\Gamma^{(d)}(s, x)$ for positive integer s into a combination of $\Gamma^{(\delta)}(0, \cdot)$ terms with $\delta < d$. For example,

$$\Gamma^{(1)}(1, x) \ = \ e^{-x} \log x \ + \ \Gamma(0, x)$$

and

$$\Gamma^{(4)}(2, x) \ = \ ((x+1) \log x \ + \ 4) \ \log^3 x\, e^{-x} + 4\, \Gamma^{(3)}(0, x) + 12\, \Gamma^{(2)}(0, x).$$

3.6 Stark–Keiper and other "summation form" strategies

The Stark–Keiper formula reads, for positive integer N but arbitrary s,

$$\zeta(s, N) = \frac{1}{s-1} \sum_{k=1}^{\infty} \left(N + \frac{s-1}{k+1}\right) (-1)^k \binom{s+k-1}{k} \zeta(s+k, N),$$

where $\zeta(s, a)$ is the Hurwitz zeta function discussed in the next section. Interestingly, Keiper was able to use this relation for *recursive* computation of various zeta values. A code example of such recursion is exhibited in [30, p. 55].

There is another "summation form" for Riemann ζ

$$\zeta(s) = \lim_{N\to\infty} \frac{1}{2^{N-s+1} - 2^N} \sum_{k=0}^{2N-1} \frac{(-1)^k}{(k+1)^s} \left(\sum_{m=0}^{k-N} \binom{N}{m} - 2^N \right) \tag{27}$$

for which it is possible to give a rigorous error bound as a function of the cutoff N and s itself [7]. This and the Stark–Keiper scheme previous should always be considered for ζ calculations because the sums involved are extremely simple. (One drawback occurs when imaginary height t is very large, for $s := \sigma + it$, in which domain the prescriptions of the Riemann–Siegel class dominate.)

Continued fraction schemes for Riemann zeta and polylogarithms are found in [34]; and, we do not refer to the incomplete-gamma fractions—instead, those authors exhibit actual continued fractions for polylogarithmic entities (the fraction elements are quite complicated).

Later in the present treatment we discuss the Stieltjes expansion

$$\zeta(s) = \frac{1}{s-1} + \sum_{n\geq 0} (-1)^n \gamma_n \frac{(s-1)^n}{n!}, \tag{28}$$

where the γ_N—essentially Taylor coefficients—start with $\gamma_0 := \gamma$, the celebrated Euler constant. A similar expansion that yields certain closed-form coefficients is discussed by Vepstas in [53], namely

$$\zeta(s) = \frac{1}{s-1} + \sum_{n\geq 0} (-1)^n b_n \frac{[s]_n}{n!},$$

where here, $[s]_n$ denotes the (falling) Pochhammer symbol, $[s]_n := s(s-1)\cdots(s-n+1)$.

4 Hurwitz zeta function

The Hurwitz ζ-function is defined for its literal-convergence region $\Re(s) > 1$ as

$$\zeta(s, a) := \sum_{n\geq 0} \frac{1}{(n+a)^s} = \overline{\Phi}(1, s, a).$$

It is interesting to look first at Algorithm 1 and infer quickly that for $a \neq 0, -1, -2, \ldots,$

$$\zeta(s, a) = \frac{1}{\Gamma(s)} \sum_{n\geq 0} \frac{\Gamma(s, \lambda(n+a))}{(n+a)^s} + \frac{1}{\Gamma(s)} \sum_{m\geq 0} \frac{(-1)^m B_m(a)}{m!} \frac{\lambda^{m+s-1}}{m+s-1}, \tag{29}$$

with free parameter $\lambda \in [0, 2\pi)$. Note the interesting pole cancellation we have seen before: At nonpositive integers s the second sum's Γ prefactor has a pole neatly cancelled by the $m = 1-s$ summand. Thus we obtain again the exact evaluations $\zeta(-m, a) = -B_{m+1}(a)/(m+1)$ for $m \in (0, 1, 2, \ldots)$.

Algorithm 3 can be simplified for, say, $\Re(a) \in (0, 1]$, so including the instance $\zeta(s, 1) := \zeta(s)$, yielding

$$\begin{aligned}\zeta(s,a) \quad = \quad & -\frac{\pi^{s/2}}{s\Gamma(s/2)}\delta_{a=1} + \frac{1}{s-1}\frac{\pi^s}{\Gamma(s/2)} + \\ & \frac{1}{2}\sum_{n\in Z}{}' \frac{1}{(A^2)^{s/2}}\left(\frac{\Gamma(s/2,\pi A^2)}{\Gamma(s/2)} + \frac{\Gamma((s+1)/2,\pi A^2)}{\Gamma((s+1)/2)}S(A)\right) + \\ \pi^{s-1/2}\sum_{u=1}^{\infty}\frac{1}{u^{1-s}} & \left(\frac{\Gamma\left((1-s)/2,\pi u^2\right)}{\Gamma(s/2)}\cos(2\pi a u) + \frac{\Gamma\left(1-s/2,\pi u^2\right)}{\Gamma((s+1)/2)}\sin(2\pi a u)\right),\end{aligned} \tag{30}$$

where $A := n + a$ as in Algorithm 3.

4.1 Generalized L-series

A generalized L-series, which includes many Dirichlet series of theoretical interest, is

$$L_s(\chi) := \sum_{n\geq 1}\frac{\chi(n)}{n^s},$$

where $\chi(n)$ is periodic with period P. (No particular number-theoretical import is required here for the character χ—mere periodicity is enough.) We have in essence a finite number of sums, each over an arithmetic progression of n values, with the immediate Hurwitz-zeta decomposition following:

$$L_s(\chi) = \frac{1}{P^s}\sum_{k=1}^{P}\chi(k)\,\zeta\left(s, \frac{k}{P}\right).$$

5 Polylogarithms

The polylogarithm Li_s is defined—when convergent—as

$$\mathrm{Li}_s(z) := \sum_{n\geq 1}\frac{z^n}{n^s} = z\,\Phi(z, s, 1). \tag{31}$$

It turns out that Algorithm 2 can be quite useful in polylogarithm computations. We have, for s not a positive integer, and $|\log z| < 2\pi$, a convergent form

$$\mathrm{Li}_s(z) = \sum_{n\geq 0}\zeta(s-n)\frac{\log^n z}{n!} + \Gamma(1-s)(-\log z)^{s-1}. \tag{32}$$

However, when $s = k+1$ for nonnegative integer k, a limiting procedure shows

$$\mathrm{Li}_s(z) \;=\; \sum_{0\le n\ne k} \zeta(k+1-n)\frac{\log^n z}{n!} \;+\; \frac{\log^k z}{k!}\left(H_k - \log(-\log z)\right), \tag{33}$$

where $H_k := \sum_{m=1}^k 1/m$ denotes the k-th harmonic number (with $H_0 := 0$). Later we explain the limiting procedure that gives (33); we shall also be able to compute, along such lines, polylogarithm derivatives in the s variable.

Algorithm 3 can again be simplified using $a := 1$, to yield a general polylogarithm analytic continuation as

$$\begin{aligned}\mathrm{Li}_s(z) \quad = \quad & -\frac{\lambda^{s/2}}{s\Gamma(s/2)} \;+\; \frac{1}{s-1}\frac{\pi^{1/2}\lambda^{(s-1)/2}}{\Gamma(s/2)}\delta_{z=1} \;+ \\ & \sum_{n=1}^{\infty}\frac{z^n}{n^s}\left(\frac{\Gamma(s/2,\lambda n^2)}{\Gamma(s/2)}\cosh(n\log z) \;+\; \frac{\Gamma((s+1)/2,\lambda n^2)}{\Gamma((s+1)/2)}\sinh(n\log z)\right) \;+ \\ & \frac{\pi^{s-1/2}}{2}\sum_{u\in Z}{}' \frac{e^{-2\pi i a u}}{(U^2)^{(1-s)/2}}\left(\frac{\Gamma\left((1-s)/2, \frac{\pi^2}{\lambda}U^2\right)}{\Gamma(s/2)} \;+\; i\,\frac{\Gamma\left(1-s/2, \frac{\pi^2}{\lambda}U^2\right)}{\Gamma((s+1)/2)}S(U)\right),\end{aligned} \tag{34}$$

where $U := u + \frac{\log z}{2\pi i}$.

5.1 Analytic properties of polylogarithms

Outside the open unit z-circle, there are two difficulties: First, there is no absolute convergence, and second, cuts in the complex plane must be carefully considered. So for example, it is known that

$$\mathrm{Li}_2\left(\frac{1}{2}\right) = \frac{\pi^2}{12} - \frac{1}{2}\log^2 2,$$

as may be verified numerically by direct summation of (31), with a precision gain of about 1 bit per summand. However, it is also standard that the analytic continuation has

$$\mathrm{Li}_2(2) = \frac{\pi^2}{4} - i\pi\log 2,$$

even though the sum (31) cannot be performed directly. Incidentally, all along the cut $z \in [1,\infty)$ there is a discontinuity in the correct analytic continuation, exemplified (for $\epsilon > 0$) by

$$\mathrm{Li}_2(2+i\epsilon) = \frac{\pi^2}{4} + i\pi\log 2,$$

and in general

$$\mathrm{Disc}\ \mathrm{Li}_s(z) = 2\pi i\frac{\log^{s-1} z}{\Gamma(s)},$$

with $\Im(\mathrm{Li})$ always being split equally across the cut—thus we know exactly the imaginary part of any $\mathrm{Li}_n(z)$ on the real ray $z \in [1, \infty)$; said part is $(i/2)\mathrm{Disc}$. This discontinuity relation is quite useful in checking of any software.

There are relations that allow analytic continuation, namely [35] [44]:

$$\mathrm{Li}_s(z) + \mathrm{Li}_s(-z) = 2^{1-s}\mathrm{Li}_s(z^2),$$

true for all complex s, z, and for n integer, and complex z,

$$\mathrm{Li}_n(z) + (-1)^n \mathrm{Li}_n(1/z) = -\frac{(2\pi i)^n}{n!} B_n\left(\frac{\log z}{2\pi i}\right) - 2\pi i \Theta(z) \frac{\log^{n-1} z}{(n-1)!}, \qquad (35)$$

where B_n is the standard Bernoulli polynomial and Θ is a domain-dependent step function: $\Theta(z) := 1$, if $\Im(z) < 0$ or $z \in [1, \infty)$, else $\Theta = 0$. That is, the final term in this latest relation is included when and only when z is in the lower open half-plane union the real cut $[1, \infty)$.

Another useful relation is, for any complex z but for $n = 0, -1, -2, -3, \ldots$,

$$\mathrm{Li}_n(z) = (-n)!(-\log z)^{n-1} - \sum_{k=0}^{\infty} \frac{B_{k-n+1}}{k!(k-n+1)} \log^k z.$$

5.2 Polylogarithm-Hurwitz relation

One interesting option we do not explore in the present treatment is the functional relation between polylogarthims and the Hurwitz ζ:

$$\mathrm{Li}_s(z) \;:=\; \frac{\Gamma(1-s)}{(2\pi)^{1-s}} \left(i^{1-s}\zeta\left(1-s, \frac{1}{2} + \frac{\log(-z)}{2\pi i}\right) + i^{s-1}\zeta\left(1-s, \frac{1}{2} - \frac{\log(-z)}{2\pi i}\right)\right). \qquad (36)$$

One application of this functional relation is to render polylogarithms into a Bernoulli-series form. Indeed, the functional relation (36) together with (29) yields the following algorithm. Considering $\mathrm{Li}_s(e^{-x})$, define $\alpha := x/(2\pi i)$. If α is an integer, return $\zeta(s)$, else use, with free parameter $\lambda \in [0, 2\pi)$, and noting if necessary that α can now be restricted such that $\Re(\alpha) \in [0, 1)$, the representation

$$\begin{aligned} \mathrm{Li}_s(e^{-x}) \;:=\; & i^{1-s} \sum_{n \geq 0} \frac{\Gamma(1-s, \lambda(n+1-\alpha))}{(n+1-\alpha)^{1-s}} \;+\; i^{s-1} \sum_{n \geq 0} \frac{\Gamma(1-s, \lambda(n+\alpha))}{(n+\alpha)^{1-s}} \;- \\ & \pi \sum_{m \geq 0} \frac{(-i)^m \lambda^{m-s}}{m!} \mathrm{sinc}\left(\frac{\pi}{2}(m-s)\right) B_m(\alpha). \end{aligned} \qquad (37)$$

Refinements on this series representation are straightforward; e.g., use real parts when x, s are real. Note that s can be a nonnegative integer, courtesy of the sinc function—in fact, for even integer s the last sum with the B_m can be especially simple. Remarkably, one hereby obtains an algorithm for the general analytic continuation of $\mathrm{Li}_s(z)$ in the complex s-plane and for any complex z—a feature not present in some of our other computational algorithms (recall, as in Algorithm 2, there are restrictions on $|\log z|$).

5.3 Lerch–Hurwitz (periodic) zeta function

The function (periodic in real x)

$$E_s(x) \;:=\; \sum_{n\geq 1} \frac{e^{2\pi i n x}}{n^s} \;=\; \Phi(e^{2\pi i x}, s, 1)$$

can also be thought of as a polylogarithm evaluation $\mathrm{Li}_s\left(e^{2\pi i x}\right)$. So E_s is susceptible to various of our algorithms. In particular, a straightforward way to calculate this periodic zeta function is to calculate an entity $\mathrm{Li}_s(e^{-2\pi i \alpha})$ using (37) as-is.

6 Digamma and polygamma functions

A convergent scheme for the polygamma functions arises from the Hurwitz-zeta representation (29) and a definition of the digamma function

$$\psi^{(0)}(z) \;:=\; \frac{d}{dz}\log\Gamma(z) = -\gamma \;+\; \sum_{n\geq 0}\left(\frac{1}{n+1} - \frac{1}{n+z}\right),$$

where we note the sum is a limiting form of the difference of two Hurwitz ζ functions. One infers a converging series ($\lambda \in (0, 2\pi)$ is the usual free parameter here)

$$\psi^{(0)}(z) \;=\; -\gamma - 1 - \log\left(1 - e^{-\lambda}\right) + \sum_{k=1}^{\infty}\left((-1)^k \frac{\lambda^k}{k!k}\left(B_k - B_k(z)\right) - \frac{e^{-\lambda(k+z-1)}}{k+z-1}\right), \tag{38}$$

then observes that higher-order polygammas, namely

$$\psi^{(n)}(z) \;:=\; \frac{d^{n+1}}{dz^{n+1}}\log\Gamma(z)$$

are simply Hurwitz-zeta evaluations:

$$\psi^{(n)}(z) \;=\; (-1)^{n+1}\, n!\; \zeta(n+1, z)$$

for positive integer n. Thus we have established convergent series for all polygammas (there are standard recurrence relations that allow us to restrict argument a in $\psi^{(m)}(1+a)$ to be in $(0, 1]$).

7 Key fundamental constants

7.1 Euler and Stieltjes constants

We begin with the alluring historical expansion (28) involving the Stieltjes constants γ_N. Expanding (15) near $s = 1$ yields

$$\gamma_1 = \frac{\pi^2}{12} - \frac{1}{2}\gamma^2 + \sum_{n\geq 1} \frac{1}{n}\left(-\Gamma(0,n) + \frac{B_n}{n!\, n}\right) \tag{39}$$

Similar series accrue for the higher-index γ_N—one may employ the derivative machinery described at the end of Section 3.5 for $\Gamma^{(d)}(0,n)$ in such a context. It is of interest that the first sum in representation (39) can be put in the form

$$\sum_{n\geq 1} \frac{1}{n}\Gamma(0,n) = \int_0^{1/e} \frac{\log(1-t)}{t\log t}\, dt, \tag{40}$$

which in turn can be cast as a series involving the Nörlund numbers from (10).

On the other hand, we can use the incomplete-gamma expansion (17) for the case of the Riemann ζ to provide a computational formula for the Euler constant, as:

$$\gamma = -2 + \log 4\pi + 2\sum_{n=1}^{\infty}\left(\frac{\operatorname{erfc}(n\sqrt{\pi}\,)}{n} + \Gamma\left(0, n^2\pi\right)\right). \tag{41}$$

Based on the material in Section 3.5 we state

Principle: Any Stieltjes constant γ_N can be cast as a convergent two-dimensional sum involving elementary summands, such that D good digits require, for α some absolute constant, $O\left(D^\alpha\right)$ operations. (It is allowed that the implied big-O constant can be N-dependent.) It is natural to conjecture that α can be taken to be $1+\epsilon$.

Incidentally, based on our previous discussion of incomplete-gamma evaluations, simply equating two different series forms (23, 25) gives us an immediate representation of Euler γ in rather simple terms of Laguerre polynomials L_n:

$$\gamma = -\frac{1}{e}\sum_{n\geq 0}\frac{1}{n+1}\frac{1}{L_n(-1)L_{n+1}(-1)} - \sum_{k\geq 1}\frac{(-1)^k}{k!\, k}. \tag{42}$$

Because of the subexponential growth of the Laguerre function, this series representation achieves D good digits of γ in $O(D^{2+\epsilon})$ operations. However, various acceleration techniques may well apply, especially as the summands of the Laguerre sum here are all rational. Indeed, the creation of the Laguerre denominators is not in itself expensive; one has an especially simple recurrence

$$L_k(-1) \; = \; 2L_{k-1}(-1) - \left(1 - \frac{1}{k}\right) L_{k-2}(-1),$$

and may create quickly each successive summand of (42). Note that the use of (41) together with the remarks of Section 3.5 should result in lower complexity. So (42) is not the fastest available scheme, but consistent with the above general principle on Stieltjes constants. It could well be, however, that these incomplete-gamma series for the γ_N turn out to be susceptible to binary-splitting or other acceleration techniques, so that current best complexity bounds for γ itself can perhaps be approached in this way. (See [18, 19, 54] for modern results on computing γ.)

7.2 The works of M. W. Coffey

As for convergence rate of such Stieltjes-constant schemes, the waters are deep. In regard to other series for the γ_n, see the excellent works of M. W. Coffey [22, 38, 39, 23, 24]. Coffey's algorithms in some cases also involve double sums, so all of these methods should eventually be assessed as to computational complexity. It is of interest that Coffey's analyses sometimes involve Meijer-G evaluations—equivalently in this context, high-order hypergeometrics—which functions amount to alternative ways to write incomplete-gamma terms. (Note that Coffey's papers are also relevant to other sections of the present work.) This complexity-of-series is a fascinating research problem; for one thing, the study of magnitude growth for the γ_n remains an imperfect science.

7.3 Glaisher–Kinkelin constant

One relation for the Glaisher–Kinkelin constant A is

$$A \; = \; (2\pi)^{1/12} e^{\gamma/12 - \zeta'(2)/(2\pi^2)},$$

which can be cast in the form

$$\log A \; = \; \frac{1}{12}(1 + \log 2\pi) - \frac{1}{2\pi^2}\frac{d}{ds}\Gamma(s)\zeta(s)|_{s=2}.$$

Now we can exploit our Bernoulli-series form (15) for $\Gamma \cdot \zeta$, to infer

$$\frac{d}{ds}\Gamma(s)\zeta(s)|_{s=2} \; = \; \sum_{n \geq 1} \frac{1}{n^2}\left((1 + \lambda n)\log \lambda + 1)e^{-\lambda n} + \Gamma(0, \lambda n)\right) \; +$$

$$\sum_{m\geq 0} \frac{B_m}{m!}\lambda^{m+1}\left(\frac{\log\lambda}{m+1} - \frac{1}{(m+1)^2}\right)$$

An instance of this convergent series is afforded by setting $\lambda := \log 2$, whence

$$\log A = \frac{1}{24} + \frac{\log^2 2}{4\pi^2} - \frac{\log^2 2\ \log\log 2}{4\pi^2} + \frac{1}{12}\log 2\pi - \frac{1}{24}\log\log 2 - \frac{1}{2\pi^2}\sum_{n\geq 1}\left(\frac{\Gamma(0, n\log 2)}{n^2} + \frac{B_{n-1}}{n!}\log^n 2\left(-\frac{1}{n} + \log\log 2\right)\right).$$

300 summands of this series yield about 100 good decimal digits for $\log A$.

The above development for $\log A$ is to show how Bernoulli-series forms may be employed. There are somewhat more efficient series; for example, (19) may be used together with [50, (8)]:

$$\int_0^{1/2} \log\Gamma(x+1)\ dx = -\frac{1}{2} - \frac{7}{24}\log 2 + \frac{1}{4}\log\pi + \frac{3}{2}\log A$$

to effect a Glaisher–Kinkelin representation in terms of a rational zeta series, in the spirit of [12]. A goal of "one decimal digit of precision per series term" can thus be met in the form

$$\log A = \frac{265}{144} - \frac{1}{12}\gamma + \frac{571}{36}\log 2 - \frac{14}{3}\log 3 - \frac{5}{3}\log 5 - \frac{7}{3}\log 7 - \frac{1}{6}\log\pi + \frac{1}{3}\sum_{n\geq 2}\frac{\left(\zeta(n) - 1 - \frac{1}{2^n} - \frac{1}{3^n} - \frac{1}{4^n}\right)(-1)^n}{n(n+1)2^n},$$

where, indeed, summands decay as 10^{-n}.

7.4 Khintchine constant

The celebrated Khintchine constant—the (almost everywhere) geometric mean of continued fraction elements, is given from the measure theory of fractions as

$$K_0 = \prod_{r\geq 1}\left(1 + \frac{1}{r(r+2)}\right)^{\log_2 r}.$$

Over the years, rapidly convergent expansions have accrued, such as [3]

$$(\log 2)(\log K_0) = \sum_{n\geq 1}\frac{\zeta(2n) - 1}{n}\sum_{k=1}^{2n-1}\frac{(-1)^{k+1}}{k},$$

a series that can be accelerated by "peeling off" terms from $\zeta(2n)$ and so involve Hurwitz-zeta values $\zeta(2n, N)$ for a chosen positive integer N.

Thus our various algorithms for computing ζ or Hurwitz-ζ can be brought to bear for the Khintchine constant. But there is more to be said. Another series for K_0 is

$$(\log 2)(\log K_0) \;=\; \log^2 2 + \mathrm{Li}_2\left(-\frac{1}{2}\right) + \frac{1}{2}\sum_{k\geq 2}(-1)^k\,\mathrm{Li}_2\left(\frac{4}{k^2}\right).$$

While this series converges rather slowly (1000 summands yield about 6 good decimals), there is the interesting research problem of somehow speeding up the polylogarithmic sum.

A modern, very efficient series is attributed to O. Pavlyk, who built on the work of Gosper [52], which series we paraphrase here as

$$\begin{aligned}(\log 2)(\log K_0) \;&=\; -\frac{\pi^2}{6}(\gamma + \log 2 + \log \pi - 12\log A) + \\ &2\sum_{k=2}^{\infty}(-1)^k\frac{\log k}{(k+2)k^{k+2}}\left(2^{k+1}\,{}_2F_1\left(1, k+2; k+3; -\frac{2}{k}\right) - {}_2F_1\left(1, k+2; k+3; -\frac{1}{k}\right)\right) + \\ &2\sum_{k=2}^{\infty}\frac{(-1)^k(2^k-1)}{k+1}\left(\zeta^{(1)}(k+1) \;+\; \sum_{j=1}^{k-1}\frac{\log j}{j^{k+1}}\right),\end{aligned}$$

where A is the aforementioned Glaisher–Kinkelin constant. Again we witness the appearance of previously studied entities, namely ζ derivatives.

Another Gosper relation is

$$(\log 2)(\log K_0) \;=\; \sum_{j\geq 2}\frac{(-1)^j(2-2^j)}{j}\,\zeta^{(1)}(j).$$

This series converges slowly, so again a good research problem is to somehow apply acceleration. It may be helpful to observe that this series may be transformed to

$$(\log 2)(\log K_0) \;=\; 2\gamma\log 2 - \sum_{j\geq 2}\frac{(-2)^j}{j}\,\eta^{(1)}(j). \tag{43}$$

7.5 The MRB constant

The M. R. Burns (MRB) constant is given by the attractive summation [51]:

$$B \;=\; \sum_{k\geq 1}(-1)^k\left(k^{\frac{1}{k}} - 1\right) \;=\; 0.1878596\ldots\,.$$

Remarkably, if we look longingly at our voluminous list of zeta variants and use a series for $k^{1/k} = e^{(\log k)/k}$, we obtain, at least formally, a true jewel of an expression:

$$B \;=\; -\sum_{m\geq 1} \frac{(-1)^m}{m!}\eta^{(m)}(m),$$

which series actually converges rather quickly (60 summands here yield > 100 correct decimal digits). It may turn out to be lucrative to employ not the eta derivatives $\eta^{(m)}(m)$ explicitly, instead to use a Taylor expansion of $\eta(d)$ around $d = 0$ to write, again formally:

$$B \;=\; \sum_{m\geq 1} \frac{c_m}{m!}\eta^{(m)}(0), \qquad (44)$$

where the c coefficients are defined

$$c_j \;:=\; \sum_{d=1}^{j} \binom{j}{d}(-1)^d d^{j-d}.$$

Interestingly, as pointed out by J. Borwein, $c_j/j!$ is the j-th Taylor coefficient in the expansion of e^{-xe^x} about $x = 0$. Though (44) converges rather slowly, it is conceivable that by focusing on the fixed argument 0 of the eta derivatives, we might uncover some algorithm advantages; see for example Section 3.2 for remarks on Riemann-zeta derivatives at argument 0.

7.6 Examples of alternating-series acceleration

The already classic paper [21] lays out historical and modern means of accelerating alternating series. The idea is that many a sum $S = \sum_n (-1)^n a_n$ can be restructured to converge—sometimes surprisingly—rapidly to its value S. As just one application of Algorithm 1 of [21], we can take our alternating relation (43) and run *Mathematica* code:

```
eta[s_] := (1 - 2^(1 - s)) Zeta[s];
s1 = 2 EulerGamma Log[2];
a[j_] := 1/(j + 2) 2^(j + 2) Derivative[1][eta][j + 2];
(* Now start accelerate algorithm for given a[0], a[1], ... *)
n = 130;  (* Number of a's involved. *)
d = (3 + Sqrt[8])^n; d = 1/2 (d + 1/d);
{b, c, s} = {-1, -d, 0};
Do[
  c = b - c;
  s = s + c a[k];
  b = (k + n) (k - n) b/((k + 1) (k + 1/2))
```

```
  , {k, 0, n - 1}
 ];
s2 = s/d;
(* s2 is now the desired sum of (-1)^k a[k]. *)
N[s1 - s2, 110]
```

Remarkably enough, the (only!) $n = 130$ evaluations of the η-derivative here yield 100 good decimal digits of the Khintchine constant K_0. A good many of our other alternating series throughout the present paper can likewise benefit from this specific acceleration technique.

Another example using the same algorithm—just different $a[\,]$ terms—is that of computing a ζ derivative. Consider that

$$\zeta^{(1)}(s) \;=\; \frac{\eta^{(1)}(s) - 2^{1-s}(\log 2)\;\zeta(s)}{1 - 2^{1-s}},$$

with

$$\eta^{(1)}(s) = -\sum_{n\geq 0} \frac{(-1)^n \log(n+1)}{(n+1)^s}.$$

Now we can apply the above coded algorithm to this alternating sum, to get for example $\zeta^{(1)}(2)$ to 100 good decimals with the same $n = 130$ total $a[j]$ terms involved. Note that even the $\zeta(2)$ appearing can be calculated in the same fashion, from the alternating $\eta(2)$. Incidentally, this example shows that $\log A$, where A is the Glaisher-Kinkelin constant, can be obtained quickly to 100 decimals, with a very short program involving only elementary-functions calls.

A good research challenge is to calculate in this accelerated fashion more general zeta variants, such as the MTW values discussed next.

8 MTW zeta values and polylogarithm derivatives

8.1 Rapidly convergent series representation

The Mordell–Tornheim–Witten (MTW) zeta function has a canonical form

$$\mathcal{W}(r,s,t) \;:=\; \sum_{m,n\geq 1} \frac{1}{m^r n^s (m+n)^t} \tag{45}$$

and has been the focus of much study in regard to symbolic identities, analyticity and so on. The literal sum converges over a certain r, s, t space, and can be analytically continued for all complex r, s, t—although there are singularities. We borrow the expedient of definite integration from Bailey, Borwein et al. [5] to represent $\mathcal{W}$ as

$$\mathcal{W}(r,s,t) \;=\; \frac{1}{\Gamma(t)} \int_0^1 \mathrm{Li}_r(z)\mathrm{Li}_s(z)(-\log z)^{t-1}\,\frac{dz}{z}. \tag{46}$$

By adroitly splitting $\int_0^1 \to \int_0^{1/e} + \int_{1/e}^1$, we may insert the series (32, 33) into the second integral, employing the evaluations

$$\begin{aligned} U_{p,q} &:= \int_{1/e}^{1} \log^p z \log^q(-\log z) \frac{dz}{z} \\ &= \frac{(-1)^{p+q}\, q!}{(p+1)^{q+1}}, \end{aligned}$$

and defining coefficients

$$\begin{aligned} A_p &:= \Gamma(1-p); \quad p \notin Z^+, \\ &:= \frac{(-1)^{p-1}}{\Gamma(p)} H_{p-1}; \quad p \in Z^+, \end{aligned}$$

where $H_k = \sum_{j=1}^k 1/j$ is the k-th harmonic number, with $H_0 := 0$. Similarly, defining

$$\begin{aligned} B_p &:= 0; \quad p \notin Z^+, \\ &:= \frac{(-1)^p}{\Gamma(p)}; \quad p \in Z^+, \end{aligned}$$

we obtain a series for $\mathcal{W}$ that is valid for any complex r, s, t, with $|\lambda| < 2\pi$:

$$\begin{aligned} \Gamma(t)\ \mathcal{W}(r,s,t) = \sum_{m,n\ge 1} \frac{\Gamma(t,(m+n)\lambda)}{m^r n^s (m+n)^t} \; + \\ \sum_{u,v\ge 0}{}' (-1)^{u+v} \frac{\zeta(r-u)\zeta(s-v)}{u!v!(u+v+t)} \lambda^{u+v+t} \; + \\ \sum_{q\ge 0}{}' (-1)^q \frac{\zeta(r-q)}{q!} \lambda^{s+q+t-1} \left(\frac{A_s + B_s \log\lambda}{(s+q+t-1)} - \frac{B_s}{(s+q+t-1)^2} \right) \; + \\ \sum_{q\ge 0}{}' (-1)^q \frac{\zeta(s-q)}{q!} \lambda^{r+q+t-1} \left(\frac{A_r + B_r \log\lambda}{(r+q+t-1)} - \frac{B_r}{(r+q+t-1)^2} \right) \; + \; \lambda^{r+s+t-2} \cdot \\ \left(\frac{(A_r + B_r\log\lambda)(A_s + B_s\log\lambda)}{r+s+t-2} - \frac{A_r B_s + A_s B_r + 2B_r B_s \log\lambda}{(r+s+t-2)^2} + \frac{2B_r B_s}{(r+s+t-2)^3} \right). \end{aligned} \tag{47}$$

The notation $\sum'$ means that we *avoid* any $\zeta(1)$ evaluations entirely.

A fascinating result from this Erdélyi-series procedure: There are singularities of $\mathcal{W}$ at $r+s+t=2$, with residue $\Gamma(1-r)\Gamma(1-s)/\Gamma(t)$ when said residue is finite. But there are *also* singularities whenever $s+t-1$ or $r+t-1$ is a nonpositive integer. Also, in the limit $t \to 0$ we see that the residual term is just the first ($u = v = 0$) term of the u, v summation, and so $\mathcal{W}(r, s, 0) = \zeta(r)\zeta(s)$ is verified. As for testing such a complicated but converging representation,

1) One should obtain the same basic numerical answer over a range of free λ.
2) One might verify numerically the Zagier triangle identity

$$\mathcal{W}(r, s, t) = \mathcal{W}(r-1, s, t+1) + \mathcal{W}(r, s-1, t+1).$$

3) A typical numerical value for three noninteger r, s, t is

$$\mathcal{W}(\pi, \pi, \pi) \approx 0.121784932649073172392415831466446\ldots\ .$$

4) A typical evaluation near a pole is, for $d := 200001/300000$,

$$\mathcal{W}(d, d, d) = 529982.9016524962105\ldots\ .$$

5) Analytic-continuation values *are* obtainable outside of the domain of literal convergence of the defining sum for $\mathcal{W}$, e.g.

$$\mathcal{W}\left(-\frac{1}{2}, -\frac{1}{2}, 1\right) = 0.6378331771492328160229422319062\ldots.$$

8.2 Multiple-zeta values

The twofold multiple-zeta function is

$$\overline{\zeta}(t, r) = \sum_{n>m\geq 1} \frac{1}{n^t}\frac{1}{m^r},$$

which is seen to be

$$= \mathcal{W}(r, 0, t).$$

Thus, the $s = 0$ case of series (47) is in play, and we get values such as

$$\overline{\zeta}\left(\frac{3}{2}, 1\right) = 4.6818144115562270356922102793371995\ldots\ ,$$

and for one of the still algebraically unresolved cases

$$\overline{\zeta}(2, 6) = 0.65156516371512690455646396209037 7\ldots\ .$$

In this connection see [28, 29]—the latter reference reveals a surprising efficiency in higher-dimensional sum calculations, which efficiency was later echoed in [14, Sec 7]. The pioneering algebraic work on such entities is exemplified in papers such as [4, 10] and references therein.

8.3 Alternating MTW variants

Alternating MTW sums are generally more numerically tractable, due to the existence of the alternating zeta function $\eta(s)$ defined below. The polylogarithmic instance of doubling relation (6) is

$$\mathrm{Li}_s(z) + \mathrm{Li}_s(-z) \;=\; \frac{1}{2^{s-1}}\mathrm{Li}_s(z^2),$$

which identity can be used in conjunction with (32) to establish an attractive, compact series (valid for $|\log z| < \pi$)

$$\mathrm{Li}_s(-z) \;=\; -\sum_{m\ge 0} \eta(s-m)\frac{\log^m z}{m!}\;, \tag{48}$$

where

$$\eta(s) \;:=\; \left(1 - 2^{1-s}\right)\zeta(s)$$

is a regular function; the $(s=1)$-pole of ζ has vanished, as $\eta(1) = \log 2$, so the sum (48) requires no singularity avoidance. Most important for certain analyses: The eta-series (48) can be differentiated with respect to the outer variable, say

$$\mathrm{Li}_s^{(k)}(-z) \;:=\; \left(\frac{\partial}{\partial s}\right)^k \mathrm{Li}_s(-z) \;=\; -\sum_{m\ge 0} \eta^{(k)}(s-m)\frac{\log^m z}{m!}.$$

We note in passing the derivatives

$$\eta^{(1)}(1) \;=\; \gamma \log 2 - \frac{1}{2}\log^2 2,$$

$$\eta^{(1)}(-2) \;=\; -\frac{1}{3}\log 2 - \frac{1}{4} + 3\log A,$$

where A is the Glaisher–Kinkelin constant; in general, though, one only needs a library of numerical Riemann-ζ derivatives to obtain η derivatives.

An immediate byproduct of this eta-expansion is a rapidly convergent series for certain MTW zeta-variants. Consider for example the entity (here we echo the notation of Borwein et al. [5]):

$$\omega^{--}_{a,b,0}(r,s,t) \;:=\; \sum_{m,n\ge 1} (-1)^{m+n}\frac{\log^a m\,\log^b n}{m^r n^s (m+n)^t}\;,$$

which can also be written

$$=\; \frac{(-1)^{a+b}}{\Gamma(t)}\int_0^1 \mathrm{Li}_r^{(a)}(-z)\mathrm{Li}_s^{(b)}(-z)(-\log z)^{t-1}\,\frac{dz}{z}\,.$$

By again splitting $\int_0^1 \to \int_0^{1/e} + \int_{1/e}^1$, and employing the eta expansion (48) for the integral over $(1/e, 1)$, we can use evaluations

$$\int_0^{1/e} z^\alpha (-\log z)^\beta \, dz \;=\; \frac{1}{(1+\alpha)^\beta}\Gamma(1+\beta, 1+\alpha)$$

we arrive at a convergent series involving the η-function. An example of such series is the case $\omega_{0,0,0}^{--}$:

$$\omega_{0,0,0}^{--}(r,s,t) \;=\; \sum_{m,n\ge 1} \frac{(-1)^{m+n}}{m^r n^s (m+n)^t} \frac{\Gamma(t, m+n)}{\Gamma(t)} \;-\; \frac{1}{\Gamma(t)} \sum_{j,k\ge 0} \frac{\eta(r-j)}{j!} \frac{\eta(s-k)}{k!} \frac{(-1)^{j+k}}{j+k+t}. \tag{49}$$

Note that for positive integer t, the incomplete gamma function here is elementary. For the case $r = s = t = 1$ we can give a limit on each summation index, say $m, n, j, k \le 240$, to obtain

$$\omega_{0,0,0}^{--}(1,1,1) \;:=\; \sum_{m,n\ge 1} \frac{(-1)^{m+n}}{mn(m+n)}$$

$$= \; 0.30051422578989857134993454037786249769124657308512472044806788883 54\ldots\;,$$

agreeing in fact with the $\omega_{0,0,0}^{--}(1,1,1) = \frac{1}{4}\zeta(3)$, a known evaluation [11].

Intriguing it is that certain apparently difficult sums can be computed more easily than one might expect. An exemplary calculation—using first derivatives of η—is

$$\omega_{1,1,0}^{--}(1,1,1) \;:=\; \sum_{m,n\ge 1} \frac{(-1)^{m+n} \log m \, \log n}{m\, n(m+n)}$$

$$= \; 0.008465459183243566000220465483\ldots$$

8.4 More difficult ω-sums

The computational situation with the ω-sums is much more problematic when the alternating sign factor $(-1)^{m+n}$ is absent. Let us consider

$$\omega_{a,b,c}^{++}(r,s,t) \;:=\; \sum_{m,n\ge 1} \frac{\log^a m \, \log^b n \, \log^c(m+n)}{m^r n^s (m+n)^t}$$

$$= \; (-1)^{a+b+c} \frac{\partial^c}{\partial t^c} \frac{1}{\Gamma(t)} \int_0^1 \mathrm{Li}_r^{(a)}(z) \mathrm{Li}_s^{(b)}(z) (-\log z)^{t-1} \, \frac{dz}{z}\,,$$

where now it will be recognized that the argument of the polylogarithms is not $-z$, but $+z$. This seemingly innocent alteration motivates us to work out the complete analytic expansion of polylogarithms near integer outer argument—a task to which we next turn.

9 Analytic expansion of Li_s for near-integer s

An intricate analysis of the Erdélyi representation (32) yields an analytic expansion of $\mathrm{Li}_s(z)$ for $s = k + 1 + \tau$, for k a fixed nonnegative integer and a new complex variable τ. It is convenient first to state the result informally:

Principle: For nonnegative integer k, the d-th derivative $\mathrm{Li}_{k+1}^{(d)}$ can be cast as

$$\mathrm{Li}_{k+1}^{(d)}(z) = (\text{series in powers of } \log z) + \log^k z \cdot (\text{degree-}(d{+}1) \text{ polynomial in } \log(-\log(z))).$$

Let us choose a nonnegative integer k and rewrite (32) with $s = k + 1 + \tau$:

$$\mathrm{Li}_s(z) \;=\; \sum_{0 \le n \ne k} \zeta(k + 1 + \tau - n)\,\frac{\log^n z}{n!} \;+\; \left\{ \Gamma(-k - \tau)(-\log z)^{k+\tau} + \zeta(1 + \tau)\,\frac{\log^k z}{k!} \right\}. \tag{50}$$

Now there is no singularity avoidance whatever in the sum, so the τ-expansion of said sum can be written in terms of derivatives of ζ. We proceed to expand the entity in braces in powers of τ. Omitting the tedious details, the full τ-expansion is, for $|\log z| < 2\pi$ and $\tau \in [0, 1)$:

$$\mathrm{Li}_{k+1+\tau}(z) \;=\; \sum_{0 \le n \ne k} \zeta(k + 1 + \tau - n)\frac{\log^n z}{n!} \;+\; \frac{\log^k z}{k!} \sum_{j=0}^{\infty} c_{k,j}(\mathcal{L})\,\tau^j, \tag{51}$$

with $\mathcal{L} := \log(-\log z)$ and the c coefficients involve the Stieltjes constants from (28):

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

for b coefficients defined in turn by

$$b_{k,j}(\mathcal{L}) \;=\; \sum_{\substack{p+t+q=j \\ p,t,q \ge 0}} \frac{\mathcal{L}^p}{p!}\frac{\Gamma^{(t)}(1)}{t!}(-1)^{t+q} f_k(q),$$

where $f_k(q)$ is the coefficient of x^q in

$$\prod_{m=1}^{k} \frac{1}{1 + x/m},$$

easily calculable via $f_{k,0} = 1$ and the recursion

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

The first instances are harmonic-number relations $f_{k,q} = -H_k$ and $f_{k,2} = \frac{1}{2}H_k^2 + \frac{1}{2}H_k^{(2)}$.

Recondite as this τ-expansion may be, the rewards are substantial. Indeed, one has

$$c_{k,0} \;=\; H_k \;-\; \mathcal{L},$$

giving immediately the Erdélyi expansion (33) at any positive integer $s = k+1$. Another instance: To get first derivatives $\mathrm{Li}_1^{(1)}(z)$ for $k=0$ we shall need the exact evaluation

$$c_{0,1} \;=\; -\gamma_1 - \frac{1}{2}\gamma^2 - \frac{\pi^2}{12} - \gamma\mathcal{L} - \frac{1}{2}\mathcal{L}^2.$$

This begets a convergent expansion for first outer derivative (again for $|\log z| < 2\pi$):

$$\mathrm{Li}_1^{(1)}(z) \;=\; \sum_{n\geq 1} \zeta^{(1)}(1-n)\frac{\log^n z}{n!} - \gamma_1 - \frac{1}{2}\gamma^2 - \frac{\pi^2}{12} - \gamma\log(-\log z) - \frac{1}{2}\log^2(-\log z). \tag{52}$$

As a sharp test of this result, a numerical value for 50 terms of the ζ'-series here works out as

$$\mathrm{Li}_1^{(1)}\left(\frac{1}{2}\right) \;=\; -0.17289680030426475956117932688102820711445969877 14\ldots,$$

correct to the implied precision, when compared to different algorithms that simply take numerical derivatives of polylogarithms.

9.1 Convergent sums for the difficult ω values

Let us employ the above analytical results to attempt an exemplary series representation of

$$\omega_{1,1,0}^{++}(1,1,1) \;:=\; \sum_{m,n\geq 1} \frac{\log m\,\log n}{mn(m+n)}$$

$$= \int_0^1 \mathrm{Li}_1^{(1)}(z)\mathrm{Li}_1^{(1)}(z)\,\frac{dz}{z}\,,$$

again using notation and integral from Borwein et al. [5]. Combining results so far, we have a series form:

$$
\begin{aligned}
\omega_{1,1,0}^{++}(1,1,1) \;=\; \beta \;+\; \sum_{m,n\geq 1} \frac{\log m\, \log n}{mn(m+n)} e^{-m-n} \;+& \\
\sum_{m,n\geq 1} \frac{\zeta^{(1)}(1-m)}{m!} \frac{\zeta^{(1)}(1-n)}{n!} U_{m+n,0} \;-& \\
\sum_{m\geq 1} \frac{\zeta^{(1)}(1-m)}{m!} \left(2\alpha\, U_{m,0} + 2\gamma\, U_{m,1} + U_{m,2}\right)\,,&
\end{aligned}
\tag{53}
$$

where constants are defined:

$$
\alpha \;:=\; \gamma_1 + \frac{1}{2}\gamma^2 + \frac{\pi^2}{12},
$$

$$
\beta = 6 + 2\alpha + \alpha^2 - 6\gamma - 2\alpha\gamma + 2\gamma^2.
$$

Taking a limit of 375 on every summation index, we obtain a 140-digit value

$$
\omega_{1,1,0}^{++}(1,1,1) \;\approx
$$

```
4.30244762034222643331985179818698942752019447430436225569749833\
  73406896458605708423834220669589660132906320814848672664367230\
  398478820315706236223995256611060718260 4
```

in evident agreement with preliminary computations of Bailey, Borwein et al. [5].

9.2 Combining series with extreme-precision quadrature

There is an interesting way to achieve precise numerics via a combination of series and quadrature. Consider the MTW sums as in (45), but now 4-dimensional:

$$
\mathcal{W}(r,s,t,u) \;:=\; \sum_{m,n,p\geq 1} \frac{1}{m^r n^s p^t (m+n+p)^u}. \tag{54}
$$

Clearly, a multidimensional sum of the type (47) can be generated, but it can become—for higher dimensions—more practical to use a simpler series together with quadrature. Indeed, it is not hard to derive

$$
\begin{aligned}
\Gamma(u)\, \mathcal{W}(r,s,t,u) \;=\; \sum_{m,n,p\geq 1} \frac{\Gamma(u, \lambda(m+n+p))}{m^r n^s p^t (m+n+p)^u} \;+& \\
\int_0^\lambda T^{u-1} \mathrm{Li}_r\left(e^{-T}\right)\, \mathrm{Li}_s\left(e^{-T}\right)\, \mathrm{Li}_t\left(e^{-T}\right)\; dT,&
\end{aligned}
\tag{55}
$$

valid for free parameter $\lambda \in [0, \infty)$. This wide parameter range also yields various theoretical truths; we obtain on the assignment $\lambda := \infty$ such cases as

$$\mathcal{W}(1,1,1,1) \;=\; 6\,\zeta(4),$$
$$\mathcal{W}(0,0,0,u) \;=\; \zeta(u) - \frac{3}{2}\zeta(u-1) + \frac{1}{2}\zeta(u-2),$$

and so on. As for the use of extreme-precision quadrature, taking $\lambda := 3$ and a limit of 80 on each summation index results in such as

$$\mathcal{W}(1,1,1,1) \;=\; 6.4939394022668291490960221792470074166485057115123614460 97\ldots,$$
$$\mathcal{W}(2,2,2,2) \;=\; 0.20455675507770602758948208328044122237213211374667483820 2\ldots,$$
$$\mathcal{W}(2,4,6,8) \;=\; 0.000157853276760225431962629891229777035954013043090624 19\ldots.$$

The first of these three approximations is consistent with $6\,\zeta(4)$.

Moreover, if one wants MTW outer derivatives, one may use such representations as (52) together with quadrature, to obtain, for free parameter $\lambda \in (e^{-2\pi}, 1]$,

$$\omega^{++++}_{1,1,1,1}(1,1,1,1) \;:=\; \sum_{m,n,p\,\geq 1} \frac{\log m\, \log n\, \log p\, \log(m+n+p)}{m\,n\,p\,(m+n+p)} \tag{56}$$
$$= \int_0^1 \left(\mathrm{Li}_1^{(1)}(z)\right)^3 (\gamma + \log(-\log z))\,\frac{dz}{z}$$
$$= \int_\lambda^1 \left(\mathrm{Li}_1^{(1)}(z)\right)^3 (\gamma + \log(-\log z))\,\frac{dz}{z} \;-$$
$$\sum_{m,n,p\,\geq 1} \frac{\log m\, \log n\, \log p}{m\,n\,p\,(m+n+p)} \left((\gamma + \log(-\log\lambda))\lambda^{m+n+p} \;+\; \Gamma(0, -(m+n+p)\log\lambda)\right)$$
$$=\; 393.95644190297417690269554547960277193912677747341826027083865338 79\ldots.$$

9.3 Alternative formulae for polylogarithm analysis

Another option for possible derivative-based analysis of polylogarithms and ω-sums is to invoke the identity

$$\mathrm{Li}_s(z) \;=\; \frac{z}{2} \;+\; \sum_{m\in Z} \frac{\Gamma(1-s, 2m\pi i - \log z)}{(2m\pi i - \log z)^{s-1}}.$$

It is suggested that if this sum be performed symmetrically—i.e. summed over $m \in [-M, +M]$ then $M \to \infty$, the relation is valid for all complex s, z [47].

9.4 Clausen function

A generalized Clausen function is

$$\mathrm{Cl}_s(x) \ := \ \sum_{n\geq 1} \frac{\sin nx}{n^s},$$

which can be formally put in Lerch–Hurwitz (complex-argument polylogarithmic) form

$$= \ \frac{1}{2i}\left(\mathrm{Li}_s\left(e^{ix}\right) - \mathrm{Li}_s\left(e^{-ix}\right)\right).$$

From the eta-decomposition (48) we quickly obtain (valid for $|\theta| < \pi$)

$$\mathrm{Cl}_s(\pi-\theta) \ = \ -\sum_{\text{odd } n>0} \frac{\eta(s-n)}{n!}(-1)^{(n-1)/2}\,\theta^n \ . \tag{57}$$

For nonnegative integer k we know $\eta(-k) \ = \ (1-2^{k+1})(-1)^k \frac{B_{k+1}}{k+1}$, so when s is a positive integer we have

$$\mathrm{Cl}_s(\pi-\theta) \ = \ -\sum_{\text{odd } n\in[1,s-1]} \frac{\eta(s-n)}{n!}(-1)^{(n-1)/2}\,\theta^n \ +$$

$$\sum_{\text{odd } n\geq s+1} \left(1-2^{n-s+1}\right)(-1)^{(n-1)/2} \frac{B_{n+s-1}}{n!(n+s-1)}\,\theta^n.$$

We have split up the eta series in this way to signal the fact of eta being elementary at nonpositive integer arguments. For example, the Catalan constant G can be written

$$G \ = \ \mathrm{Cl}_2\left(\frac{\pi}{2}\right) \ := \sum_{n\geq 1} \frac{\sin(\pi n/2)}{n^2} \ = \ \frac{1}{1^2} \ - \frac{1}{3^2} \ + \ \frac{1}{5^2} \ - \cdots$$

$$= \ \frac{\pi}{2}\log 2 \ + \sum_{\text{odd } n\geq 3} \left(2^{n-1}-1\right)(-1)^{(n-1)/2} \frac{B_{n-1}}{n!(n-1)} \left(\frac{\pi}{2}\right)^n.$$

A more exotic example is

$$\mathrm{Cl}_8\left(\frac{\pi}{2}\right) \ := \sum_{n\geq 1} \frac{\sin(\pi n/2)}{n^8} \ = \ \frac{1}{1^8} \ - \frac{1}{3^8} \ + \ \frac{1}{5^8} \ - \cdots$$

$$= \frac{\pi^5\zeta(3)}{5120} - \frac{5\pi^3\zeta(5)}{256} + \frac{63\pi\zeta(7)}{128} - \frac{\pi^7\log 2}{645120} + \sum_{\text{odd } n\geq 9} \left(2^{n-7}-1\right)(-1)^{(n-1)/2} \frac{B_{n-7}}{n!(n-7)} \left(\frac{\pi}{2}\right)^n.$$

For some θ the convergence of (57) may be slow, in which case an alternative series may be derived from the polylogarithm representation (33). Taking $s = 2$ for example, we find

$$\mathrm{Cl}_2(t) \;=\; t\left(1 - \frac{1}{2}\log t^2\right) \;+\; \sum_{\mathrm{odd}\ n\ge 3} (-1)^{(n-3)/2}\frac{B_{n-1}}{n!(n-1)}t^n,$$

valid for $|t| < 2\pi$, so one may switch between this series or (57) (with $s = 2$) to achieve rapid convergence over the useful range $t \in [-\pi, +\pi]$. Extension to arbitrary integer s is straightforward.

Incidentally, in [13] it is mentioned that a single Clausen series can also be accelerated using the duplication rule

$$\frac{1}{2}\mathrm{Cl}_2(2\theta) \;= \mathrm{Cl}_2(\theta) - \mathrm{Cl}_2(\pi - \theta).$$

In addition, those authors also mention yet another use of Bernoulli multisectioning to facilitate extreme-precision Clausen evaluation (see our Section 2.2). The importance of Clausen functions in modern experimental mathematics is exemplified by the questions raised in [31].

In the recent literature [5] there appear such entities as outer Clausen derivatives. We record here a certain, striking instance via our polylogarithm derivative form (52):

$$\begin{aligned}\mathrm{Cl}_1^{(1)}(\theta) \;&=\; -\sum_{n\ge 1}\frac{\log n}{n}\sin(n\theta)\\ &=\; \frac{\pi}{2}(\gamma + \log\theta) \;+\; \sum_{\mathrm{odd}\ n>0}\zeta^{(1)}(1-n)(-1)^{(n-1)/2}\,\frac{\theta^n}{n!},\end{aligned} \qquad (58)$$

valid for real $\theta \in (0, 2\pi)$. It is fascinating that the $\log\Gamma$ forms (19, 20) now imply a direct connection between a zeta-sum and the zeta-derivative-sum here in (58). Indeed, denote by $\sum_\zeta$ the zeta-sum in (19), and by $\sum_{\zeta'}$ the derivative-sum in (58) with $\theta := 2\pi z$. Then

$$\sum_\zeta \;+\; \frac{1}{\pi}\sum_{\zeta'} \;=\; 1 - \gamma - z(1 + \log 2\pi) - \frac{1}{2}\log\frac{\sin\pi z}{\pi z},$$

which relation also means that we can cast the Clausen derivative in question in terms of a zeta-sum (devoid of zeta-derivatives). This connection is currently not fully understood; certainly, one would like to avoid zeta derivatives in sums, in favor of zeta values per se. (See [12] for various "recycling" methods that generate and process large sets of zeta values.)

10 Epstein zeta functions and lattice sums

For a higher-dimensional analogue of our algorithm developments, we consider a certain generalized (Epstein) zeta function of four parameters. Specifically, assume A is a D-by-

D, real, positive definite matrix, s is a complex number, and c, d are real vectors. We adopt the definition

$$Z_A(s; c, d) \ := \ \sum_{n \in Z^D}{}' \frac{e^{2\pi i c \cdot An}}{|An - d|^s}, \tag{59}$$

where the vector n runs over the full, D-dimensional integer lattice and the notation $\sum'$ means as usual that any singularities are to be ignored in the course of summation. As to the very existence of the sum, there will generally be some real threshold σ for which the constraint $\Re(s) > \sigma$ yields an absolutely convergent $\sum'$. Then we may infer the analytic continuation to $\Re(s) \leq \sigma$ by standard methods. We note that Z_A has a one-dimensional instance that coincides with the Riemann ζ function. For $A = 1$ (the identity matrix) we have

$$Z_1(s; 0, 0) = 2\zeta(s).$$

Just as with the Riemann zeta itself, there exist attractive closed-form evaluations of Z_A, in various dimensions D, as we present later.

Over the years, the sums Z_A have arisen in chemistry and physics research. Calculation of electrostatic energies of crystals use such sums in a natural way. In fact, in this context the matrix A is what characterizes the very structure of a periodic crystal, so that Z_A is related to physical energy. Interesting also is that the avoidance of the singularity in the Σ' is manifest in the physical scenario as avoidance of self-energy at an ionic center. There is a large and long-standing literature on such chemical application, grouped under such topical headings as "lattice sums," or "Madelung problem," and so on (see [27] for some survey material). In theoretical physics, vacuum energy—-or Casimir—calculations may also involve Epstein zeta functions [1]. The Epstein sums also figure into analytic number theory, for example in problems regarding sum-of-squares representations.

There are some interesting optimizations we can state right off. First, it will turn out to be computationally efficient to handle matrices of unit determinant. To this end we observe a scaling property, valid for positive real γ:

$$Z_A(s; c, d) = \gamma^{-s} Z_{A/\gamma}(s; \gamma c, d/\gamma). \tag{60}$$

Now the choice

$$\gamma = (\det A)^{1/D}$$

allows us to carry out calculations for the right-hand side of (60), with its matrix A/γ having unit determinant. In the common case where A is a diagonal matrix, the γ parameter is simply the geometric mean of the diagonal elements.

A second initial optimization is this: we need not evaluate Z_A for unconstrained c, d vectors, because one can always reduce them according to the integer lattice Z^D. Define the inverse transpose:

$$B = A^{-T}$$

and reduce c, d with respect to the Z^D lattice by:

$$c' = B((B^{-1}c) \bmod 1),$$

$$d' = A((A^{-1}d) \bmod 1),$$

where it is intended that each component of a vector be reduced (mod 1); i.e., so that each component is in the interval $[0, 1)$. It turns out, then, that under such reduction to the lattice we have

$$Z_A(s; c, d) = e^{2\pi i c' \cdot (d-d')} Z_A(s; c', d'). \tag{61}$$

In this way the magnitudes of the c, d parameters can be controlled during computation. Accordingly, we shall heretofore assume c, d have been *a priori* reduced. In particular, a c or d parameter now belongs to the Z^D lattice if and only if it is the zero vector.

10.1 Riemann splitting for Epstein zeta

Along the lines of Algorithm 3 a dimensionally generalized form for Epstein zeta function Z_A works out to be

$$\begin{aligned} e^{-\pi i c \cdot d} \frac{\Gamma(s/2)}{\pi^{s/2}} Z_A(s; c, d) \quad = \quad & \frac{\delta(c) \det B}{s/2 - D/2} - \frac{\delta(d)}{s/2} \ + \\ & e^{-\pi i c \cdot d} \sum_n{}' \frac{\Gamma(\frac{s}{2}, \pi |An - d|^2) e^{2\pi i c \cdot An}}{(\pi |An - d|^2)^{s/2}} \ + \\ & \frac{e^{\pi i c \cdot d}}{\det A} \sum_k{}' \frac{\Gamma(\frac{D-s}{2}, \pi |Bk - c|^2) e^{-2\pi i d \cdot Bk}}{(\pi |Bk - c|^2)^{\frac{D-s}{2}}}. \end{aligned} \tag{62}$$

This incomplete-gamma series together with our preceding optimization discussion suggests the following:

Algorithm 4 Riemann-splitting algorithm for Epstein zeta function $Z_A(s; c, d)$.

1) Invoke the reduction formulae (60, 61) as necessary, so that inputs A, c, d have these properties: That $\det A = 1$ and for $B = A^{-T}$ all components of $B^{-1}c, A^{-1}d$ lie in $[0, 1)$ via (mod 1) reduction to the integer lattice.

2) Next we handle the two possibilities $s = 0, D$. First check for the known evaluation at $s = 0$: If $s = 0$ return either -1 (in the case d vanishes), or return zero (in the case $d \neq 0$). Then check for possible singularity at $s = D$: If both $s = D$ and $c = 0$, return with indication of singularity, otherwise continue to step (3).

3) Choose a summation limit L (so that computational error will be, roughly speaking, $e^{-\pi L^2}$). Find also the least and greatest eigenvalues, respectively λ, μ, of A.

4) Sum the first series of (62) over each component $n_i \in [-L/\lambda, +L/\lambda]$, evaluating only those summands having $|An - d| \leq L$. Then sum the second series of (62) similarly, but using instead $k_i \in [-\mu L, +\mu L]$, resolving only those summands with $|Bk - c| \leq L$.

5) Using the rest of the terms in (62), and any reduction formulae that were invoked in step(1), return an evaluation of the original Z_A.

10.2 Exact theoretical evaluations as sharp algorithm tests

There exist a host of closed-form results and known evaluations of the Epstein zetas. These results are extremely useful—if not indispensable—for proper testing of any computational engine that is supposed to be evaluating Z_A. Happily, there are known evaluations for different classes of parameters; e.g., d or c or both $\neq 0$, and so on. In what follows, we remind ourselves that c, d parameters are assumed reduced to the Z^D lattice, as was explained for reduction relation (61).

First there is the functional equation, which we can infer from the Riemann strategy. From (62) it is evident that the entity:

$$\Lambda_A(s; c, d) = \sqrt{\det A}\, e^{-\pi i c \cdot d} \frac{\Gamma(s/2)}{\pi^{s/2}} Z_A(s; c, d)$$

is invariant under a specific parametric transformation. Indeed,

$$\Lambda_A(s; c, d) = \Lambda_B(D - s; -d, c).$$

This functional equation is of course a higher-dimensional analogue of the celebrated relation for $\zeta(s)$.

An exact evaluation at $s = 0$ also follows from (62); namely:

$$Z_A(0; c, d) = -\delta(d),$$

from which the well known evaluation $\zeta(0) = -1/2$ follows in the one-dimensional setting. Likewise, the fact of a pole at $s = D$ depends, as we see in (62), on whether c vanishes: there is a pole at $s = D$ if and only if $c = 0$, and the residue is easy to infer as $2\pi^{D/2}(\det B)/\Gamma(D/2)$.

A beautiful class of closed-form evaluations has arisen over the years in the art of applying Z_A in the sciences. Many such relations arise in the theory of Jacobi theta-functions; often combinatorics and number theory are involved in fascinating ways. Here and elsewhere, 1_D means either the D-dimensional identity matrix, or a D-vector consisting of all 1's as appropriate by context; while α_D denotes a D-vector $\{\alpha, \alpha, ..., \alpha\}$. In addition, we define some specific L-series which figure into some of the closed-form evaluations:

$$\beta(s) = 1^{-s} - 3^{-s} + 5^{-s} - ...,$$

$$\eta(s) = (1 - 2^{1-s})\zeta(s) = 1^{-s} - 2^{-s} + 3^{-s} - ...,$$

$$\lambda(s) = (1 - 2^{-s})\zeta(s) = 1 + 3^{-s} + 5^{-s} + ...,$$

$$L_{-3}(s) = 1^{-s} - 2^{-s} + 4^{-s} - 5^{-s} + 7^{-s} - ...,$$

$$L_{-8}(s) = 1^{-s} + 3^{-s} - 5^{-s} - 7^{-s} + 9^{-s} + 11^{-s} - ...$$

$$L_{+8}(s) = 1^{-s} - 3^{-s} - 5^{-s} + 7^{-s} + 9^{-s} - 11^{-s} - ...$$

Some of these series themselves enjoy exact evaluation, such as $\beta(1) = \pi/4$ and the analytic continuation evaluation $\beta(0) = 1/2$.

Various exact evaluations are known for $D = 2$ dimensions, for example

$$Z_{1_2}(s; 0_2, 0_2) = \sum_{m,n \in Z}{}' \frac{1}{(m^2 + n^2)^{s/2}} = 4\zeta(s/2)\beta(s/2),$$

$$Z_{1_2}(s; (\frac{1}{2})_2, 0_2) = \sum_{m,n \in Z}{}' \frac{(-1)^{m+n}}{(m^2 + n^2)^{s/2}} = -4\eta(s/2)\beta(s/2).$$

Note that the second zeta above is a "Madelung constant" for $D = 2$, i.e. the potential energy of the origin charge in a certain 2-dimensional charge lattice. About the physically genuine, 3-dimensional Madelung constant we shall have more to say later. For the moment, we note that 2-dimensional zeta evaluations have been taken yet further, for example the Madelung problem on an hexagonal lattice has been solved, in the sense of exact evaluation. The relevant hexagonal sum is taken to be:

$$H(s) = \sum_{m,n \in Z}{}' \frac{(\frac{n-m+1}{3})}{((n + m/2)^2 + 3(m/2)^2)^{s/2}},$$

where $(\frac{x}{3})$ is the Legendre symbol, which runs $1, -1, 0, 1, -1, 0, ...$ as x runs $1, 2, 3, 4, 5, 6, ...$ Now $H(x)$ can be written as a superposition of four complex Epstein zetas. However, it is argued in [8] that one can instead evaluate just two (real) zetas:

$$H(s) = \frac{1-3^{1-s/2}}{2}(2Z_A(s;0_2,0_2) - Z_A(s;(\frac{1}{2})_2,0_2)),$$

with matrix

$$A = \{\{1, 1/2\}, \{0, \sqrt{3}/2\}\},$$

and by such means arrive at the exact value

$$H(s) = 3(1-3^{1-s/2})\zeta(s/2)L_{-3}(s/2),$$

so that the "Madelung" value is $H(1)$, while the case $s = 2$ comes down to the attractive result $H(2) = \pi \ln 3\sqrt{3}$. Beyond this, but still in two dimensions, sums with denominators $(m^2 + |d|n^2)^{s/2}$ have been evaluated, through adroit application of number-theoretical and transform techniques, for certain classes of discriminant d [37]. An example of the beauty of some of the known two-dimensional Epstein zeta evaluations is Zucker's sum:

$$\sum{}' \frac{(-1)^{m+n}}{(4m-1)^2 + 13(4n-1)^2} = \frac{\pi}{16\sqrt{13}} \log \frac{(1+\sqrt{2})^3}{5+\sqrt{26}}.$$

Further dimensional generalizations include the following collection for $D = 4$, starting with an attractive chain of evaluations [56] [37] [32]:

$$\log 2 = -\frac{1}{4}Z_{1_4}(2,(\frac{1}{2})_4,0_4) = -\frac{1}{4}\sum_{\{a,b,c,d\}\in Z^4} \frac{(-1)^{a+b+c+d}}{a^2+b^2+c^2+d^2}$$

$$= -\frac{\pi}{2} - Z_{1_4}(2;((\frac{1}{2})_3,0),0_4)$$

$$= -\frac{1}{2}Z_{1_4}(2;((\frac{1}{2})_2,0_2),0_4)$$

$$= \frac{\pi}{2} - Z_{1_4}(2;(\frac{1}{2},0_3),0_4)$$

$$= -\frac{1}{8}Z_{1_4}(2;0_4,0_4).$$

Some of which being instances of the following:

$$Z_{1_4}(s;(\frac{1}{2},0_3),0_4) = 4\beta(s/2)\beta(s/2-1) - 2^{3-s}\eta(s/2)\eta(s/2-1),$$

$$Z_{1_4}(s;((\frac{1}{2})_3,0),0_4) = -4\beta(s/2)\beta(s/2-1) - 2^{3-s}\eta(s/2)\eta(s/2-1),$$

$$Z_{1_4}(s;0_4,((\frac{1}{2})_3,0)) = 2^s(\lambda(s/2)\lambda(s/2-1) - \beta(s/2)\beta(s/2-1)),$$

$$Z_{1_4}(s; 0_4, (\frac{1}{2}, 0_3)) = 2^s(\lambda(s/2)\lambda(s/2-1) + \beta(s/2)\beta(s/2-1)),$$

$$Z_{1_4}(s; ((\frac{1}{2})_3, 0), (0_3, \frac{1}{2})) = 2^s(L_{-8}(s/2)L_{-8}(s/2-1) + L_{+8}(s/2)L_{+8}(s/2-1)),$$

$$Z_{1_4}(s; (\frac{1}{2}, 0_3), (0, (\frac{1}{2})_3)) = 2^s(L_{-8}(s/2)L_{-8}(s/2-1) - L_{+8}(s/2)L_{+8}(s/2-1)),$$

Then there are some isolated evaluations in even higher dimension, such as the beautiful 6-dimensional result of Zucker:

$$\sum{}' \frac{(-1)^{a+b+c+d+e+f}}{(a^2+3b^2+3c^2+3d^2+3e^2+3f^2)^{3/2}} = -\frac{2\pi\zeta(3)}{3\sqrt{3}} - \frac{4\pi^3\log 2}{81\sqrt{3}},$$

and an 8-dimensional result:

$$Z_{1_8}(8; (\frac{1}{2})_8, 0_8) = \sum_{n\in Z^8}{}' \frac{(-1)^{n_1+\ldots+n_8}}{(n_1^2+\ldots+n_8^2)^4} = -\frac{8\pi^4\log 2}{45}.$$

For the remainder of this section we focus on $D = 3$, which cases include evaluations applicable in the physical sciences.

10.3 Madelung constant

The celebrated Madelung constant of chemistry and physics is a 3-dimensional construct

$$M = Z_{1_3}(1; (\frac{1}{2})_3, 0_3) = \sum_{(x,y,z)\in Z^3}{}' \frac{(-1)^{x+y+z}}{\sqrt{x^2+y^2+z^2}},$$

which has never been cast into any convenient closed form.[4] It is of interest that this 3-dimensional setting is in many ways more difficult than any of the 2,4,8-dimensional settings previous. This discrepancy could be thought of as a relative paucity of relations for odd powers of Jacobi theta functions.[5] It should be remarked, however, that literally dozens of three-dimensional Epstein zetas admit of closed-form evaluation, as in [57] [58], yet none of these is precisely the Madelung M. Nevertheless, using the method of the present treatment—which amounts to a long-known "Ewald expansion" for such a crystal energy—one is able to obtain numerical values such as

$$M \sim -1.74756459463318219063621203554439740348516143662474175815282535076\ldots$$

[4]There is an attempt to do so in [27], where a few closed-form terms come rather close to the known M value.

[5]Although, the present author does use in [27] the compelling Andrews identity for θ^3, and such a procedure results in a *finite-domain definite integral* for M.

in a short time, and, in practice, carry out such numerics to thousands of decimal places. Incidentally one reason for attaining such precision would be somewhat more than recreational: The Madelung constant enjoys relations with other Z_A evaluations, for example the following nontrivial connections are known [55] [58] [33]:

$$M = \frac{3}{\pi} Z_{1_3}(2; ((\frac{1}{2})_2, 0), 0_3) = \frac{3}{\pi} \sum_{(x,y,z)\in Z^3}{}' \frac{(-1)^{x+y}}{x^2+y^2+z^2}$$

$$= \frac{3}{\pi} \sum_{(x,y,z)\in Z^3}{}' \frac{(-1)^{x+y+z}}{x^2+2y^2+2z^2}$$

$$= \frac{6}{\pi} \sum_{(x,y,z)\in Z^3}{}' \frac{(-1)^{x}}{x^2+y^2+2z^2}$$

$$= \frac{1}{\pi} Z_{1_3}(2; 0_3, (\frac{1}{2})_3) = \frac{4}{\pi} \sum_{(x,y,z)\in (2Z+1)^3} \frac{1}{x^2+y^2+z^2},$$

this last form defined over all odd triples (and, as always, as an analytic continuation since the literal sum does not converge).

There are other interesting approaches to precise estimation of M. Indeed, J. Buhler and R. Crandall [32] showed that one need not necessarily invoke Riemann splitting to achieve a rapidly convergent series. For example,

$$M \;=\; -\lambda + \sum_{\vec{v}\in Z^3}{}' \frac{(-1)^{\sum v_i}}{|\vec{v}|}(1-\tanh\lambda|\vec{v}|) \;+\; \frac{2\pi}{\lambda}\sum_{\vec{u}\in O^3} \frac{\operatorname{cosech}(\pi^2|\vec{u}|/(2\lambda))}{|\vec{u}|},$$

where O^3 denotes the odd-integers 3-dimensional lattice, and λ is a free parameter. It follows that

$$M \;=\; \lim_{\lambda\to\infty}\left(-\lambda + \frac{2\pi}{\lambda} S\left(\frac{\pi}{2\lambda}\right)\right)$$

where

$$S(x) \;:=\; \sum_{\vec{u}\in O^3} \frac{\operatorname{cosech}(\pi x|\vec{u}|)}{|\vec{u}|}.$$

Through the efforts of S. Tyagi and I. J. Zucker, S values are known exactly for certain arguments. The deepest known such result is Zucker's $S(1/\sqrt{24})$, which gives a Madelung estimate as the argument of lim above,

$$M \;\approx\; -\pi\sqrt{6} \;+\; \frac{\sqrt{\frac{1}{6}\left(3\sqrt{2}-6\sqrt{3}+6\sqrt{6}\right)}\;\Gamma\left(\frac{1}{8}\right)^2}{\pi\;\Gamma\left(\frac{1}{4}\right)} \;=\; -1.74756\ldots,$$

which is correct to the implied precision. For some ruminations on hyperclosed numbers and how the mighty Madelung might fit into the universe of fundamental constants, see [15].

One of the mysteries in regard to the Madelung M is the lack of closed-form representation *in spite of* the existence of closed forms for related entities. There is, for example, the attractive relation:

$$\sum{}' \frac{3(-1)^x + 3(-1)^{x+y} + (-1)^{x+y+z}}{(x^2+y^2+z^2)^{3/2}} = -4\pi \log 2,$$

which can be cast as an identity involving $Z_{1_3}(3, b/2, 0_3)$ for a certain three binary vectors b.

In any test suite for numerical evaluation, all the above are useful checking relations. We have seen – for the hexagonal lattice sum $H(s)$–a nontrivial A matrix. Another case of nontrivial A, in fact for the matrix $A = diag(\{2, \sqrt{2}, \sqrt{2}\})$, is:

$$Z_A(s, (\frac{1}{4}, 0_2), (\frac{1}{2}, 0_2)) = \sum_{(x,y,z)\in Z^3} \frac{(-1)^m}{((2x-\frac{1}{2})^2 + 2y^2 + 2z^2)^{s/2}} = 2^s L_{-8}(s-1).$$

One may also test further some nontrivial instances of c, d parameters such as:

$$Z_{1_3}(s, (\frac{1}{2}, 0_2), (0_2, \frac{1}{2})) = \sum_{(x,y,z)\in Z^3} \frac{(-1)^x}{(x^2+y^2+(z-\frac{1}{2})^2)^{s/2}} = 2^{s+1}\beta(s-1).$$

In particular, setting $s = 2$ yields the Catalan constant $G = \beta(2) = 1 - 1/3^2 + 1/5^2 - 1/7^2 + ...$ as:

$$G = \frac{1}{16} Z_{1_3}(3, (\frac{1}{2}, 0_2), (0_2, \frac{1}{2})),$$

while for $s = 1$ we would obtain the exact potential energy at a certain point within a peculiar, alternating charge-plane crystal. Another example of nontrivial—but physically meaningful—parameters is the following attractive evaluation of [36], which can be thought of as the potential energy at the point $(x, y, z) = (\frac{1}{6}, \frac{1}{6}, \frac{1}{6})$ within the (sodium chloride) lattice of the basic Madelung problem:

$$Z_{1_3}(1, (\frac{1}{2})_3, (\frac{1}{6})_3) = \sum_{(x,y,z)\in Z^3} \frac{(-1)^{x+y+z}}{\sqrt{(x-\frac{1}{6})^2 + (y-\frac{1}{6})^2 + (z-\frac{1}{6})^2}} = \sqrt{3}.$$

Of course, this last formula is *not* the most efficient way to calculate the square root of three!

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