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Computational Strategies for the Riemann Zeta Function

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Abstract. We provide a compendium of evaluation methods for the Riemann zeta function, presenting formulae ranging from historical attempts to recently found convergent series to curious oddities old and new. We concentrate primarily on practical computational issues, such issues depending on the domain of the argument, the desired speed of computation, and the incidence of what we call "value recycling."

1 Motivation for Efficient Evaluation Schemes

It was of course a profound discovery of Riemann that a function so superbly exploited by Euler, namely

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \prod_{p \text{ prime}} (1 - p^{-s})^{-1}, \tag{1}$$

could be interpreted—to great advantage—for general complex s-values. The sum (1) defines the *Riemann zeta function* in the half-plane of absolute convergence $\Re(s) > 1$, and in the entire complex plane (except for the pole at $s = 1$) by analytic continuation. The purpose of the present treatise is to provide an *overview* of both old and new methods for evaluating $\zeta(s)$.

Starting with Riemann himself, algorithms for evaluating $\zeta(s)$ have been discovered over the ensuing century and a half, and are still being developed in earnest. But why concentrate at all on computational schemes? One reason, of course, is the intrinsic beauty of the subject; a beauty which cannot be denied. But another reason is that the Riemann zeta function appears—perhaps surprisingly—in many disparate domains of mathematics and science, well beyond its canonical domain of analytic number theory. Accordingly, we shall provide next an overview of some such connections, with the intent to underscore the importance of efficient computational methods.

Typically, a particular method is geared to a specific domain, such as the critical strip $0 < \Re(s) < 1$, or the positive integers, or arguments lying in arithmetic progression, and so on. We shall honor this variety of purpose in presenting both old and new evaluation methods with a view to the specific domain in question. Just as the method of choice for evaluation tends to depend on the domain, the domain in turn typically depends on the theoretical or computational problem at hand. Though much of the present treatment involves new results for s-values in *integer* arithmetic progression, we shall digress presently to mention the primary historical motivation for ζ evaluation: analytic number theory applications.

There are well-known and utterly beautiful connections between number-theoretical facts and the behavior of the Riemann zeta function in certain complex regions. We shall summarize some basic connections with a brevity that belies the depth of the subject. First we state that ζ evaluations in certain complex regions of the s-plane have been used to establish theoretical bounds. Observe from the definition (1) that, in some appropriate sense, full knowledge of ζ behavior should lead to full knowledge of the prime numbers. There is Euler's rigorous deduction of the infinitude of primes from the appearance of the pole at $s = 1$; in fact he deduced the stronger result that the sum of the reciprocals of the primes diverges. There is the known [59] equivalence of the *prime number theorem* [54]:

$$\pi(x) \sim \mathrm{li}(x) := \int_0^x \frac{du}{\log u} \sim \frac{x}{\log x} \tag{2}$$

with the nonvanishing of $\zeta(s)$ on the line $\Re(s) = 1$. Here, the li integral assumes its Cauchy principal value. (Note that some authors define li in terms of an integral starting at $u = 2$ and differing from our present integral by an absolute constant.)

Another way to witness a connection between prime numbers and the Riemann zeta function is the following. We observe that behavior of $\zeta(s)$ on a line such as $\Re(s) = 2$ in principle determines $\pi(x)$. In fact, for any non-integer $x > 1$,

$$\pi^*(x) := \pi(x) + \tfrac{1}{2}\pi(x^{1/2}) + \tfrac{1}{3}\pi(x^{1/3}) + \cdots = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \frac{x^s}{s} \log\zeta(s)\, ds, \tag{3}$$

for *any* real $c > 1$. If one can perform the contour integral to sufficient precision, then one has a value for π^* and may peel off the terms involving $\pi(x^{1/n})$ successively, for example by recursive appeal to the same integral formula with reduced x. This notion underlies the Lagarias-Odlyzko method for evaluation of $\pi(x)$ [75]. Those authors suggest clever modification, based on Mellin transforms, of the contour integrand. The idea is to transform x^s/s to a more convergent function of $\Im(s)$, with a relatively small penalty in necessary corrections to the π^* function. Experimental calculations using standard 64-bit floating point arithmetic for the ζ evaluations for quadrature of the contour integral—with, say, Gaussian decay specified for the integrand—can evidently reach up to $x \sim 10^{14}$ but not much further [57] [46]. Still, it should eventually be possible via such analytic means to exceed current records such as:

$$\pi(10^{20}) = 2220819602560918840$$

obtained by M. Deléglise, J. Rivat, and P. Zimmerman via nonanalytic (i.e. combinatorial) means. In fact the Lagarias-Odlyzko remains the (asymptotically) fastest known $\pi(x)$ counting method, requiring only $O(x^{1/2+\epsilon})$ bit complexity and $O(x^{1/4+\epsilon})$ memory. The primary remaining obstacle to analytic superiority is the sheer difficulty of high-precision ζ evaluations, especially in regard to rigorous error bounds, of which there is historically a definite paucity when one looks away from the critical line.

Then there are profound bounds on the fluctuations of prime densities—that is, error bounds on the prime number formula—depending on the celebrated *Riemann hypothesis*, that all the zeros in the critical strip $0 < \Re(s) < 1$—call these the critical zeros—lie on the *critical line* $s = 1/2 + it$. In this regard, a different way of exploring the connection between ζ and prime numbers runs as follows. Riemann established the following relation, valid for non-integer $x > 1$:

$$\pi^*(x) = \mathrm{li}(x) - \sum_\rho \mathrm{li}(x^\rho) + \int_x^\infty \frac{du}{u(u^2-1)\log u} - \log 2,$$

where ρ runs over all zeros in the critical strip, that is $0 < \Re(\rho) < 1$, and counting multiplicity. Incidentally the conditionally convergent sum over zeros $\rho = \sigma + it$ is to be interpreted as the limit of the sum over $|t| \le T$ as $T \to \infty$ [61] [54] [63]. Arising from this kind of analysis is a highly refined prime-number estimate—due in essence to Riemann—involving not π^* but the elusive π function itself. Since one can write

$$\pi(x) = \sum_{m=1}^\infty \frac{\mu(m)}{m}\pi^*(x^{1/m}),$$

where μ denotes the *Möbius function*, it should be the case that, in some appropriate sense,

$$\pi(x) \sim \mathrm{Ri}(x) - \sum_\rho \mathrm{Ri}(x^\rho), \tag{4}$$

with Ri denoting the *Riemann function* defined:

$$\mathrm{Ri}(x) = \sum_{m=1}^\infty \frac{\mu(m)}{m}\mathrm{li}(x^{1/m}). \tag{5}$$

This relation (4) has been called "exact" [93], yet we could not locate a proof in the literature; such a proof should be nontrivial, as the conditionally convergent series involved are problematic. In any case the relation (4) is quite accurate (see below), and furthermore the Riemann function Ri can be calculated efficiently via evaluations of ζ at *integer* arguments in the Gram formula we encounter later (relation (70)).

The sum in (4) over critical zeros is not absolutely convergent, and furthermore the phases of the summands interact in a frightfully complicated way. Still, we see that the known equivalence of the Riemann hypothesis with the "best possible" prime number theorem:

$$\pi(x) - \mathrm{li}(x) = O(\sqrt{x}\log x)$$

makes heuristic sense, as under the celebrated hypothesis $|x^\rho|$ would be $\sqrt{x}$ for every relevant zero in (4). Incidentally, as far as this equivalence goes, it is even possible to give explicit values for the implied big-O constant [11]. For example, for $x > 2700$ the magnitude of the left hand side—under the Riemann hypothesis–never exceeds $\frac{1}{8\pi}\sqrt{x}\log x$.

One way to find rigorous, explicit bounds on certain sums over critical zeros (on the Riemann hypothesis) is to use the known [11] exact relation

$$\sum |\rho|^{-2} = 1 + \tfrac{1}{2}\gamma - \tfrac{1}{2}\log(4\pi),$$

which incidentally is one possible overall check on any computational runs over many zeros. For example, the left-hand sum above, over the first 200 zeros (with $t > 0$) and their conjugate zeros, is ~ 0.021 while the right-hand constant is ~ 0.023.

Let us consider numerical experiments pertaining to $\pi(x)$ itself. If one uses the Ri formalism together with the first 200 critical zeros (with $t > 0$) and their conjugates, a numerical estimate from relation (4) is:

$$\pi(10^{20}) \sim 2220819602591885820,$$

evidently correct to about 1 part in 10^{11}. This is certainly more accurate than the direct, prime-number-theorem estimate:

$$\mathrm{li}(10^{20}) \sim 2220819602783663484.$$

It is in this way that Riemann critical zeros reveal, albeit somewhat unforgivingly, truths about prime numbers. Incidentally, as a computational matter, a convenient way to obtain numerical evaluations for li is to use the formal identity $\mathrm{li}(z) = \mathrm{E}i(\log z)$, where $\mathrm{E}i$ denotes the standard exponential integral, the latter standard function often having the superior machine implementation.

Because of such analytical connections, each of which underscoring the importance of the Riemann hypothesis, massive numerical calculations have been carried out over certain complex regions, such manipulations in turn depending on rapid evaluation of $\zeta(s)$. In 1979 R. Brent [31] showed that the first 81 million critical zeros lie on the critical line. In 1986 van de Lune et al. [81] showed that the first 1.5 billion critical zeros also lie on the critical line. The Odlyzko-Schönhage method for ζ evaluation in complex regions—which method we discuss in later sections—can be used to extend such massive calculations yet further. Indeed, Odlyzko showed efficacy by calculating 1.5×10^8 zeros with imaginary part near 10^{20}. Then there is the *Mertens conjecture*, that

$$|\sum_{n \le x} \mu(n)| < \sqrt{x} \text{ for all } x \ge 1,$$

where μ denotes the Möbius function, which conjecture was disproved by numerical efforts involving computation of the first 2000 critical zeros [87]. We note here that an exploratory discussion—from various vantage points—of the Riemann hypothesis appears in Section 8.

In the earlier part of the 20th century Littlewood [80] performed a *tour de force* of analysis by establishing that $\pi(x)$ and $\mathrm{li}(x)$ trade dominance infinitely often, in fact

$$\pi(x) - \mathrm{li}(x) = \Omega_{\pm}\left(\frac{\sqrt{x}\log\log\log x}{\log x}\right),$$

although we know not a single explicit $x > 2$ such that $\pi(x)$ is the greater. After Littlewood's proof an upper bound on the first instance of integer x with $\pi(x) > \mathrm{li}(x)$ was given, on the Riemann hypothesis, as a gargantuan, triply-exponentiated "Skewes number:"

$$10^{10^{10^{34}}}.$$

Skewes later removed the dependency to give an even larger, unconditional bound [97] [98]. Through the work of Lehman and te Riele the bound has been brought down to 10^{371}, again using numerical values of critical zeros [99]. Rosser and Schoenfeld have likewise analyzed complex zeros of related functions to establish interesting bounds on yet other number-theoretical conjectures. For example, they show that every integer greater than or equal to 2 is a sum of at most 7 primes [83]. More recently, Bays and Hudson [14] have shown how to use zeros of Dirichlet L-functions to quite efficiently compute the difference $\pi_1(x) - \pi_3(x)$, for large $x \sim 10^{300}$ say, with $\pi_k(x)$ here being the number of primes $\equiv k (\mathrm{mod}\ 4)$ and not exceeding x. Because of the obvious relevance to number theory, we shall touch upon the problem of computational complexity for $\zeta(1/2 + it)$ in Section 7.

But there are likewise beautiful, less familiar connections between the Riemann zeta function and number-theoretical conjectures. Consider for example, as proposed by E. Bach [7] [8] and analyzed in part also by P. Flajolet and I. Vardi [55] the following three constants: the *Artin constant* A, the *Mertens constant* B, and the *twin-prime constant* C:

$$A = \prod_p \left(1 - \frac{1}{p(p-1)}\right), \tag{6}$$

$$B = \gamma + \sum_p \left(\log(1 - p^{-1}) - p^{-1}\right), \tag{7}$$

$$C = \prod_{p>2} \left(1 - \frac{1}{(p-1)^2}\right), \tag{8}$$

in which the product (6) and the sum (7) run over all primes p, and the product (8) runs over all odd primes $p > 2$. The constant A arises in the theory of primitive roots, B arises in the powerful asymptotic relation $\sum_{p \le x} 1/p \sim B + \log\log x$, and C arises in detailed conjectures regarding the density of twin prime pairs. Relevant series developments for these constants are:

$$
\begin{aligned}
-\log A &= \sum_{n=2}^{\infty} \frac{\log \zeta(n)}{n} \sum_{m<n, m|n} \mu(m) a_{n/m-1}, &(9)\\
B - \gamma &= \sum_{n=2}^{\infty} \frac{\log \zeta(n)}{n} \mu(n), &(10)\\
-\log C &= \sum_{n=2}^{\infty} \frac{\log((1-2^{-n})\zeta(n))}{n} \sum_{m<n, m|n} \mu(m)(2^{n/m}-2), &(11)
\end{aligned}
$$

where $a_0 = 0$, $a_1 = 1$, otherwise $a_k = a_{k-1} + a_{k-2} + 1$. A fascinating aspect of these relations is this: whereas the original definitions (6) (7) (8), if used directly for computation, involve agonizingly slow convergence (not to mention determination of primes), the three series (9) (10) (11) each converge so rapidly that any of A, B, C may be determined to hundreds of digits in a convenient sitting. Incidentally there are yet more interesting relations between number-theoretical constants and such entities as the logarithmic derivative $\zeta'(s)/\zeta(s)$ [9].

It is worthwhile to observe that the so-called "prime-ζ" function

$$P(s) = \sum_{p \text{ prime}} p^{-s}$$

can be evaluated to surprisingly high precision due to the identity

$$P(s) = \sum_{n=1}^{\infty} \frac{\mu(n)}{n} \log \zeta(ns).$$

For example, a certain problem in connection with the arrangement of pairs of coprime planar coordinates [105] amounts to analyzing the product

$$f(z) = \prod_{p \text{ prime}} \left(1 - \frac{z}{p^2}\right),$$

for some $z \neq -1, 0, 1$ (for each of which three values the product is well known). The problem can be solved in one sense by observing that

$$\log f(z) = -\sum_{m=1}^{\infty} P(2m) \frac{z^m}{m},$$

whence the Taylor coefficients of $\log f$ can be obtained to extreme precision without one having to know a vast collection of primes. Incidentally, one theoretically convenient aspect of the prime-ζ is that in the prime-counting relation (3), if one replaces $\zeta(s)$ with $P(s)$, and $x > 0$ is again not an integer, then the left-hand side is just $\pi(x)$.

Still in connection with analysis, many interesting identities are manifestations of what we shall call *"rational ζ-series,"* being explicit representations of some real number x, in the form

$$x = \sum_{n=2}^{\infty} q_n \zeta(n, m), \tag{12}$$

where each q_n is a rational number, m is fixed, and the $\zeta(n, m)$ are instances of the standard *Hurwitz zeta function*

$$\zeta(s, m) = \sum_{n=0}^{\infty} \frac{1}{(n+m)^s}. \tag{13}$$

Note that $\zeta(s, 1) = \zeta(s)$; the easy rule-of-thumb is that for integer m the Hurwitz $\zeta(s, m)$ is a zeta-like sum that starts with $1/m^s$. Thus for integer m the rational ζ-series (12) takes the form

$$x = \sum_{n=1}^{\infty} q_n \left(\zeta(n) - \sum_{j=1}^{m-1} j^{-n} \right),$$

in which the nth term decays roughly as q_n/m^n. We shall see in Section 4 that many fundamental constants enjoy convenient, rational ζ-series representation; and we shall be concentrating, then, on the variety involving $\zeta(n, 2)$.

The relations (9) (10) (11) involve collections of ζ-values and thus provide additional motive for what we call "value recycling" (Section 6). By this we refer to scenarios in which initial calculated values convey some information in regard to other values; so for instance some set of known ζ-values are used to get others, or many values interact symbiotically. (We had thought to call such approaches "parallel" schemes, but that is a slight misnomer because a single, scalar processor can benefit full well from most of the strategies we describe.) The motive for recycling ζ-values at integer arguments is especially strong when a rational ζ-series is essentially the only known recourse for numerical evaluation, for in such cases one desires large collections of ζ-values. In Section 4 we give examples to show that this last resort—when one is compelled to rely upon a rational ζ-series—does arise in practice.

2 Collected Relations

We next list standard properties of the *Riemann zeta function*. For $\Re(s) > 1, \Re(\mu) > -1$ we have a Hurwitz zeta representation:

$$\zeta(s, \mu+1) = \frac{1}{\Gamma(s)} \int_0^\infty \frac{t^{s-1} e^{-\mu t}}{e^t - 1} dt, \quad \zeta(s) = \zeta(s, 1), \tag{14}$$

whereas over the somewhat larger region $\Re(s) > 0$ the Riemann zeta function can be determined in proportion to the η function:

$$\eta(s) = (1 - 2^{1-s})\zeta(s) = \frac{1}{\Gamma(s)} \int_0^\infty \frac{t^{s-1}}{e^t + 1} dt.$$

As we shall see in Section 3, these integrals themselves already yield interesting, convergent expansions suitable for computation; not, however, always the fastest available. In Riemann's own works one finds integral representations that define $\zeta(s)$ for all complex s, for example:

$$\pi^{-s/2}\Gamma(\tfrac{1}{2}s)\zeta(s) = -\frac{1}{s} - \frac{1}{1-s} + \frac{1}{2}\int_1^\infty (t^{(1-s)/2} + t^{s/2})(\theta_3(e^{-\pi t}) - 1)\frac{dt}{t}, \tag{15}$$

in which the *Jacobi theta-function* [20] is $\theta_3(q) = \sum_{n=-\infty}^{\infty} q^{n^2}$. This representation will give rise to an (extremely) rapidly converging series (30), although the summands will be non-elementary. The collection of entire representations is by no means limited to (15). For example there is the Jensen formula:

$$\zeta(s) = \frac{1}{2} + \frac{1}{s-1} + 2\int_0^\infty \frac{\sin(s \tan^{-1} t)\ dt}{(1+t^2)^{s/2}(e^{2\pi t} - 1)},$$

also valid for all $s \neq 1$, and useful in certain proofs of the prime number theorem [59].

From (15), there follows immediately the celebrated *functional equation*. If we define

$$\xi(s) = \tfrac{1}{2}s(s-1)\pi^{-s/2}\Gamma(\tfrac{1}{2}s)\zeta(s), \tag{16}$$

then the functional equation can be written elegantly [54] as

$$\xi(s) = \xi(1-s). \tag{17}$$

Furthermore, by considering complex values $s = 1/2 + it$, one sees that the Riemann hypothesis is true if and only if all zeros of the function

$$\Xi(t) = -\tfrac{1}{2}(t^2 + \tfrac{1}{4})\xi(\tfrac{1}{2} + it) \tag{18}$$

are real [100]. The idea of forging a real-valued facsimile on the critical line is a good one, conducive to numerical analysis such as locating critical zeros. But the Ξ-function decays rapidly for large t, so in practice a more reasonable choice is the function (sometimes called the *Hardy function* [71]):

$$Z(t) = \exp(i\vartheta(t))\zeta(\tfrac{1}{2} + it), \tag{19}$$

where we define ϑ implicitly by:

$$e^{i\vartheta(t)} = \chi(1/2 + it)^{-1/2}, \tag{20}$$

and the square root is defined continuously, with fixation $\sqrt{\chi(1/2)} = 1$. In general one may write

$$\chi(s) = \pi^{s-1/2}\frac{\Gamma((1-s)/2)}{\Gamma(s/2)}. \tag{21}$$

Now for real t, the Hardy Z-function is real and the equality $|Z(t)| = |\zeta(\frac{1}{2} + it)|$ holds. These convenient properties render Z useful in modern searches for critical zeros [31] [81]. In particular, simple zeros of $\zeta(1/2+it)$ on the critical line are signified by sign changes—as t increases—of the Z-function, and this notion can be made rigorous by careful constraint on numerical error, so that a machine can *prove* that all zeros in the critical strip interval $t \in [0, T]$ for some fixed T do in fact lie precisely on the critical line [83]. Later in Section 3 we shall describe the kinds of error contributions that appear in prevailing series developments of the Z-function.

It is well known that for positive even integer arguments we have exact evaluations

$$\zeta(2n) = -\frac{(2\pi i)^{2n} B_{2n}}{2(2n)!}, \tag{22}$$

in terms of the *Bernoulli numbers* $1, -\frac{1}{2}, \frac{1}{6}, 0, \frac{1}{30}, 0, \frac{1}{42}, \ldots$ defined by the generating series

$$\frac{t}{e^t - 1} = \sum_{m=0}^{\infty} \frac{B_m}{m!} t^m, \tag{23}$$

in which $B_{2n+1} = 0$ for $n > 0$. For computational purposes it will turn out to be important that the series (23) has radius of convergence 2π. Now from the functional equation (17) one may deduce the analytic continuation value $\zeta(0) = -\frac{1}{2}$ and the values at negative integer arguments

$$\zeta(-2n) = 0, \quad \zeta(1-2n) = -\frac{B_{2n}}{2n} \tag{24}$$

for positive integer n. An elegant and computationally lucrative representation for the even-argument ζ-values is

$$\pi t \cot \pi t = -2 \sum_{m=0}^{\infty} \zeta(2m) t^{2m}. \tag{25}$$

The series (25) converges for $|t| < 1$, and with this constraint in mind can be used in many different computational algorithms, including some recycling ones, as we shall discuss. On the issue of whether a convenient generating function can be obtained for *odd*-argument ζ-values, there is at least one candidate, namely the following relation involving the logarithmic derivative of the gamma function, i.e. the *digamma function* $\psi(z) = d \log \Gamma(z)/dz$:

$$\psi(1-t) = -\gamma - \sum_{n=2}^{\infty} \zeta(n) t^{n-1}, \quad |t| < 1, \tag{26}$$

which will be useful in the matter of recycled evaluation.

Standard recurrence relations for Bernoulli numbers can be invoked to provide relations such as

$$\sum_{k=0}^{m} \frac{(\pi i)^{2k}}{(2k+1)!} (1 - 2^{2k-2m+1}) \zeta(2m-2k) = 0, \tag{27}$$

and for integer $k \geq 2$,

$$\sum_{j=1}^{k-1} \zeta(2j)\zeta(2k-2j) = (k + \tfrac{1}{2})\zeta(2k).$$

See [51] for generalizations to sums of products of $N \geq 2$ ζ-values, Bernoulli/Euler polynomials, and the like. Similar relations for odd-argument ζ-values are difficult if not fundamentally impossible to obtain. There are, however, some interesting relations between the values at odd integer arguments if we allow easily computed residual terms, which can be cast as rational ζ-series, as we shall see in Section 5.

Many interrelations between ζ values can be inferred from the following series development for the *complex Lerch*, or *periodic zeta function* [6] [49]:

$$\sum_{n=1}^{\infty} \frac{e^{2\pi i n x}}{n^s} = -\sum_{j=0}^{\infty} \frac{(\pi i)^j}{j!} \eta(s-j)(2x-1)^j, \tag{28}$$

valid for $\Re(s) > 0$ and real x with $|2x-1| \leq 1$. An immediate representation obtains on setting $x = 0$:

$$\zeta(s) = -\sum_{j=0}^{\infty} \frac{(-\pi i)^j}{j!} \eta(s-j),$$

valid for $\Re(s) > 0$. Note that if $\zeta(s)$ be real, then the imaginary part of the right-hand side vanishes, and this gives certain ζ-series representations. On the other hand, using just the real part of the right-hand side yields, for even integer s, the previous relation (27) for $\zeta(\text{even})$; while for odd s we obtain certain representations of $\zeta(\text{odd})$. The Lerch-series approach will be discussed later as a computational tool.

3 Evaluations for General Complex Arguments

Until the 1930s the workhorse of the evaluation art for the Riemann zeta function was Euler-Maclaurin expansion. The standard *Euler-Maclaurin formula* applied to $x \mapsto x^{-s}$ yields, for two cutoff integers M, N:

$$\zeta(s) = \sum_{n=1}^{N-1} \frac{1}{n^s} + \frac{1}{2N^s} + \frac{N^{1-s}}{s-1} + \sum_{k=1}^{M} T_{k,N}(s) + E(M, N, s) \tag{29}$$

where

$$T_{k,N}(s) = \frac{B_{2k}}{(2k)!} N^{1-s-2k} \prod_{j=0}^{2k-2} (s+j).$$

If $\sigma := \Re(s) > -2M - 1$ the error is rigorously bounded as [86] [39]:

$$|E(M, N, s)| \le \left| \frac{s + 2M + 1}{\sigma + 2M + 1} T_{M+1,N}(s) \right|.$$

One disadvantage of such expansions is universal; i.e. relegated not only to the Riemann zeta function. The problem is, one does not obtain a manifestly convergent expansion; rather, the expansion is of asymptotic character and one is compelled to rescale the cutoff parameters when attempting a new precision goal. With this in mind, we proceed for much of the rest of this treatment to focus on convergent series.

Since $(s-1)\zeta(s)$ is entire, we may write

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

The coefficients are generally referred to as the *Stieltjes constants* and are given by

$$\gamma_n = \lim_{m \to \infty} \left\{ \sum_{k=1}^{m} \frac{\log^n(k)}{k} - \frac{\log^{n+1}(m)}{n+1} \right\}.$$

Note that $\gamma_0 = 0.5772156649\ldots$ is the *Euler constant*. In principle, the Stieltjes expansion here gives a scheme for evaluation of Euler's constant, provided one has a sufficiently sharp scheme for $\zeta(1+\varepsilon)$.

From (15), one has

$$\zeta(s)\Gamma(\tfrac{1}{2}s) = \frac{\pi^{s/2}}{s(s-1)} + \sum_{n=1}^{\infty} n^{-s}\Gamma(\tfrac{1}{2}s, \pi n^2) + \pi^{s-1/2}\sum_{n=1}^{\infty} n^{s-1}\Gamma(\tfrac{1}{2}(1-s), \pi n^2), \tag{30}$$

in principle a consummately convergent expansion, the only obstacle to high efficiency being the evaluations of the *incomplete gamma function*, given (at least for $\Re(z) > 0$) by:

$$\Gamma(a,z) = \int_z^{\infty} t^{a-1}e^{-t}dt = \frac{2z^a e^{-z}}{\Gamma(1-a)}\int_0^{\infty}\frac{t^{1-2a}e^{-t^2}}{t^2+z}dt,$$

where the latter integral representation is valid for (an important region) $\Re(a) < 1$. But the evaluation of $\Gamma(a,z)$ is not as problematic as it may seem; many computer systems of today have suitable incomplete-gamma machinery. There are the special cases $\Gamma(s,0) = \Gamma(s)$ and $\Gamma(1,z) = e^{-z}$, with a recursion

$$a\Gamma(a,z) = \Gamma(a+1,z) - z^a e^{-z} \tag{31}$$

that proves useful, as we shall see, in the art of value recycling. The recursion also reveals that when a is a positive integer $\Gamma(a,z)$ is an elementary function of z. There is an at least threefold strategy for evaluating the incomplete gamma [43]. For $a \neq 0, -1, -2, \ldots$ one has an ascending hypergeometric series and transformed counterpart:

$$\begin{aligned}\Gamma(a,z) &= \Gamma(a) - a^{-1}z^a\,{}_1F_1(a; a+1; -z),\\ &= \Gamma(a)\left(1 - z^a e^{-a}\sum_{m=0}^{\infty}\frac{z^m}{\Gamma(a+m+1)}\right),\end{aligned}$$

while for larger values of $|z|$ one may use the continued fraction (when it exists—the convergence issues for general complex a are intricate and fascinating, see [59] or the recent treatment [3]):

$$\Gamma(a,z) = \cfrac{z^a e^{-z}}{z + \cfrac{1-a}{1 + \cfrac{1}{z + \cfrac{2-a}{1 + \ddots}}}}$$

where pairs of consecutive numerators here take the form $\{n-a, n\}$ as n runs through the positive integers. For extremely large $|z|$ values one has a standard asymptotic series:

$$\Gamma(a, z) \sim z^{a-1} e^{-z}\left(1+\frac{a-1}{z}+\frac{(a-1)(a-2)}{z^2}+\cdots\right),$$

valid at least for $\Im(z) > 0$. Convergence and error-bounding issues can be resolved via proper analysis of appropriate Mellin-Barnes contour integrals, as discussed in [46]. For the moment we underscore the rapid convergence of series (30) by noting the behavior for positive real $z > \sigma$:

$$|\Gamma(\sigma+it, z)| < \max(1, 2^\sigma) z^{\sigma-1} e^{-z}.$$

This bound is quite convenient in practice, and means that only $O(\sqrt{D})$ terms of a summand in series (30) are required to achieve D correct digits. A generalization of the incomplete-gamma series is useful in higher dimensions, specifically when Epstein zeta functions (generalizations of the Riemann zeta function) are to be evaluated [45].

The series (30) should always be considered as a possible expedient for evaluating ζ. We note that, especially for large $|\Im(s)|$, the Riemann-Siegel formula can be superior, easier to apply in practice, and also supports recycled evaluation of the Odlyzko-Schönhage type. But a recycling option also exists—albeit in a different sense and over different complex domains—for relation (30); for example the recursion relation (31) allows recycling for certain arithmetic progressions of arguments, as we shall see later.

It is sometimes noted that a formula such as (30) suffers from precision loss when $|\Im(s)|$ is large, due to the factor $\Gamma(s/2)$ on the left, which factor in such instances being an exponentially small one, decaying as $\sim \exp(-\pi|\Im(s)|/4)$. But there is the notion of using a free parameter in formula (30), and furthermore allowing said parameter to attain complex values in order to reduce this precision loss. The interesting work of Rubinstein [95] on more general L-function evaluation contains analysis of this type, along with yet more incomplete-gamma representations. Other treatments of ζ on the critical line depend also on incomplete-gamma asymptotics, such as the Temme formulae [88]. In the same spirit there is ongoing research into the matter of casting series of the type (30) in more elementary terms, with a view to practical computation, by using a combination of: complex free parameter, rigorous error bounds, and special expansions of the incomplete gamma at certain saddle points [47].

¿From the integral representation (14) together with the generating series (23), we can choose $|\lambda| < 2\pi$ and obtain

$$\zeta(s)\Gamma(s) = -\frac{\lambda^s}{2s}+\frac{\lambda^{s-1}}{s-1}+\sum_{n=0}^{\infty} n^{-s}\Gamma(s, \lambda n) - 2\lambda^{s-1}\sum_{n=1}^{\infty}\left(\frac{\lambda}{2\pi i}\right)^{2n}\frac{\zeta(2n)}{2n+s-1}, \qquad (32)$$

which is valid over the entire complex s-plane, provided we properly handle the limiting case $s \to n$ for a negative integer n. In fact, the pole in $\Gamma(s)$ on the left corresponds to the pole in the relevant summand in the second sum, and we derive all at once the evaluations (24). Now (32) is an intriguing and sometimes useful expansion. The free parameter λ allows one to test quite stringently any numerical scheme: one must obtain invariant results for any λ chosen in the allowed domain. For positive integer arguments s, the incomplete gamma is *elementary*; furthermore, for such s and rational $\lambda/(2\pi)$, the second sum in (32) has all rational coefficients of the $\zeta(2n)$. We shall have more to say about this expansion in Section 7.

An interesting method for development of manifestly convergent series such as (30) and (32) starts with the representation (28) for the Lerch function. If we set $x = 1/2 + i\lambda/(2\pi)$ then, formally at least:

$$(1 - 2^{1-s})\zeta(s) = \eta(s) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n^s} e^{-\lambda n} - \sum_{j=1}^{\infty} \frac{(-\lambda)^j}{j!} \eta(s-j). \tag{33}$$

It can be shown that this relation is valid for all complex s, with free parameter $\lambda \in (0, \pi]$. Later, in Section 5 we discuss specific applications for integer arguments s.

The *Stark formula*, also analyzed by J. Keiper [42] [106], provides a different approach for general complex s and N a positive integer:

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

which by its very construction admits of interesting recursion schemes: one can write a Hurwitz-ζ function that calls itself. Reminiscent of the Stark-Keiper approach is the formula

$$\zeta(s) = \lim_{N \to \infty} \frac{1}{2^{N-s+1} - 2^N} \sum_{k=0}^{2N-1} \frac{(-1)^k}{(k+1)^s} \left(\sum_{m=0}^{k-N} \binom{N}{m} - 2^N \right) \tag{34}$$

for which it is possible to give a rigorous error bound as a function of the cutoff N and s itself [21] [25]. Very recently there appeared the interesting Woon formula, which amounts to a relation involving Bernoulli numbers that generalizes the celebrated formula (24). We paraphrase the Woon formula thus: for free real parameter $w > 0$ and $\Re(s) > 1/w$, one has

$$\zeta(s) = -\pi(2\pi w)^{s-1} \sec(\tfrac{1}{2}\pi s) \sum_{n=0}^{\infty} \frac{(-1)^n b(w, n)\Gamma(s)}{n!\Gamma(s-n)},$$

where we define

$$b(w, n) = \tfrac{1}{2} + 2w \sum_{m=2}^{n+1} \left(\frac{i}{2\pi w}\right)^{2m} \binom{n}{2m-1} \zeta(2m).$$

Note that for positive even integer s, this whole scheme boils down to a tautology, because we have intentionally replaced (on the right-hand side of the b definition) the Bernoulli coefficients of Woon's original rendition with ζ(even) values. It is of interest that this formula becomes singular only at odd integer values of s (where the secant diverges), although Woon has specified a limiting process in such cases [107].

We end this section with a discussion of practical issues for the *Riemann-Siegel formula.* This formula and its variants amount to the most powerful evaluation scheme known for s possessed of large imaginary part—the quite elegant and profound developments are referenced in [31] [100] [54] [16] [86] [18] [62] [63]. Another unique aspect of the Riemann-Siegel formula is that it is relatively difficult to implement, having several terms each requiring its own special strategy. Yet another is the fact that different variants apply best in different complex regions, with different error-bounding formula applicable in problem-dependent fashion. Loosely speaking, the Riemann-Siegel formulae apply in two modes. Representatives of these modes are first, calculations on the critical line $s = 1/2 + it$ (for which the Z-function (19) is appropriate); and second, evaluations with $\Re(s) > 1$, as in the evaluation algorithms for the integral (3) (for which $\log \zeta$ is desired). In all such instances any bounding formula must take into account the decay of error as a function of the imaginary part t.

The Riemann-Siegel formula for ζ itself—as opposed to variants attendant on the Hardy Z-function—can be written as an "approximate functional equation:"

$$\zeta(s) = \sum_{n=1}^{M} \frac{1}{n^s} + \chi(s) \sum_{n=1}^{M} \frac{1}{n^{1-s}} + E_M(s),$$

where M is a certain cutoff value, the χ-function is from relation (21), and E_M is an error term that, although depending in a complicated way on the intended domain of s, can be bounded explicitly for computations in certain useful regions of the complex s-plane [86]. We note that the formula admits of more general rendition—in which the limits on the summands are unequal—and that an optimized inequality of said limits may be called for when one is working off the critical line. There is a long-studied theory for this kind of approximation, and there remain open questions on the precise asymptotic nature of the errors [100] [63] [54] [16]. In particular there is a distinct paucity of useful explicit bounds for s off the critical line, but research is ongoing into this dilemma [46].

The Riemann-Siegel formula above is certainly a streamlined rendition. The detailed error terms are complicated [86] [100] [63] [56]; moreover the level of asymptotic correction, the number of error terms to add in, and so on depend on the required precision and the complex domain of s. Accordingly, we shall give below just one practical variant and some explicit error bounds. As for the Hardy function (19), a similarly stripped-down rendition is [62]:

$$Z(t) = 2\sum_{1\le n\le\tau} n^{-1/2}\cos(t\log(n^{-1}\tau) - \tfrac{1}{2}t - \tfrac{1}{8}\pi) + O(t^{-1/4}), \quad t>0,$$

where $\tau = \sqrt{t/(2\pi)}$. It turns out the big-O error term here is best possible, because the indicated error is actually $\Omega_\pm(t^{-1/4})$ (not surprising—for one thing, the discontinuity implicit in the summation cutoff is of this magnitude). We now give just one reliable form of an expanded Riemann-Siegel formula for Z. In their numerical researches on the critical zeros, Brent et al. [31] [32] [81] used the following practical variant. To simplify notation, let $m = \lfloor\tau\rfloor$, $z = 2(\tau - m) - 1$. Then the variant involves the angle ϑ from definition (20), which angle is relatively easy to calculate from gamma-function asymptotics, and reads:

$$\begin{aligned} Z(t) &= 2\sum_{n=1}^{m} n^{-1/2}\cos(t\log n - \vartheta(t)) \\ &+ (-1)^{m+1}\tau^{-1/2}\sum_{j=0}^{M}(-1)^j\tau^{-j}\Phi_j(z) + R_M(t). \end{aligned} \tag{35}$$

Here, M is a cutoff integer of choice, the Φ_j are entire functions defined for $j\ge 0$ in terms of a function Φ_0 and its derivatives, and $R_M(t)$ is the error. For computational rigor one needs to know an explicit big-O constant. A practical instance is Brent's choice $M=2$, for which we need

$$\begin{aligned} \Phi_0(z) &= \frac{\cos(\frac{1}{2}\pi z^2 + \frac{3}{8}\pi)}{\cos(\pi z)}, \\ \Phi_1(z) &= \frac{1}{12\pi^2}\Phi_0^{(3)}(z), \\ \Phi_2(z) &= \frac{1}{16\pi^2}\Phi_0^{(2)}(z) + \frac{1}{288\pi^4}\Phi_0^{(6)}(z). \end{aligned}$$

All of this notational tangle may appear stultifying, but the marvelous benefit is this: the errors R_M have been rigorously bounded, in computationally convenient fashion by various investigators—notably W. Gabcke [56]—to achieve such as the following, for $t\ge 200$, $M\le 10$:

$$|R_M(t)| < B_M t^{-(2M+3)/4},$$

for a set of bounding numbers:

$$\{B_0,\ldots,B_{10}\} = \{0.127, 0.053, 0.011, 0.031, 0.017, 0.061, 0.661, 9.2, 130, 1837, 25966\}.$$

Now the computationalist does not have to interpret big-O notation in numerical experiments. Perhaps surprisingly, regardless of these beautiful bounds the Riemann-Siegel formula with just $M = 1$—so that R_1 is in force—was enough to resolve the first 1.5 billion zeros, in the following sense. The optimized strategy in [81] for finding and *proving* that zeros lie exactly on the critical line, which strategy stems from that used originally by Brent [31], was reported never to have failed with the R_1 bound in hand. Incidentally the zero-location method is ingenious: one uses known rigorous bounds on the number of zeros in a vertical segment of the critical strip. For example the number of zeros having $t \in [0, T]$ can be obtained from [100]:

$$N(T) = 1 + \pi^{-1}\vartheta(T) + \pi^{-1}\Delta \arg \zeta(s),$$

where ϑ is the angle from the assignment (20) and Δ signifies the variation in the argument, defined to start from $\arg \zeta(2) = 0$ and varying continuously to $s = 2 + iT$, then to $s = 1/2 + iT$. If some number of sign changes of $Z(t)$ has been counted, and this count saturates the theoretical bound (e.g., bound says $N(t) < 15.6$ zeros and we have found 15), then all the zeros in the segment must have been found: they must lie precisely on $\Re(s) = 1/2$ and furthermore they must be simple zeros because Z sustained changes in sign.

It should be pointed out that most of the work in these hunts for critical zeros is in the evaluation of a finite sum:

$$\sum_{n=1}^{m} n^{-1/2} \cos(t \log n - \vartheta). \tag{36}$$

where we recall that $m = \lfloor \tau \rfloor$ is the greatest integer not exceeding $\sqrt{t/(2\pi)}$. The authors of [81] in fact vectorized this sum in supercomputer fashion. Computational issues aside, one can also envision—by pondering the phase of the cosine—how it is that zeros occur, and with what (approximate) frequency [100].

There is an interesting way to envision the delicate inner workings of the Riemann-Siegel formula (35). Note the implicit discontinuity of the n-summation; after all, the summation limit $m = \lfloor \tau \rfloor$ changes suddenly at certain t. The idea is, the M terms of the j-summation must cancel said discontinuity, up to some hopefully insignificant error. As Berry and Keating note [16], the summation limit m itself is a kind of critical-phase point during the analysis of those integral representations of ζ that underlie the Riemnann-Siegel formalism. Berry and Keating gave, in fact, an alternative, free-parameter representation of the Z-function, which representation avoids discontinuities in summation. Though their leading sum is more complicated, it is also more accurate (instead of a discontinuous cutoff there is a smooth, error-function decay near the Riemann-Siegel critical-phase point m), and the same kind of accuracy-complexity tradeoff occurs for their ensuing correction terms. Thus the Berry-Keating form is perhaps a viable computational alternative; at the very least it has theoretical importance in connection with semi-classical quantum theory and stationary states of operators (see Section 8).

Since the Riemann-Siegel formula can be derived by application of saddle point methods to integral representations, W. Galway [57] has noted such integrals themselves are well suited for numerical integration. This allows computation of ζ values to arbitrary accuracy while still retaining many of the advantages of the Riemann-Siegel formula. Another advantage of this method is that the analysis of the error terms is simplified.

We observe that the Riemann-Siegel formula exhibits properties in common with both the Euler-Maclaurin formula (29) and the incomplete-gamma expansion (30). As for the former similarity, the Riemann-Siegel form is asymptotic in nature, at least in the sense that one chooses a set of M correction terms depending, in principle, on *both* the range of the argument and the required accuracy. As for the similarity with the incomplete-gamma formula, note that both formulae tend to require $O(t^{1/2})$ summands—the Riemann-Siegel by its very construction, and the incomplete-gamma by accuracy requirements. Of course, the Riemann-Siegel summands involve exclusively elementary functions, which is a strong advantage. We shall have more to say about such computational matters in Section 7.

4 Rational Zeta Series

Consider a natural specialization of the rational ζ-series (12), obtained by setting $m = 1$ in the Hurwitz zeta function (13). We shall discuss representations of real numbers x in the form

$$x = \sum_{n=2}^{\infty} q_n(\zeta(n) - 1), \tag{37}$$

where the rational coefficients q_n are, in some appropriate sense, well-behaved. It is not hard to prove that *any* real x admits a rational ζ-series of the form (37) for unrestricted rational q_n; but we are concerned with expansions for which the q_n are particularly simple in structure. One might demand the $|q_n|$ be bounded, or constrain the denominator of q_n to possess $O(\log n)$ bits, and so on. This kind of series for some desired number x tends to be computationally convenient because, of course, $\zeta(n) - 1$ decays like $1/2^n$ for increasing n. It will turn out that many fundamental constants enjoy simple representations. To mention a few: π (in fact any positive integer power of π), $\log \pi$, $\log r$ for any rational

r, Euler's constant γ, the *Catalan constant* G[1], the *Khintchine constant* K_0 (actually $(\log K_0)(\log 2)$), and any quadratic surd $(A+\sqrt{B})/C$ (including for example the golden mean $(1+\sqrt{5})/2$) are representable with relatively simple, explicit coefficients.

Let us consider some fundamental numbers from such disparate classes. First, there is a "representation of unity"

$$1 = \sum_{n=2}^{\infty} (\zeta(n) - 1), \tag{38}$$

which has tremendous value in testing evaluation schemes—in particular the recycling schemes—for the $\zeta(n)$ themselves. Curiously, this representation can be partitioned into disjoint sums over even and odd n respectively; the even-indexed sum having the value $3/4$, the odd-indexed sum having the value $1/4$. There are attractive representations for $\log 2$ and Euler's constant γ:

$$\log 2 = \sum_{n=1}^{\infty} \frac{\zeta(2n) - 1}{n},$$

$$1 - \gamma = \sum_{n=2}^{\infty} \frac{\zeta(n) - 1}{n}. \tag{39}$$

As we shall see, the convergence of these and many related series can be duly accelerated. To give just one side example of the analytic depth of this subject, we note that Ramanujan once observed that a formula of Glaisher:

$$\gamma = 2 - 2\log 2 - 2 \sum_{n=3,\ \mathrm{odd}} \frac{\zeta(n) - 1}{n(n+1)}$$

(as one can deduce from identities above and below this one) could be generalized to *infinitely-many* different formulae for γ [92].

Many relations can be obtained upon manipulation of identities such as

$$\sum_{n=1}^{\infty} t^{2n}(\zeta(2n) - 1) = \tfrac{1}{2} - \tfrac{1}{2}\pi t \cot \pi t - t^2(1-t^2)^{-1}, \quad |t| < 2, \tag{40}$$

$$\sum_{n=2}^{\infty} t^{n}(\zeta(n) - 1) = -t(\gamma + \psi(1-t) - t(1-t)^{-1}), \quad |t| < 2, \tag{41}$$

[1] G, γ and $\zeta(5)$ are quintessential examples of constants whose irrationality though suspected is unproven. Efficient high precison algorithms allow one to prove in these and many other cases that any rational representation must have an enormous denominator. See for example [33].

which arise from the expansions (25) and (26), respectively. Thus for example one may integrate (41) to achieve a formal expansion involving Euler's constant:

$$t(1-\gamma)+\log\Gamma(2-t)=\sum_{n=2}^{\infty} n^{-1}t^{n}(\zeta(n)-1), \tag{42}$$

which expansion will have application later in Section 8. For $t = 3/2$ we obtain a representation of $\log\pi$:

$$\log\pi=\sum_{n=2}^{\infty} n^{-1}(2(\tfrac{3}{2})^{n}-3)(\zeta(n)-1).$$

Evaluations of rational ζ-series with simple coefficients q_n can take attractive forms. For example, whereas (40) can be used to derive:

$$\sum_{n=1}^{\infty}\frac{\zeta(2n)-1}{2^{2n}}=\frac{1}{6}, \tag{43}$$

and one of many ζ-series for π:

$$\sum_{n=1}^{\infty}\frac{\zeta(2n)-1}{4^{2n}}=\frac{13}{30}-\frac{\pi}{8}, \tag{44}$$

it also leads to

$$\sum_{n=1}^{\infty}\frac{\zeta(2n)-1}{8^{2n}}=\frac{61}{126}-\frac{\pi}{16}\sqrt{\frac{\sqrt{2}+1}{\sqrt{2}-1}}.$$

Not only can we establish such series for certain $\pi\alpha$, with α a nontrivial algebraic number; we may also insert appropriate roots of unity as t-parameters in (40) to obtain such as:

$$\sum_{n=1}^{\infty}(\zeta(4n)-1)=\tfrac{7}{8}-\tfrac{1}{4}\pi\left(\frac{e^{2\pi}+1}{e^{2\pi}-1}\right).$$

We note that in (43), $q_n = 1/2^n$ for n even, else $q_n = 0$, provides an alternative representation of unity, to be contrasted with (38). In fact, there are infinitely many representations of unity. For example the case $q_n = 1$ can be generalized to the following, valid for any nonnegative integer k:

$$1=\sum_{n=k+2}^{\infty}\binom{n-1}{k}(\zeta(n)-1).$$

Likewise (41) leads to interesting series, such as the following obtained by integration:

$$\begin{aligned}\sum_{n=2}^{\infty} \frac{\zeta(n)-1}{(-1)^n(n+1)} &= \tfrac{1}{2}\gamma + \tfrac{1}{2} - \log 2 - \int_1^2 \log\Gamma(z)dz \\ &= \tfrac{1}{2}(\gamma + 3 - \log 2\pi) - \log 2, \end{aligned} \tag{45}$$

which result has a theoretical application we encounter in Section 8.

There are yet other rational ζ-series that interrelate various *Dirichlet series*. One way to derive such relations is to know, first, a cotangent integral such as

$$I_n := \int_0^{1/2} x^n \cot \pi x \, dx,$$

then use the expansion (25) within the integral. Actually, this integral I_n is known exactly for every positive integer n in terms of logarithms and values of $\zeta(\text{odd})$ [49]. One example provides a relation involving $\pi^{-2}\zeta(3)$:

$$\sum_{n=1}^{\infty} \frac{\zeta(2n)-1}{4^n(n+1)} = \tfrac{3}{2} - 9\log 2 + 4\log 3 + \tfrac{7}{2}\pi^{-2}\zeta(3). \tag{46}$$

Consideration of integrals over $0 < x < 1/4$ provide representations for $\pi^{-1}G$, where $G = 1 - 1/3^2 + 1/5^2 - 1/7^2 + \cdots$ is Catalan's constant:

$$\sum_{n=1}^{\infty} \frac{\zeta(2n)-1}{16^n(2n+1)} = \tfrac{3}{2} - \pi^{-1}G - \tfrac{1}{4}\log 2 - 2\log 5 + 2\log 3 \tag{47}$$

and

$$\sum_{n=1}^{\infty} \frac{\zeta(2n)-1}{16^n(2n+1)n} = 2\pi^{-1}G - 3 + 5\log 5 + \log\pi - 5\log 2 - 3\log 3. \tag{48}$$

Incidentally not only rationals but logarithms of rationals as appear in (45) (46) (47) (48) are easy to absorb, if necessary, into the ζ sum. We shall encounter a general logarithmic representation later in this section.

A rational ζ-series can often be accelerated for computational purposes, provided one can resolve the exact sum

$$\sum_{n=2}^{\infty} \frac{q_n}{a^n}$$

for some contiguous sequence $a = 2, 3, 4, \ldots, A$. One simply "peels off" these terms, leaving a series involving the Hurwitz terms $\zeta(n, A+1)$; i.e., ζ-like sums starting with

$1/(A+1)^n$. For example, it turns out that one may peel off *any* number of terms from (46) [42]. The exact corrections for $a = 2, 3, \ldots$ simply add to the detail of the logarithmic term. Perhaps the canonical example of "peeling" is the γ series (39) previously encountered. By peeling of N terms (including 1) from the ζ summand, one has

$$\gamma = \sum_{j=1}^{N} j^{-1} - \log N - \sum_{m=2}^{\infty} m^{-1}\zeta(m, N+1),$$

in which one witnesses the classical limit expression for γ plus an exact (always negative) correction. Computational complexity issues for this peeling—and other evaluation schemes—are discussed in Section 7. For the moment, we observe that if peeling be taken to its extreme limits, there may be no special advantage. For example, if we peel *all* summands in relation (46) for $\zeta(3)$, so that the whole rational ζ-series vanishes, we get the peculiar relation

$$\begin{aligned}\zeta(3) \;=\; & \frac{5\pi^2}{36} - \frac{2\pi^2}{3}\sum_{n=1}^{\infty}\Big\{ -5/12 - 2n^2 + n(n+1)(2n+1)\log(1+1/2n) \\ & \qquad -n(n-1)(2n-1)\log(1-1/2n)\Big\},\end{aligned} \tag{49}$$

a slowly converging series indeed. Thus the primary motivation for peeling is to optimize sums for actual computation—by peeling an optimal number of terms.

We next mention results of Flajolet and Vardi [55] [101], who demonstrate that if $f(z) = \sum_{m\geq 2} f_m z^m$ is analytic on the closed unit disk, then

$$\sum_{n=1}^{\infty} f(1/n) = f(1) + \sum_{m=2}^{\infty} f_m(\zeta(m) - 1),$$

along with peeled such forms involving $\zeta(m, N)$ for $N > 2$. Some of the immediate results along these lines are for π:

$$\pi = \tfrac{8}{3} + \sum_{m=1}^{\infty} 4^{-m}(3^m - 1)(\zeta(m+1) - 1) \tag{50}$$

and for Catalan's constant:

$$G = \tfrac{8}{9} + \tfrac{1}{16}\sum_{m=1}^{\infty}(m+1)4^{-m}(3^m - 1)(\zeta(m+2) - 1).$$

The latter arises from the identity

$$(1-3z)^{-2} - (1-z)^{-2} = \sum_{m=1}^{\infty}(m+1)4^{-m}(3^m - 1)z^m.$$

It is of interest that we thus know rational ζ-series for both G and, as formula (47) yields, G/π. One may also derive a series for π^3, starting with the generating function $f(z) = z^3(1-3z/4)^{-3} - z^3(1-z/4)^{-3}$. In fact, any odd power of π can be cast first as a Dirichlet series (actually, a rational multiple of the *beta function*, $\beta(d) = 1^{-d} - 2^{-d} + 3^{-d} - \cdots$), then one constructs $f(z)$, quickly obtaining a series for π^d. Flajolet and Vardi [55] were able to augment the aforementioned number-theoretical representations described in Section 1 by casting such as the Landau-Ramanujan and Hafner-Sarnak-McCurley constants in terms of convergent ζ constructs.

These curious and attractive series aside, there can actually be practical import for rational ζ-series, thus motivating efficient schemes for evaluation of the relevant $\zeta(n)$. One of the most interesting applications is a result from the measure theory of continued fractions [108] [12]. The celebrated Khintchine constant K_0, defined as the limiting geometric mean of the elements of almost all simple continued fractions, can be bestowed with an efficient series development. The development is particularly compelling in that one of the standard definitions of K_0 is a cumbersome, slowly converging, infinite product. The rational ζ-series we have in mind is the Shanks-Wrench form [108] which for $N > 2$ can be peeled $N-2$ times to yield [12]:

$$\begin{aligned}(\log K_0)(\log 2) &= \sum_{n=1}^{\infty} \frac{\zeta(2n)-1}{n}\left(1 - \frac{1}{2} + \frac{1}{3} - \cdots + \frac{1}{2n-1}\right) \\ &= \sum_{k=3}^{N} \log\left(1 - \frac{1}{k}\right) \log\left(1 + \frac{1}{k}\right) \\ &+ \sum_{n=1}^{\infty} \frac{\zeta(2n, N)}{n}\left(1 - \frac{1}{2} + \frac{1}{3} - \cdots + \frac{1}{2n-1}\right). \end{aligned} \tag{51}$$

The peeled form has been used, together with recycling methods for evaluating ζ at the even positive integers, to obtain K_0 to thousands of digits. In like manner, for negative integers p the *p-Hölder means* (for almost all reals) denoted K_p, of which the harmonic mean K_{-1} is an example, can be given representations:

$$(K_p)^p \log 2 = \sum_{n=2}^{\infty} Q_{np}(\zeta(n + |p|) - 1),$$

where all Q coefficients have been given explicit rational form [12]. Again there is a peeled form, and the harmonic mean K_{-1} in particular is now known, via such machinations, to more than 7000 decimal places [12].

Beyond the evident beauty of the world of ζ-expansions, there are important computational questions partially addressed by such high-precision efforts. For example, is the geometric mean of the partial quotients in the simple continued fraction for K_0 equal to K_0? The various formulae of [12] relevant to the Khintchine constant and its relatives depend in general on all integer arguments n for $\zeta(n)$, not just the even ones. For such reasons, rapid evaluation schemes—including recycling ones—for positive integer n are always of special interest.

Here is another example of the utility of the series forms of our present interest. The classical acceleration formula [78](4.28)

$$\frac{\mathrm{C}l_2(\theta)}{\theta} = 1 - \log|\theta| + \sum_{n=1}^{\infty} \frac{\zeta(2n)}{n(2n+1)} \left(\frac{\theta}{2\pi}\right)^{2n}, \quad |\theta| < 2\pi$$

for the *Clausen function*

$$\mathrm{C}l_2(\theta) := \sum_{n=1}^{\infty} \frac{\sin(n\theta)}{n^2}, \quad \theta \text{ real},$$

is useful for computing certain Dirichlet L-series values; e.g. $\mathrm{C}l_2(\pi/2) = G$, the Catalan constant. For actual computations an accelerated, "peeled" form

$$\frac{\mathrm{C}l_2(\theta)}{\theta} = 3 - \log\left(|\theta|\left(1 - \frac{\theta^2}{4\pi^2}\right)\right) - \frac{2\pi}{\theta}\log\left(\frac{2\pi+\theta}{2\pi-\theta}\right) + \sum_{n=1}^{\infty} \frac{\zeta(2n)-1}{n(2n+1)}\left(\frac{\theta}{2\pi}\right)^{2n}$$

could be used.

We next describe one way to generate a vast collection of examples of rational ζ-series, by establishing a certain connection with *Laplace transforms*. Observe the following formal manipulations, where we disregard for the moment issues of convergence and summation interchange. Let μ be a fixed complex number and let f be the exponential generating series of the (presumed rational) sequence $f_0, f_1, \ldots$

$$f(x) = \sum_{n=0}^{\infty} \frac{f_n}{n!} x^n. \tag{52}$$

Proceeding formally, we derive

$$\begin{aligned} \int_0^{\infty} f(x/a) e^{-\mu x}\, dx &= \int_0^{\infty} f(x/a) e^{-\mu x} (e^x - 1)^{-1} \sum_{k=1}^{\infty} x^k/k!\, dx \\ &= \sum_{n=0}^{\infty}\sum_{k=1}^{\infty} \frac{a^{-n} f_n}{k!\, n!} \int_0^{\infty} \frac{e^{-\mu x} x^{n+k}}{e^x - 1}\, dx. \end{aligned} \tag{53}$$

Now we invoke the integral representation (14) for the Hurwitz zeta function to arrive at the formal Laplace transform

$$\int_0^\infty f(x/a)e^{-\mu x}dx = \sum_{n=2}^\infty \zeta(n, \mu+1)\sum_{k=0}^{n-2}\binom{n-1}{k}\frac{f_k}{a^k},$$

where a is so far arbitrary, but eventually to be constrained by convergence requirements. Up to this point μ is likewise unrestricted; if we specify $\mu = 1$ and assume the coefficients f_n be rational, then we have a formal relation

$$\int_0^\infty f(x)e^{-ax}dx = \sum_{n=2}^\infty q_n(\zeta(n)-1),$$

where the q_n are explicit and rational:

$$q_n = \sum_{k=0}^{n-2}\binom{n-1}{k}\frac{f_k}{a^{k+1}}.$$

The recreational possibilities of the Laplace transform approach seem endless. One may use a *Bessel function* of the first kind, $f(x) = J_0(x) = 1-(x^2/4)/(1!)^2+(x^2/4)^2/(2!)^2-\cdots$, whose Laplace transform is known

$$\int_0^\infty J_0(x)e^{-ax}dx = (1+a^2)^{-1/2}$$

to obtain (again, merely formally as yet)

$$\frac{1}{\sqrt{1+b}} = \sum_{n=2}^\infty(\zeta(n)-1)\sum_{k=0}^{n/2-1}(-b/4)^k\binom{2k}{k}\binom{n-1}{2k}, \tag{54}$$

which already shows the importance of convergence considerations; evidently $|b|$ must be sufficiently small; certainly $|b| < 2$ suffices. Now observe that for integers μ, ν a square root of μ/ν may be written

$$\sqrt{\frac{\mu}{\nu}} = \frac{1}{\sqrt{1+(\nu/\mu-1)}}$$

if $\mu > \nu$, otherwise we use $(\mu/\nu)\sqrt{\nu/\mu}$, and so the ζ-series (54) applies with

$$b = \min(\mu,\nu)/\max(\mu,\nu) - 1$$

to yield $\sqrt{q}$ for any rational q and therefore any quadratic surd. Along these lines one may establish infinitely many different rational ζ-series for the golden mean, $\tau = (1+\sqrt{5})/2$. For example, setting $b = 1/465124$, for which $\sqrt{1+b} \in Q[\tau]$, results in just one explicit series.

To represent π as a rational ζ-series, one may use the integral

$$\int_0^\infty \frac{e^{-x}\sin x}{x}\,dx = \frac{\pi}{4}$$

to obtain the series

$$\begin{aligned} \frac{\pi}{4} &= \sum_{n=2}^{\infty}(\zeta(n)-1)\sum_{k=0}^{n/2-1}\frac{(-1)^k}{2k+1}\binom{n-1}{2k} \\ &= \sum_{n=2}^{\infty} n^{-1}(\zeta(n)-1)\Im((1+i)^n - 1 - i^n) \end{aligned} \tag{55}$$

where interestingly enough the coefficients q_n vanish for $n = 4, 8, 12, \ldots$. This rational ζ-series for π, like the form (50) and the aforementioned scheme for π^{odd}, is nontrivial in the sense that, whereas π^{2n}, being a rational multiple of $\zeta(2n)$, is trivially representable, odd powers of π evidently require some nontrivial analysis.

We have intimated that logarithms of rationals can always be given an explicit ζ-series. One may show this by invoking the Laplace transform:

$$\int_0^\infty \frac{e^{-x}(1-e^{-ax})}{x}\,dx = \log(1+a)$$

to infer

$$\log(1-a) = \sum_{n=2}^{\infty} n^{-1}(\zeta(n)-1)(1+a^n-(1+a)^n).$$

Though this series has a finite domain of convergence, one may forge a series for $\log N$ for any integer $N \ge 2$ by using $\log N = -\log(1+(1/N-1))$. Thus $\log M/N$ for any integers M, N can be cast as a rational ζ-series. And the story by no means ends here. One may take

$$f(x) = \frac{\sinh\sqrt{x}}{\sqrt{x}}$$

to obtain a series for the error function at rational points z. (More precisely, one obtains a series for $\sqrt{\pi}\exp(z^2)\mathrm{erf}(z)$.) As the error function is essentially an incomplete gamma function, there is the possibility of casting more general incomplete gammas in rational ζ-series.

There is the intriguing possibility that one may effect numerical integration for some Laplace-transform integrands by way of appropriate rational ζ-series. There is also the possibility of discovering new identities by inversion; that is, one may work the Laplace transform technique backwards, to observe (let us say formally, as before):

$$\sum_{n=2}^{\infty} q_n(\zeta(n)-1) = \sum_{k=0}^{\infty} f_k,$$

where the f_k are defined via the recurrence

$$(k+1)f_k = q_{k+2} - \sum_{j=0}^{k-1} \binom{k+1}{j} f_j.$$

A different—and elegant—integral transform technique was enunciated by Adamchik and Srivastava [1], in the following form to which our Laplace-transform method stands as a kind of complement. Working formally as before, one can quickly derive from the representation (14) a general relation

$$\sum_{n=2}^{\infty} q_n(\zeta(n)-1) = \int_0^{\infty} \frac{F(t)e^{-t}}{e^t-1}\,dt, \tag{56}$$

where

$$F(t) = \sum_{n=1}^{\infty} q_{n+1}\frac{t^n}{n!}.$$

As with our Laplace-transform technique, when one can do the integral one obtains a rational ζ-series. Adamchik and Srivastava went on to derive in this fashion such attractive series as

$$\sum_{n=1}^{\infty} n^{-1}t^n(\zeta(2n)-1) = \log((1-t)\pi\sqrt{t}\csc(\pi\sqrt{t})),$$

which can also be derived by integration of relation (40); and the following curiosity which involves a derivative of ζ:

$$\sum_{n=2}^{\infty} \frac{\zeta(n)-1}{(n+1)(n+2)} = -\tfrac{1}{6}(1+\gamma) - 2\zeta'(-1).$$

Adamchik and Srivastava also employed their ζ-summation methods together with a certain polylogarithm series from [12] to derive an alternative representation for the Khintchine constant:

$$(\log K_0)(\log 2) = \tfrac{1}{12}\pi^2 + \tfrac{1}{2}\log^2 2 + \int_0^{\pi} t^{-1}\log(t|\cot t|)\,dt.$$

This kind of analysis analysis shows again that a rational ζ-series can enjoy, quite beyond its natural allure, some theoretical importance. Incidentally, when a successful Laplace-transform kernel is used in the Adamchik-Srivastava formalism, the effects can be appealing. As just one example, if we use a Bessel kernel not as in the previous quadratic-surd analysis, but for F in the relation (56), the result is a convergent scheme for certain sums $\sum_m (x^2+m^2)^{-s}$, which can in turn be summed over x to yield such as:

$$\begin{aligned}\sum_{N=1}^{\infty} \frac{d(N)}{(1+N^2)^{3/2}} &= \sum_{n=1}^{\infty} 4^{-n}(\zeta(2n+1)-1)2n\zeta(2n+1)(-1)^{n-1}\binom{2n}{n} \\ &= 0.1977854807156750630882363015 82\ldots\end{aligned}$$

where $d(N)$ is the number of divisors of N. Though the relevant coefficents this time are not rational (as they involve the $\zeta(2n+1)$ themselves), the indicated numerical value would evidently be difficult to achieve without the aid of such manifest convergence.

Because the series of choice for practical calculation of some constants (such as the Khintchine constant as just one example) is some form of rational ζ-series, we are interested in ζ-evaluations for integer arguments, to which subject we next turn.

5 Integer Arguments

Because of existing fast algorithms for computation of π and its powers in (22), not to mention finite recurrences between the ζ-values at even positive integer arguments, computations for positive odd integer arguments are relatively more difficult.

Our first observation is that various of the formulae of previous sections may be applied directly when s is a positive odd integer. As just one example, the free-parameter choice $\lambda = i\pi$ in (32), together with the recursion relation (31), gives rise to an interrelation between the ζ-values at odd positive integer arguments in the following form. Let m be a positive integer. With $s = 2m+1$, we obtain

$$-\frac{(1-2^{-2m-1})2\zeta(2m+1)}{(\pi i)^{2m}} = \sum_{k=1}^{m-1} \frac{(1-4^{-k})\zeta(2k+1)}{(\pi i)^{2k}(2m-2k)!}$$

$$+\quad \frac{1}{(2m)!}\Big\{\log 2-\frac{1}{2m}+\sum_{n=1}^{\infty}\frac{\zeta(2n)}{4^n(n+m)}\Big\}. \qquad (57)$$

When $m=1$, the formula yields

$$\zeta(3)=\frac{2\pi^2}{7}\Big\{\log 2-\frac{1}{2}+\sum_{n=1}^{\infty}\frac{\zeta(2n)}{4^n(n+1)}\Big\},$$

which can be peeled once to give relation (46). Such as $\zeta(5)$ could be obtained in terms of $\zeta(3)$ and a convergent series, and so on. It is interesting that the weight factor $1/(2m)!$ of the troublesome series part decays so rapidly; that is, we have for large m an "almost exact" interrelation between the relevant $\zeta(\text{odd})$, in the spirit of, say, the even-argument relation (27).

¿From the Lerch expansion (33) one can derive other interrelations amongst ζ evaluations. Using the functional equation (17) we can write, for example:

$$\tfrac{3}{4}\zeta(3)=\tfrac{1}{12}\left(1+\pi^2\right)-\tfrac{1}{2}\log 2+\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n^3e^n}-2\sum_{j=1}^{\infty}\left(\frac{i}{2\pi}\right)^{2j}\frac{(1-4^j)\zeta(2j)}{2j(2j+1)(2j+2)},$$

where the last sum on the right has purely rational summands decaying as π^{-2j}.

There are other similar series for $\zeta(\text{odd})$, for example that of Boo [26]:

$$\zeta(3)=-\frac{4\pi^2}{7}\sum_{n=0}^{\infty}\frac{\zeta(2n)}{(2n+1)(2n+2)4^n}.$$

and of K. Williams [109]:

$$\zeta(3)=-2\pi^2\sum_{n=0}^{\infty}\frac{\zeta(2n)}{(2n+2)(2n+3)4^n}.$$

Specific hyperbolic series, to be chosen as odd positive integer s is $1,-1 \pmod 4$ respectively, are essentially due to Ramanujan and ála Zagier run as follows:

$$p\,\zeta(4p+1) = \frac{1}{\pi}\sum_{n=0}^{2p+1}(-1)^n\,(n-\tfrac{1}{2})\,\zeta(2n)\,\zeta(4p+2-2n) - 2\sum_{n>0}\frac{n^{-4p-1}}{\exp(2\pi n)-1}\left(p+\frac{\pi n}{1-\exp(-2\pi n)}\right) \qquad (58)$$

$$\zeta(4p-1) = -\frac{1}{\pi}\sum_{n=0}^{2p}(-1)^n\,\zeta(2n)\,\zeta(4p-2n)-2\sum_{n>0}\frac{n^{-4p+1}}{\exp(2\pi n)-1} \qquad (59)$$

For $p = 0$, (58) evaluates to $1/4$ and (59) to $-1/12 = \zeta(-1)$, as might be hoped.

Note that there is no longer an infinite set of ζ-values required; the sums involving ζ are finite in (58) and (59). Moreover, while these require evaluation of $e^{2\pi k}$, the number e^{π} can be computed once and recycled.

Recently, similar but demonstrably different series have been found (the first few cases empirically by Simon Plouffe). A most striking example—which can be obtained, *ex post facto*, from ([15], Ch. 14, Entry 21(i))—in implicit form is:

$$\begin{aligned}
&\left(2-(-4)^{-n}\right)\left(2\sum_{k=1}^{\infty}\frac{1}{\left(e^{2k\pi}-1\right)k^{4n+1}}+\zeta(4n+1)\right)\\
&\qquad-(-4)^{-2n}\left(-2\sum_{k=1}^{\infty}\frac{1}{\left(e^{2k\pi}+1\right)k^{4n+1}}+\zeta(4n+1)\right)\\
&=\pi^{4n+1}\sum_{k=0}^{2n+1}(-1)^{k+1}\left(4^k+(-1)^{k(k-1)/2}(-4)^n 2^k\right)\frac{B_{4n+2-2k}}{(4n+2-2k)!}\frac{B_{2k}}{(2k)!}
\end{aligned} \tag{60}$$

in which Bernoulli numbers can be replaced by even ζ-values using (24); and whose first case yields:

$$\zeta(5) = -\frac{72}{35}\sum_{k=1}^{\infty}\frac{1}{\left(e^{2k\pi}-1\right)k^5} - \frac{2}{35}\sum_{k=1}^{\infty}\frac{1}{\left(e^{2k\pi}+1\right)k^5} + \frac{\pi^5}{294}.$$

A classical formula

$$\zeta(2) = 3\sum_{k=1}^{\infty}\frac{1}{k^2\binom{2k}{k}}$$

has analogue

$$\zeta(4) = \frac{36}{17}\sum_{k=1}^{\infty}\frac{1}{k^4\binom{2k}{k}}$$

given in Comtet [40](p. 89), or see [20]. The next formula—which has no known single term analogue yielding $\zeta(5)$—played a signal role in Apéry's proof of the irrationality of $\zeta(3)$. (These matters are discussed further in [22, 23].) The precise formula, due to Hjortnaes [60] is:

$$\zeta(3) = \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}. \tag{61}$$

There is however a two-term analogue yielding $\zeta(5)$, namely this due to Koecher: [72, 73]

$$\zeta(5) = 2\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^5\binom{2k}{k}} - \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^2}, \tag{62}$$

and, more generally we have the following formal expansion in powers of z:

$$\sum_{k=1}^{\infty} \frac{1}{k^3(1-z^2/k^2)} = \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\left(\frac{1}{2}+\frac{2}{1-z^2/k^2}\right)\prod_{j=1}^{k-1}(1-z^2/j^2).$$

Borwein-Bradley: [22, 23, 4] established:

$$\zeta(7) = \frac{5}{2}\sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^7\binom{2k}{k}} + \frac{25}{2}\sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4}, \tag{63}$$

and, more generally the power series in z:

$$\sum_{k=1}^{\infty} \frac{1}{k^3(1-z^4/k^4)} = \frac{5}{2}\sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\frac{1}{1-z^4/k^4}\prod_{j=1}^{k-1}\frac{j^4+4z^4}{j^4-z^4}. \tag{64}$$

Note that (64) contains (61) and (63) as its constant term and next term (coefficient of z^4) respectively. Formula (64) was discovered empirically and reduced in [22] to an equivalent finite form by a process of "creative telescoping" and analytic continuation. This finite form was subsequently proven by Almkvist and Granville. The formulae (61, 62, 63) are well-suited for numerical computation due to the fact that the series terms decay roughly geometrically with ratio $1/4$. Algorithms 1, 2 and 3 below are based on the Hjortnaes formula (61), the Koecher formula (62), and the Borwein-Bradley formula (63), respectively [22].

Algorithm 1 *Given D, compute $\zeta(3)$ to D digits using (61). Computations are performed to D digits.*

> $N = 1 + \lfloor 5D/3 \rfloor;\ c = 2;\ s = 0;$
>
> *for* $n = 1$ *to* N *do begin*
>
> $s = s + (-1)^{n+1}/(n^3 c);$
>
> $c = c(4n+2)/(n+1);$
>
> *end;*
>
> *return* $5s/2;$

Note that this kind of algorithm can be naturally extended to yet more efficient $\zeta(3)$ series, such as the accelerated formula (68) appearing later in this paper.

Algorithm 2 *Given D, compute $\zeta(5)$ to D digits using* (62). *Computations are performed to D digits.*

$N = 1 + \lfloor 5D/3 \rfloor;\ a = 0;\ c = 2;\ s = 0;$

for $n = 1$ *to* N *do begin*

$g = 1/n^2;\ s = s + (-1)^{n+1}(4n - 5a)/(n^3 c);$

$c = c(4n+2)/(n+1);\ a = a + g;$

end;

return $s/2;$

Algorithm 3 *Given D, compute $\zeta(7)$ to D digits using* (63). *Computations are performed to D digits.*

$N = 1 + \lfloor 5D/3 \rfloor;\ a = 0;\ c = 2;\ s = 0;$

for $n = 1$ *to* N *do begin*

$g = 1/n^2;\ s = s + (-1)^{n+1}(5a + g)/(n^3 c);$

$c = c(4n+2)/(n+1);\ a = a + g;$

end;

return $5s/2;$

The operational complexity of Algorithms 1, 2 and 3 will be discussed in Section 7. Generally speaking, for fixed precision (say D digits) these are the fastest schemes available for the indicated ζ(integer) values. One should keep in mind that there are asymptotically (very large D) even faster ways of handling the relevant summations, using a so-called FEE method also discussed in Section 7.

6 Value Recycling

We have mentioned the multivalue computations of Odlyzko and Schönhage [86], such an approach being of interest for complex s lying, say, in some (complex) arithmetic progression. It turns out that for certain sets of arguments with integer differences (the arguments not necessarily in arithmetic progression) one can invoke alternative value-recycling schemes. The basic notion of recycling here is that previously calculated ζ-values—or initialization tables of those calculations—are re-used to aid in the extraction of other ζ-values, or many ζ-values at once are somehow simultaneously determined, and so on. So by value recycling we mean that somehow the computation of a collection of ζ-values is more efficient than would be the establishment of independent values.

First, one can use either of (30) or (32) to efficiently evaluate ζ at each of N arguments $\{s, s+2, s+4, \ldots, s+2(N-1)\}$ for any complex s. This approach might be fruitful for obtaining a collection of ζ-values at odd positive integers, for example. The idea is to exploit the recursion relation (31) for the incomplete gamma function and thereby, when N is sufficiently large, effectively unburden ourselves of the incomplete gamma evaluations. One may evaluate such as $\Gamma(\{s/2\}, x), \Gamma(\{(1-s)/2\}, x)$ where $\{z\}$ denotes generally the fractional part of z, over a collection of x-values, then use the above recursion either backward or forward to rapidly evaluate series terms for the whole set of desired ζ-values. Given the initial $\Gamma(\{s/2\}, x)$ evaluations, the rest of the calculation to get all the ζ-values is sharply reduced. In the case that the $\{s+2k\}$ are odd integers, the precomputations involve only $\Gamma(0, x)$ and $\Gamma(1/2, x)$ values; known classically as exponential-integral and error-function values. Reference [42] contains explicit pseudocode for a recycling evaluation of $\zeta(3), \zeta(5), ..., \zeta(L)$ via the series (30), in which evaluation one initializes error function and exponential-integral values, respectively:

$$\{\Gamma(1/2, \pi n^2) \ : \ n \in [1, \lfloor D \rfloor]\}, \tag{65}$$

$$\{\Gamma(0, \pi n^2) \ : \ n \in [1, \lfloor D \rfloor]\},$$

where D decimal digits of precision are ultimately desired for each ζ value. The notion of "recycling" takes its purest form in this method, for the incomplete-gamma evaluations above are reused for every $\zeta(\text{odd})$.

A second recycling approach, relevant for *even* integer arguments, involves a method of series inversion pioneered by J. P. Buhler for numerical analyses on Fermat's "Last Theorem" and on the Vandiver conjecture [35] [36] [37]. One uses a generating function for Bernoulli numbers, and invokes the Newton method for series inversion of the key elementary function. To get values at even positive integers, one may use an expansion related to (25). One has:

$$\frac{\sinh(2\pi\sqrt{t})}{4\pi\sqrt{t}} \frac{2\pi^2 t}{\cosh(2\pi\sqrt{t}) - 1} = -\sum_{n=0}^{\infty} (-1)^n \zeta(2n) t^n,$$

which we have derived and written in this particular form to allow the algorithm following. Note that we have separated the left-hand side into to two series, each in the t variable: one series being essentially of the form $(\sinh\sqrt{z})/\sqrt{z}$ and the other being $(\cosh\sqrt{z} - 1)/z$.

The idea, then, is to invert the latter series via a fast polynomial inversion algorithm (Newton method). Using t as a place-holder throughout, one then reads off the ζ-values as coefficients in a final polynomial. In the algorithm display following, we assume that $\zeta(2), \zeta(4), \ldots \zeta(2N-2)$ are desired. The polynomial arithmetic is most efficient when truncation of large polynomials occurs at the right junctures. For a polynomial $q(t)$, we denote by $q(t) \bmod t^k$ the truncation of q through the power t^{k-1} inclusive; that is, terms t^k and beyond are dropped. Also in what follows, a polynomial multiplication operation is signified by "$*$".

Algorithm 4 *Recycling scheme for a sequence $\zeta(0), \zeta(2), \zeta(4), \ldots, \zeta(2(N-1))$.*

1) [Denominator setup]

Create the polynomial $f(t) = (\cosh(2\pi\sqrt{t}) - 1)/(2\pi^2 t)$,

through degree N (i.e., through power t^N inclusive);

2) [Newton polynomial inversion, to obtain $g := f^{-1}$]

$p = g = 1$;

while($p < \deg(f)$) do begin

$p = \max(2p, \deg(f))$;

$h = f \bmod t^p$;

$g = (g + g * (1 - h * g)) \bmod t^p$;

end;

3) [Numerator setup]

Create the polynomial $k(t) = \sinh(2\pi\sqrt{t})/(4\pi\sqrt{t})$, through degree N;

$g = g * k \bmod t^{2N-1}$;

For $n \in [0, 2N-2]$, read off $\zeta(2n)$ as $-(-1)^n$

times the coefficient of t^n in polynomial $g(t)$.

It is important to note that this algorithm can be effected in *either* numerical or symbolic mode. That is, in step 1) the polynomial in question can have floating point coefficients, or symbolic ones with their respective powers of π and so on. If symbolic mode is in force, the ζ values of the indicated finite set are all exact, through $\zeta(2N-2)$ inclusive. The method has actually been used—in numerical mode so that fast Fourier transform methods may also be applied to the numerical multiplications—to calculate the relevant ζ-values for high-precision values of the Khintchine constant [12]. Incidentally, if one worries about memory storage in such a Buhler inversion, there is a powerful technique called "multisectioning," whereby one calculates all the $\zeta(2k)$ for k lying in some congruence class (mod 4, 8 or 16 say), using limited memory for that calculation, then moving on to the next congruence class, and so on. Observe first that, by looking only at even-indexed Bernoulli numbers in the previous algorithm, we have effectively multisectioned by 2 already. To go further and multisection by 4, one may observe:

$$\frac{x \cosh x \sin x \pm x \cos x \sinh x}{\sinh x \sin x} = 2 \sum_{n \in S^{\pm}} \frac{B_n}{n!} (2x)^n,$$

where the sectioned sets are $S^+ = \{0, 4, 8, 12, \ldots\}$ and $S^- = \{2, 6, 10, 14, \ldots\}$. The key is that the denominator $(\sinh x \sin x)$ is, perhaps surprisingly, x^2 times a series in x^4, namely we have the attractive series

$$\sinh x \sin x = \sum_{n \in S^-} (-1)^{(n-2)/4} 2^{n/2} \frac{x^n}{n!}, \tag{66}$$

so that the key Newton inversion of a polynomial approximant to said denominator only has *one-fourth* the terms that would accrue with the standard Bernoulli denominator $(e^x - 1)$ (and one-half as many terms as required in Algorithm 5). Thus, reduced memory is used to establish a congruence class of Bernoulli indices, then that memory is reused for the next congruence class, and so on. Thus, these methods function well in either parallel or serial environments.

Multisectioning was used by Buhler and colleagues—as high as level-16 sections—to verify Fermat's "Last Theorem" to exponent 8 million [37]. They desired Bernoulli numbers modulo primes, and so employed integer arithmetic, but the basic Newton iteration is the same for either symbolic (rational multiples of powers of π) or numerical (floating-point) ζ-values.

A third approach is to contemplate continued fraction representations that yield ζ-values. For example, the well known fraction for $\sqrt{z} \coth \sqrt{z}$ gives:

$$\cfrac{\pi^2 z}{3 + \cfrac{\pi^2 z}{5 + \cfrac{\pi^2 z}{7 + \ddots}}} = 2 \sum_{n=1}^{\infty} (-1)^{n-1} \zeta(2n) z^n.$$

The computational advantage here would obtain if one already had in hand an efficient, continued fraction engine. There is also the possibility of fast evaluation of the convergents, although it is unclear whether this technique could be brought to the efficiency of the Buhler approach above. Incidentally, if one desires not values at the even positive integers but the actual Bernoulli numbers as exact rational numbers, there is an alternative fraction due to Bender:

$$\cfrac{1}{1+\cfrac{b(1)z}{1+\cfrac{b(2)z}{1+\cfrac{b(3)z}{1+\ddots}}}} = 1 + 6\sum_{n=2}^{\infty} B_{2n} z^{n-1},$$

with

$$b(n) = \frac{n(n+1)^2(n+2)}{4(2n+1)(2n+3)}.$$

Note that the series does not converge in any obvious sense; it is a symbolic series. Again, this form might be recommended if a good continued fraction calculator were in place. As a last alternative for fast evaluation at even positive integer arguments, there is an interesting approach of Plouffe and Fee [89], in which the Von-Staudt-Clausen formula for the fractional part of B_n is invoked, then asymptotic techniques are used to ascertain the integer part. In this way the number B_{200000} has been calculated in exact, rational form. Yet another strategy for Bernoulli numbers—untested as far as we know—is to resolve B_n via Chinese remainder methods, where one would establish via Voronoi formulae the values $B_n (\mathrm{mod}\ p_i)$ for sufficiently many small primes p_i.

A fourth approach stands as a kind of complement to the previous, even-argument method. There is actually a way to calculate ζ-values at consecutive positive integers in recycled fashion. The generating function will not now be a cotangent function but the ψ function defined in (26). Previous implementations of a ψ-based recycling algorithm, as in [42], do work but are not of the fast algorithm class. More recently [46], there has appeared an asymptotically "fast" rendition of the idea, which method we now briefly describe.

Since the standard gamma function can be estimated via such approximations as [20]

$$\left| \Gamma(z) - N^z \sum_{k=0}^{6N} \frac{(-1)^k N^k}{k!(k+z)} \right| \le 2Ne^{-N},$$

valid for real $z \in [1, 2]$, one might expect that the kind of sum appearing would, if the series inversions of the $(k + z)$ were carried out as polynomials in z, provide a reasonable series for the ψ function (the logarithmic derivative of Γ). Indeed, it turns out [46] that the logarithmic derivative of a function with summation limit $4N$, namely:

$$g(z) = \sum_{k=0}^{4N-1} \frac{(-1)^k N^k}{k!(k + 1 - z)}$$

is an appropriate power series in z, in fact

$$\frac{d}{dz} \log g(z) \sim (\log N + \gamma) + \zeta(2)z + \zeta(3)z^2 + \zeta(4)z^3 + \ldots,$$

in some appropriate asymptotic sense [46]. Thus, the same polynomial arithmetic ideas as for the Buhler method previous can be used in principle to evaluate ζ at consecutive positive integer arguments. The following algorithm display follows the treatment in [46]:

Algorithm 5 *Recycling scheme for a collection of the L values: $\zeta(2), \zeta(3), \zeta(4), \ldots, \zeta(L+1)$.*

1) [Set precision]

Choose a power-of-two N, such that 2^{-N} is less than

the required precision (i.e., N is greater than the required bit-precision).

and also $N \geq L$ (a common condition in numerical settings) .

2) [Quotient array]

Create $g[k] = P[k]/Q[k]$, for $k \in [0, 4N - 1]$, where

$P[k] = (-N)^k$, $Q[k] = k!(k + 1 - z)$,

with z being a place-holder as in standard polynomial computations.

3) [Resolve g function]

$p = 1$;

while $p \leq 2n$ *do begin*

for $q = 0$ *to* $4N - 1 - p$ *step* p *do begin*

$g[q] = g[q] + g[q + p]$;

Resolve the new $g[q]$ into numerator/denominator,

each clipped mod z^{L+1}*);*

end;

$p = 2p$*;*

end;

4) [Monic reversion]

Now $g[0] = P[0]/Q[0]$, each of P, Q being of degree at most L, so force a reverse-monic property, by dividing each of P, Q through by its constant coefficient;

5) [Inversion]

Perform Newton inversions as in step (2) of Algorithm 4, to create the reciprocal polynomials P^{-1} and Q^{-1};

6) [Coefficient computation]

Compute the coefficients R_k in the polynomial

$$R(z) = \sum_{k=0}^{L} R_k z^k = ((dP/dz)P^{-1} - (dQ/dz)Q^{-1}) \bmod z^{L+1};$$

7) [Read off the ζ values]

Optionally read off $\gamma \sim R_0 - \log N$ and in any case read off, for $k \in [2, L+1]$, the desired ζ approximations as

$$\zeta(k) \sim R_{k-1}.$$

A typical experiment with Algorithm 5 works out as follows. Take $N = L = 16$, meaning that degree-16 polynomials will be used and we shall obtain in recycling fashion a set of 16 separate ζ values, together with an approximation to γ.

$$R(x) \sim \log N + 0.57721 + 1.64493x + 1.20205x^2 + 1.08232x^3 + 1.03692x^4 +$$

$$\cdots + 1.000122713347x^{12} + \cdots$$

where we indicate good digits by virtue of their appearance. Note that $\zeta(13)$ as the coefficient of x^{12} is more accurate than the low-lying coefficients. This trend is universal to the algorithm, and in some ways is a good thing because if the values $\zeta(n) - 1$ are employed, we enjoy relative precision after the 1 is subtracted. Note also that even the low-lying coefficients have errors of order 2^{-16} as expected. Of course, the algorithm can be modified to yield only values at odd positive integers, for example by subtracting off at a key juncture a truncated cotangent series. Detailed error analysis and asymptotics are described in [46], though we do touch upon complexity issues for Algorithm 5 in the next section. It should also be observed that fast, single-argument evaluation of the gamma function and functions such as our $g(z)$ were worked out by Karatsuba [65] [68] [67] [66], about which we have more to say in the enxt section; so perhaps her methods may be used to accelerate even further the series computations of Algorithm 5.

7 Computational Complexity

Herein we focus on evaluations of ζ-values for integer arguments and arguments in certain arithmetic progressions. However, in a spirit of completeness, let us first comment on the complexity issue for those analytic number theory computations briefly reviewed in Section 1. Consider first the highly important evaluation of $\zeta(1/2+it)$ where t is positive but otherwise unrestricted; and say we desire the evaluation to have a fixed precision (one only needs enough precision actually to locate zeros, say) but that t is unrestricted. It should be stated right off that for this problem there is no known polynomial-time algorithm, say an algorithm of $O(\log^k t)$ operation complexity to perform a *single* ζ evaluation. We note the interesting remarks in [18], where the author suggests outright that the calculation of $\zeta(1/2 + it)$ is fundamentally of exponential operation complexity $O_\varepsilon(t^{1/2-o(1)})$ to achieve errors bounded by a fixed ε and furthermore that this is a special property of the critical line (indeed, off the critical line the complexity is reduced). Whereas it is known that the classical Euler-Maclaurin approach has operation complexity $O(t)$, the Riemann-Siegel formula allows $O(t^{1/2+\varepsilon})$. Indeed, we recall that most of the work for the latter method is a sum over $O(\sqrt{t})$ elementary summands. Furthermore, the Odlyzko-Schönhage approach allows the (approximately $T^{1/2}$) critical zeros of the interval $t \in [T, T + T^{1/2})$ to be found in $O(T^{1/2+\varepsilon})$ operations [83] [86] [85]. So the average operation complexity per critical zero works out to be impressive: $O(T^\varepsilon)$. To summarize,

Riemann-Siegel formula (35), $\Re(s = \sigma + it) > 0$ fixed, , $t > 0$ arbitrary, and precision fixed:

Operation complexity $O(t^{1/2+\varepsilon})$.

Odlyzko-Schönhage enhancement, for $t \in [T, T + T^{1/2}]$:

Operation complexity $O(T^{\varepsilon})$ per each of $O(T^{1/2+\varepsilon})$ ζ values.

Note that the Odlyzko-Schönhage method enjoys its tremendous efficiency because it is, in our present sense of the word, a recycling scheme. As the reference [86] describes, the evaluation of multiple ordinates t simultaneously can be done via FFT-like methods, in particular rational-complex function evaluation which can also be considered as fast interpolation along the lines of the works of Dutt, Rokhlin et al. [52] [53]. The essential idea is to attempt to perform sums of the form (36) for a set of t values (which may or may not be equispaced). Sometimes, depending on the problem at hand, a simple FFT approach with the Euler-Maclaurin formula (29) is a good option. For example, $\pi(x)$ calculations, for moderate x, carried out in the style described after relation (3) may benefit from such a simplified approach [46].

Incidentally, the Euler-Maclaurin series (29) for fixed precision and arbitrary t is not as good as the Riemann-Siegel series, in fact:

Euler-Maclaurin formula (29), $\Re(s = \sigma + it) > 0$ fixed, $t > 0$ arbitrary, and precision fixed:

Operation complexity $O(t^{1+\varepsilon})$.

Incidentally, because the Euler-Maclaurin method also starts out with a sum of terms $n^{-\sigma-it}$, the Odlyzko-Schönhage acceleration applies equally well, with the ultimate complexity being reduced accordingly to $O(T^{1/2+\varepsilon})$ for resolution of $O(T^{1/2+\varepsilon})$ zeros in $[T, T + T^{1/2}]$. Note also that the Bernoulli components of the Euler-Maclaurin sum can be obtained in recycled fashion, as we discuss below. Such methods can sometimes pull computationally (perhaps not always theoretically) important logarithmic factors off of complexity bounds. There is a moral here: regardless of superior asymptotic behavior, the Riemann-Siegel formulae may sometimes involve too many practical details when Euler-Maclaurin, far simpler to implement, and susceptible to some interesting optimizations, would suffice. The Euler-Maclaurin scheme can be used, for example, in serious practical evaluations of ζ (see for example [39], where careful Euler-Maclaurin error bounds are developed).

Unlike the analysis for fixed σ and large t, most every other aspect of the present treatment involves the following scenario: the argument s, or arguments $\{s_1, s_2, \ldots\}$ (and their population) are fixed, and we consider varying the precision, measured say as D digits.

Let us start with the incomplete-gamma series (30). Because an incomplete gamma function can be evaluated via fast Fourier transform acceleration in $O(D^{1/2} \log^2 D)$ operations [20], and because we require $O(D^{1/2})$ summands of either sum, and because elementary functions (e.g. arbitrary powers) require $O(\log^k D)$ operations, for some k [29] [30], we conclude:

Incomplete-gamma formula (30), for fixed complex s, to D-digit precision:

Operation complexity $O(D^{1+\varepsilon})$.

Recycling enhancement to incomplete-gamma formula (based on precomputations 65), for set of arguments $\{s, s+2, s+4, \ldots, s+2(N-1)\}$:

Operation complexity $O(D^{1/2+\varepsilon})$ per ζ value.

This average complexity in recycling mode is impressive; we know of no simple schemes for say $\zeta(\text{odd})$ that run faster than $O(D)$; however see the material later in this section for low bit-complexity schemes that exploit dynamically changing precision, such as Karatsuba's FEE method and possible hybrid alternatives that might stem from it.

Because the values at even positive integers appear in so many studies, we next discuss the Buhler recycling scheme, Algorithm 4. It is evident that the even-argument values $\zeta(2), \ldots, \zeta(2N)$ can all be obtained in $O(\log N)$ Newton iterations. However, these iterations can be done with dynamically increasing precision, so that the asymptotic complexity is dominated by that for the last Newton step: a single polynomial multiply for polynomials of degree $O(N)$. One can achieve such by using a fast convolution algorithm for the polynomial multiplication, such as the Nussbaumer method [42], thus obtaining all the indicated ζ-values in $O(N \log N)$ operations. To summarize

Buhler recycling scheme, Algorithm 4, for $\zeta(0), \zeta(2), \zeta(4), \ldots, \zeta(2N-2)$ each to D-digit precision:

Operation complexity $O(\log N)$ per ζ value.

This estimate now has implications for various formulae, such as the Bernoulli-based series (32) and the Euler-Maclaurin method (29), as both depend on the values at even positive integers.

As for the more general recycling scheme of Algorithm 5, the complexity analysis can be found in [46], the essential idea being that the recombination of polynomials in Step (3) involves $N/2, N/4, N/8, \ldots$ pairwise polynomial-ratio combinations respectively on successive loop passes, and these are of growing degree, yet fast polynomial multiplication can be used, with the result that the complexity is $O(N \log^2 L)$ operations for the very construction of the g function as the ratio of two polynomials each of degree L. We conclude:

Psi-function recycling scheme, Algorithm 5, for $\gamma, \zeta(2), \zeta(3), \ldots, \zeta(L+1)$ each to D-digit precision (with $L \sim D$ also):

Operation complexity $O(L^{-1} N \log^2 L)$ per each of the L evaluations of ζ.

Note that for $L \sim N$, equivalently: one desires about D different ζ values each to D digits, the average cost is $O(\log^2 D)$ per value. This is somewhat worse than the cost of Algorithm 4, but certainly falls into the "fast algorithm" category: for both algorithms we could say that "polynomial rate" is achieved, meaning polynomial time complexity $O(\log^k D)$ as a per-evaluation average.

Next we look at the Euler-Maclaurin scheme. For precision 10^{-D} we can take $M = O(D/\log N)$ in the Bernoulli summation of series (29). But we have just estimated the operation complexity as $O(M \log M)$ for the generation of the relevant Bernoulli numbers. As general exponentiation is $O(\log^k D)$ operations for some k [29] [30], the work for first summation in the Euler-Maclaurin formula requires $O(N \log^k D)$ operations. Thus for any (fixed) complex s, we end up with operation complexity $O(N \log^k D) + O(D \log(D/\log N)/\log N)$, and we conclude:

Euler-Maclaurin formula (29), for s fixed, D-digit precision:

Operation complexity $O(D^{1+\varepsilon})$.

Of course, for integer s the Euler-Maclaurin method will—as with most other schemes—be somewhat more efficient.

For the Bernoulli series (32) to D-digit precision, we again apply the recycling of Buhler for $O(D/\log(1/\lambda))$ summands in the second sum, with $O(D/\lambda)$ summands in the first. This means we optimize the free parameter as: $\lambda \sim (\log\log D)/\log D$ and conclude:

Free-parameter formula (32), for s fixed, D-digit precision:

Operation complexity $O(D \log D / \log\log D)$.

This is of course also $O(D^{1+\varepsilon})$, but the analysis is particularly straightforward for the free-parameter formula, so we exhibit the detailed complexity. Note that the asymptotic decay of the free parameter λ is consistent with the hard constraint on the allowed range $0 \le \lambda < 2\pi$. Incidentally the "peeled series" approach, whereby one peels terms from a rational-ζ series, is in complexity terms very similar to the free-parameter series. Writing

$$\sum_{n=2}^{\infty} q_n(\zeta(n) - 1) = \sum_{m=2}^{M} \sum_{n=2}^{\infty} \frac{q_n}{m^s} + \sum_{n=2}^{\infty} q_n \zeta(n, M+1) \tag{67}$$

we see that if the last summation above is over $n \in [2, N]$ then for D-digit precision we require $N = O(D/\log M)$. If the (we presume closed-form) peeled terms are each of polynomial operation complexity, and we use recycling, we have overall cost $O(M \log^k D) + O(D \log D/\log M)$. If we set $M \sim D/\log^k D$ and $N \sim D/\log M$ we obtain:

General peeled-series form (67), for s fixed, D-digit precision:

Operation complexity $O(D^{1+\varepsilon})$.

Heretofore in this section we have concentrated on *operation* counts, whereby one takes each summand of a series to full precision. Also, s arguments have heretofore been general. But for certain series of our immediate interest, notably some old and new series for $\zeta(\text{odd})$, one can adroitly adjust precision so that very low *bit* complexity is achieved. Our first observation is that a modern series having rational summands, and exhibiting linear convergence can be evaluated to D good digits, for fixed integer argument s, in $N = O(D)$ summands. Thus the operation complexity is simply:

Rational-summand series, such as (61) and many others, as in Algorithms 1, 2 and 3 , for D-digit precision:

Operation complexity $O(D)$.

This is as good as any of the previous complexity estimates, except for the recycling cases (when the average, per-value complexity may be genuinely less than $O(D)$); furthermore the terms in the various series are generally simple in structure.

But now we wish momentarily to drop the notion of "operation complexity for D digits" and concentrate instead on *bit* complexity for, let us say, N-bit precision. In modern times there has been a revolution of sorts in the matter of bit-complexity estimates for ζ evaluation, or for that matter the evaluation of more general series. The idea is to combine subseries of a given, well-convergent series in certain, efficient ways, employing recursion relations and other algebraic expedients cleverly. We shall refer to this as the FEE (fast E-function evaluation) method of E. Karatsuba. The algorithm has sometimes been called "binary splitting," which was foreshadowed in the works of Schönhage and Brent [29] [30] [96] [20] for decimal-base conversion, calculation of fundamental constsnts and some elementary functions; yet was brought into powerful, general, and rigorous form by Karatsuba,resulting in unprecedented low bit complexity for hypergeometric series of algebraic parameters and argument (see [65] [68] [68] [67] [66] [64] [69], the reference [70] being especially informative).[2]

One way to think of the FEE method is to imagine, in the words of [58], pushing "as much multiplication work as possible to the region where multiplication becomes efficient." The complexity of the FEE method, when said method applies, turns out to be:

$$O(M(N)\log^2 N),$$

where $M(N)$ is either the bit-complexity of multiplying two integers each of N bits by grammar-school (naive, $O(N^2)$ means), or the bit complexity that is the lowest known. As for minimal-complexity multiplication, the celebrated Schönhage-Strassen bit-complexity bound, namely [96]:

$$M(N) = O(N \log N \log\log N),$$

thus yields a bit complexity for the FEE method in the form

$$O(N \log^3 N \log\log N),$$

for evaluation of appropriate series to N-bit precision, which bound can be thought of as $O(N^{1+\epsilon})$ and thus "near-optimal;" and we remind ourselves that this bound thus applies to a very wide class of series.[3] In this class are computations of certain constants such as ζ-values at odd positive integers, Euler's constant γ, powers e^x for bounded x, and generally to series whose k-th terms are rational, possessed of $O(\log k)$ bits in numerator and denominator; and yet more generally to hypergeometric series with suitably bounded algebraic argument and parameters [70].

[2]There is also a succinct and accessible modern treatment of such technique, by Haible and Papanikolaou [58], yet those authors unfortunately were unaware of the original works of Karatsuba. For reasons of scholarship therefore, we choose to refer to the general series-manipulation paradigm in question as the FEE method.

[3]Incidentally there is another multiplication algorithm enjoying the same bit complexity as Schönhage-Strassen; we speak of Nussbaumer convolution which is at least as easy to implement, as described in say [42] [50].

It should be remarked right off that the FEE method gives no gain whatsoever— over direct summation— if standard, grammar-school multiplication (of bit-complexity $O(NN')$ for two respective N, N'-bit operands) be used. To see this, consider a typical series to which the FEE method applies:

$$S = \sum_{n=0}^{\infty} \frac{a(n)}{b(n)} \prod_{j=0}^{n} \frac{p(j)}{q(j)},$$

where each of a, b, p, q is an integer-valued function of $O(\log n)$ bits, and assume (as is typically required for the FEE method) that a truncation error bound of 2^{-N}, for N-bit precision, obtains after $O(N)$ terms of the series. It is not hard to see that if each term be evaluated to N bits, we require under grammar-school multiplication $O(N \log j)$ bit operations per term, so that the summation of the required N terms has bit complexity $O(N^2 \log N)$. Thus if the grammar-school bound is used with FEE, the bit complexity is $O(M(N)\log^2 N) = O(N^2 \log^2 N)$ which amounts to no gain over conventional summation.

For the present compendium we have carefully chosen an illustrative FEE example. It is neither the simplest (perhaps the calculation of e or some such constant would qualify for that), nor is it the most recondite (one can even apply FEE to special functions of applied science, such as Bessel functions and so on). But the example shows the essential ingredients of FEE, and intentionally moves a little away from the above S form to underscore the possibility of algebraic-irrational arguments. Consider the polylogarithm evaluation

$$L = \mathrm{Li}_3(\tau^{-2}) = \sum_{n=1}^{\infty} \frac{\tau^{-2n}}{n^3},$$

where $\tau = (1+\sqrt{5})/2$ is the (patently algebraic) golden mean. This L constant is especially interesting because knowing it is essentially to know $\zeta(3)$, as we see discuss in Section 8. Now if we truncate the L series through the $(n = N)$-th term inclusive, we have at least N-bit precision, so let us for algorithmic convenience choose some suitable $N = 2^k$, and note first that

$$\sum_{n=1}^{N} \frac{\tau^{-2n}}{n^3} = \sum_{m=1}^{N/2} \tau^{2m-1} \frac{8m^3 + (8m^3 - 12m^2 + 6m - 1)\tau}{8m^3(2m-1)^3},$$

where we have pairwise combined terms from the left-hand sum, to forge a half-length sum with, in Karatsuba's words, "obvious denominators." Likewise, the right-hand sum can be pairwise processed to forge a yet shorter sum:

$$\sum_{p=1}^{N/4} \tau^{4p-3} \frac{A + B\tau}{C},$$

where A, B, C are more complicated polynomials in the index p; e.g., A, B now have degree 6. In general one obtains, as Karatsuba showed, a recurrence relation for ever more complicated numerator terms. In our case, one must use the quadratic reduction $\tau^2 = 1 + \tau$ to keep all numerators in $Z[\tau]$. Upon detailed analysis of the work to perform the pairwise combinations and so on, one finds that the bit complexity to perform $k = \lg N$ such series contractions—which work yields just*one* final term, a singleton summation—is a sum:

$$\sum_{j=1}^{k} \frac{N}{2^j} M(O(2^j \log N)) = O(M(N) \log^2 N)$$

for either grammar-school or minimal-complexity multiply, as claimed.

Let us perform an example of evaluation of the L constant through $N = 16$ summands. This means that we carry out four recursion levels, obtaining on the first level eight terms:

$$\{\tau\frac{8+\tau}{8}, \ldots, \tau^{15}\frac{4096+3375\tau}{13824000}\},$$

the sum over which eight being exactly the original 16-fold sum intended. At recursion bottom we end up with s solitary term, namely

$$L \sim \frac{842439095385706230219 - 376615379847138777145\sqrt{5}}{748737728234496000} \sim 0.4026839629\ldots,$$

where we have taken the liberty to cast the result in the form of a surd $(a + b\sqrt{5})/c$. The numerical value is incidentally correct to the ten places shown. To convey an idea of the efficiency of the method, we note that for $N = 32$ summands and so five recursion levels, the numerical value of the solitary surd is correct to 17 decimals, which makes sense because to jump from 16 to 32 summands we only have to do a little more than twice the multiplication work.

It is especially intriguing that the final result of such FEE processing is not only a single term, but an *exact* term in the sense that it could be used later in a truncated series of twice the length; i.e. the single term in hand can act as the left-hand term of a one-higher recursion level. Likewise, FEE is a *parallel* method in that separate processors can in principle handle separate pairings of terms at any recursion level.

We have merely sketched the technique in brief fashion. For the rigorous details of such applications of FEE, a good reference is [67], where the celebrated formula (61) for $\zeta(3)$ is used to establish the $O(M(N)\log^2 N)$ bit complexity for N-bit precision; and therein of course the numerator recursions are of pure-integer form.

As an example application of such techniques for very-high-precision work, in [58] the identity of Amdeberhan and Zeilberger [5]:

$$\zeta(3) = \frac{1}{2}\sum_{m=1}^{\infty} \frac{(-1)^{m-1}(205m^2 - 160m + 32)}{m^5 \binom{2m}{m}^5} \tag{68}$$

is noted, together with the (S-series) assignments: $a(n) = 205n^2 + 250n + 77$, $b(n) = 1$, $p(0) = 1$, $p(n) = -n^5$ for positive n, and $q(n) = 32(2n + 1)^5$.

In spite of Karatsuba's FEE and its wide applicability, there remain some interesting open questions. For example, note that one can in principle use FEE recursion, but *symbolically*, in the following sense. One recurses down only "half way," to render an original sum of N terms as a new sum of $O(\sqrt{N})$ terms, each new term now being rational-polynomial with each numerator and denominator having say $O(\sqrt{N})$ degree with integer coefficients. (In our above example for the L constant, just one level yields a degree-3 numerator, and we are saying one would continue the construction of higher-degree numerators but only to a certain depth.) Now it is known that a degree-d polynomial can be evaluated at $O(d)$ points in $O(d \log^2 d)$ operations with fast algorithms [42], so perhaps there is a compromise in some cases, between full FEE recursion and a mixed, symbolic-FEE-polynomial scheme. At the very least, these considerations lead out of the bit-complexity paradigm into a world in which $O(D^{1/2+\epsilon})$ *operation* complexity—meaning full-precision operations for every term—suffices for D good digits.

8 Curiosities and Open Questions

We end this treatise with a tour of some attractive curiosities from the annals of ζ function studies. We do this not only because of the allure of such oddities, but also because there may well be algorithmic consequences in the verification or application of various of our recollections and observations.

Let us first focus on the special case $\zeta(3)$, which number is for many reasons a kind of celebrity in the world of ζ evaluation. The Apéry proof of the irrationality of $\zeta(3)$ which invokes formula (61), is by now legendary [103]. But within what we might call the Apéry formalism, there are yet more interesting relations. If, like the present authors, one believes that polylogarithms of algebraic arguments are fundamental functions, then there is a "closed-form" expression for $\zeta(3)$ due to Landen [77] [78](6.13) namely:

$$\zeta(3) = \tfrac{5}{4}\mathrm{L}i_3(\tau^{-2}) + \tfrac{1}{6}\pi^2 \log\tau - \tfrac{5}{6}\log^3\tau,$$

where τ is as before the golden mean $(1+\sqrt{5})/2$, and the polylogarithm is standardly defined:

$$\mathrm{L}i_s(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^s}.$$

An equivalent form is the integral [78](6.14)

$$\zeta(3) = 10 \int_0^{\log \tau} t^2 \coth t \, dt,$$

with equivalence following from known polylogarithm relations [78]. An open question is whether, in view of the fact that there are coth expansions available, the $\mathrm{L}i_3$ form above can be computationally accelerated. Another byproduct of the Apéry formalism is the remarkable continued fraction:

$$\zeta(3) = \cfrac{6}{d(0) - \cfrac{1^6}{d(1) - \cfrac{2^6}{d(2) - \cfrac{3^6}{d(3) - \ddots}}}}$$

in which $d(n) = 34n^3 + 51n^2 + 27n + 5$. Such continued fractions can be used to prove irrationality, in yielding theoretical bounds on rational approximations of $\zeta(3)$, although Apéry's original proof and the accepted variants of same do not really concentrate on the fraction *per se* [103]. Complementary to the theoretical value of the continued fraction, there are intriguing computational questions. One should not rule out the continued fraction as a computational expedient. For one thing, the usual recurrence relations for the convergents p_n/q_n of the fraction need not consume $O(n)$ operations. Because the fraction above has polynomial forms for the elements, one may consider the application of fast polynomial evaluation methods. An open question is, just how efficient can such an evaluation approach be made?

Still on the topic of the illustrious $\zeta(3)$, D. Broadhurst [34] gave a remarkable formula, amounting to a

$$\zeta(3) = \frac{8}{7} \sum_{k=1}^{\infty} \frac{1}{k^3} \left(\frac{6a_k}{2^{\lfloor (k+1)/2 \rfloor}} + \frac{4b_k}{2^{\lfloor 3(k+1)/2 \rfloor}} \right),$$

$$\begin{aligned} \{a_k\} &= \{1, -7, -1, 10, -1, -7, 1, 0, \ldots\} \\ \{b_k\} &= \{1, 1, -1, -2, -1, 1, 1, 0\}. \end{aligned}$$

The Broadhurst formula is an extension of the discovery of Bailey, Borwein, and Plouffe [13], that numbers such as π and other constants can be cast in such periodic forms. The forms permit the determination of isolated digits—albeit in restricted bases. In this way, Broadhurst gives the hexadecimal digits, starting from the 10 millionth place (inclusive) of $\zeta(3)$, as: CDA01... It should be remarked that Broadhurst was also able to determine isolated digits of $\zeta(5)$ using a more complicated summation involving three periodic coefficient sequences. Open questions include this one: as all summands are rational and the terms decay geometrically in k, how best to adapt the Broadhurst series to the FEE method of Karatsuba, for example what should be the "obvious denominators" during series contractions?

It seems as if research on $\zeta(3)$ will never end. As just one example of new directions in this regard, Lan [76] recently proposed a possible avenue for proving $\zeta(3)$, or in fact any $\zeta(\text{odd})$ transcendental. His method involves the theory of certain cyclic fields, to arrive at a formula

$$\zeta(2k+1) = \zeta(2k)\frac{2q^{2k+1} - q^{2k} - q}{q^{2k+1} - 1}A_k(q),$$

where q is a prime and the A_k coefficient can be approximated via calculations in "tamely ramified cyclic fields.". The point is, if an A_k could be shown to be algebraic, then $\zeta(2k+1)$ is automatically shown transcendental.

Interdisciplinary appearances of $\zeta(\text{integer})$ can be amusing, attractive. In physics, because the so-called Planck radiation law has terms of the form $(e^x - 1)^{-1}$, the theory of "blackbody radiation" involves the integral (14) and perforce a ζ value. For example $\zeta(3), \zeta(4)$ thus become embedded in certain physical constants involving the theoretical rate at which a hot body radiates energy (in two, three dimensions respectively). Another amusing—and totally different—connection is in number theory, where asymptotic relations can involve $\zeta(\text{integer})$. Here is a well known such relation: the probability that two random integers be relatively prime is $1/\zeta(2)$. But sometimes one encounters a more obscure relation. For example, one has the result of [28] that, if n be a power of two, the number $\#(n)$ of solutions to $n = p + xy$ with p prime and x, y positive integers enjoys the asymptotic relation

$$\frac{\#(n)}{n} \sim \frac{105\zeta(3)}{2\pi^4}.$$

It is unclear how to attempt high-precision numerical verification of this peculiar result. One may calculate for example that $\#(2^{29}) = 382203245$, giving the poor approximation $\zeta(3) \sim 1.320...$ which is off the mark by ten per cent.

Next we mention a computational connection between ζ-values and the gamma function. One can derive intriguing limit relations for values at the odd positive integers, such as

$$\zeta(3) = \lim_{\varepsilon \to 0} \frac{1}{2\varepsilon^3} \log \frac{\Gamma^3(1+\varepsilon)\Gamma(1-\varepsilon)}{\Gamma(1+2\varepsilon)},$$

which shows that a fast algorithm for general Γ evaluation implies an analogous algorithm for $\zeta(3)$. This limiting Γ-formula can be derived from the aforementioned expansion (26) for the ψ function. Incidentally, in practice the actual error in this approximation to $\zeta(3)$ is just about 2ε. Conversely, the functional equation for the Riemann zeta function and duplication formula for the gamma function allow one to compute Γ as efficiently as ζ. We mention in passing that $\Gamma(n/24)$ for positive integers n may be computed with the same reduced complexity as $\pi = \Gamma(1/2)^2$ (see [24]), via elliptic integral evaluations.

One may use the recycling ideas of Algorithm 5 to deduce evaluations for specific arguments, for example:

$$\zeta(3) = -G(1,N)^3 - 3G(1,N)G(2,N) - 3G(3,N) + O(e^{-N}),$$

where we define the G-function as a finite sum:

$$G(s,N) = \sum_{k=1}^{4N} \frac{(-N)^k}{k!\,k^s}.$$

In fact, $\zeta(2n+1)$ for any positive integer n can be expressed in terms of similar series [67] [66]. It is intriguing that this approach yields so simply to the FEE method Karatsuba: the rational G coefficients are so very simple, the summation limit on G can conveniently be made a power of two, and so on.

As for interesting interrelations involving general s we note the formulae of Landau:

$$\frac{1}{s-1} = \sum_{n=0}^{\infty} \binom{s+n-1}{n-1} \frac{\zeta(s+n)-1}{n}$$

and of Ramaswami:

$$(1-2^{1-s})\zeta(s) = \sum_{n=1}^{\infty} \binom{s+n-1}{n} \zeta(s+n).$$

Remarkably, either formula is valid for all complex s; each one may be used to define the complete analytic continuation of ζ [100]. We present them here on the idea that perhaps they have computational value. The Landau formula may possibly be used to accelerate other rational ζ-series we have encountered.

An intriguing formula of quite a different character is the following remarkable, van der Pol integral representation, valid on the (open) critical strip, which representation amounts to a complete Fourier decomposition of $\zeta(s)/s$:

$$\zeta(s) = s \int_{-\infty}^{\infty} e^{-\sigma\omega}(\lfloor e^{\omega} \rfloor - e^{\omega}) e^{-i\omega t} \, d\omega.$$

where $s = \sigma + it$, and $\Re(s) \in (0, 1)$. (Actually, the representation can be extended to the half-plane $\Re(s) > 0$ by integrating only over $(0, \infty)$ and adding back a pole term $s/(s-1)$ on the right-hand side.) The representation is especially intriguing for the Riemann critical line, that is for $\sigma = 1/2$. This Fourier approach was actually used fifty years ago by van der Pol, who went so far as to construct an electronic circuit to estimate—in what is called analog fashion—the critical behavior of the Riemann zeta function [11] [102]. An open computational question is: can discrete fast Fourier transform methods be efficiently used to estimate the Fourier integral? Of course one cannot rule out possible convergent schemes arising from theoretical manipulations *per se* of the van der Pol integral representation. One connection between the van der Pol representation and our rational ζ-series runs as follows. One of the known asymptotic relations for ζ on the Riemann critical line is [100]:

$$\int_{-T}^{T} |\zeta(1/2 + it)|^2 dt \sim 2T \log T.$$

But we can say something similar by appeal to the Fourier integral above. What might be called the "signal power" relevant to the van der Pol decomposition is:

$$\begin{aligned} P = \int_{-\infty}^{\infty} \left| \frac{\zeta(1/2 + it)}{1/2 + it} \right|^2 dt &= 2\pi \int_{-\infty}^{\infty} e^{-\omega}(\lfloor e^{\omega} \rfloor - e^{\omega})^2 \, d\omega \\ &= 4\pi \left\{ \frac{3}{2} - \log 2 - \sum_{m=2}^{\infty} \frac{\zeta(m) - 1}{(-1)^m (m+1)} \right\} \qquad (69) \end{aligned}$$

This last relation can be shown via the substitution $\omega \mapsto \log R$ in the power integral, then partitioning the R domain into intervals $[n, n+1)$. At any rate, we have come full circle back to a ζ-series, and provided at least one means for numerical evaluation of the power integral on the critical line. Indeed the ζ-series (69) admits of exact evaluation, as in relation (45), yielding the exact signal power value:

$$P = 2\pi(\log 2\pi - \gamma) = 7.920969195282313657947\ldots.$$

It is likewise intriguing that the Riemann hypothesis can be formulated in terms of the collection of ζ-values at the even positive integers. There is the theorem of Riesz, that the Riemann hypothesis is equivalent to the following big-O behavior of a certain, peculiar *Riesz function* R [100]:

$$R(x) = \sum_{n=1}^{\infty} \frac{(-x)^n}{\zeta(2n)(n-1)!} = O(x^{1/4+\varepsilon}).$$

Alternatively the Riemann hypothesis is equivalent to a different big-O condition of Hardy and Littlewood [100]:

$$\sum_{n=1}^{\infty} \frac{(-x)^n}{\zeta(2n+1)n!} = O(x^{-1/4}),$$

It is unclear whether there be any computational value whatsoever to these equivalencies, especially as the big-O statement is involved and therefore infinite computational complexity is implicit, at least on the face of it. Still, if there be any reason to evaluate such sums numerically, the aforementioned methods for recycling of $\zeta(\text{even})$ or $\zeta(\text{odd})$ values would come into play.

Predating the Riesz function is the Riemann function defined by (5), together with its fascinating connection with the distribution of prime numbers. What makes such connections yet more compelling from a practical viewpoint is that various computational expedients exist for accelerating certain evaluations. For example we have the *Gram formula* (see [94] for a derivation) as:

$$\mathrm{Ri}(x) = 1 + \sum_{n=1}^{\infty} \frac{(\log x)^n}{n\zeta(n+1)n!}, \tag{70}$$

whose very form may provide additional motivation for performing recycled computations of ζ-values at positive integer arguments.

We should mention an interesting new foray into the world of asymptotic equivalencies for the Riemann hypothesis: an application of the so-called Carleman continuation problem, described in a treatment due to Aizenberg et al. [2]. Let us paraphrase here the authors' proposition, that the Riemann Hypothesis is true if and only if we have the (large-n) behavior:

$$\limsup_n |a_n^-|^{1/n} = \limsup_n |a_n^+|^{1/n} = 1,$$

where

$$a_n^{\pm} = \int_{(1\pm 1)/4}^{(3\pm 1)/4} \left(\frac{(z^2-1)i \pm 2z\cos 2\pi x}{1+z^2 \pm 2z \sin 2\pi x} \right)^n \frac{dx}{\zeta(x)},$$

where $0 < z < 1$ is otherwise unrestricted. It is possible to take the power n as high as $N = 10^{20}$, for which the authors find

$$|a_N^-|^{1/N} \sim 0.99999999999999999999956\ldots,$$

$$|a_N^+|^{1/N} \sim 0.99999999999999999982\ldots$$

It is not yet known what is a proper scale in this asymptotic behavior; that is whether such numerical results imply compelling bounds on locations of critical zeros.

More recent, but in the same general vein of integral equivalencies, is a theorem [10], to the effect that the Riemann hypothesis is true if and only if the integral

$$I = \int \frac{\log|\zeta(s)|}{|s|^2} dt,$$

taken along the critical line $s = 1/2 + it$, vanishes. This would perhaps not be so compelling if it were not for the exact expression those authors derived for the above integral, namely a sum formula:

$$I = 2\pi \sum_{\Re(\rho) > 1/2} \log\left|\frac{\rho}{1-\rho}\right|,$$

where ρ denotes any zero in the critical strip, but to the *right* of the critical line as indicated, counting multiplicity. It is interesting to plot the defining I integral for ever-increasing integration limits, say, and witness a slow but chaotic tendency toward $I = 0$. For example, the approximation

$$I(T) = \int_{t=0}^{T} \frac{\log|\zeta(1/2+it)|}{1/4+t^2} dt$$

appears to oscillate between about 10^{-9} and 10^{-6} in the vicinity of $T \sim 1000$. One interesting question is: even if the Riemann hypothesis be true, what is a valid positive α such that

$$I(T) = O(T^{-\alpha}) \quad ?$$

On the basis of preliminary numerical evidence (the aforementioned $T \sim 1000$ data) we are moved to conjecture that $\alpha = 2$ is admissible. It is intriguing that such a numerically-motivated statement about a positive α is *stronger* than the Riemann hypothesis. Moreover, the sum formula for I could conceivably be used to infer bounds on possible violations of the Riemann hypothesis. For example, here is another interesting question: what could be inferred from sheer computation and the sum formula if one assumed the existence of a *single* errant zero $(\sigma_1 > 1/2) + i(t_1 > 0)$ and its redundant reflections?

Also recent is the tantalizing result of [91], to the effect that the Riemann hypothesis is equivalent to a positivity condition on the ξ function defined in (16), which condition applies at a *single* point $s = 1/2$ as:

$$\frac{d^n\xi}{ds^n}\left(\frac{1}{2}\right) > 0,$$

for every $n = 2, 4, 6, \ldots$. This brings up an interesting computational exercise; namely, to provide numerical values for a great number of such derivatives. It is nontrivial even to produce the first few, which we list here (to unguaranteed, but suspected implied precision):

$$\frac{d^2\xi}{ds^2}\left(\frac{1}{2}\right) = 0.022971944315145437535249\ldots,$$
$$\frac{d^4\xi}{ds^4}\left(\frac{1}{2}\right) = 0.002962848433687632165368\ldots,$$
$$\frac{d^6\xi}{ds^6}\left(\frac{1}{2}\right) = 0.000599295946597579491843\ldots,$$

with the 18-th derivative being of order 2×10^{-6}, and so on. Some possible, numerically-motivated conjectures are that the sequence of such derivatives is monotone decreasing, but that the successive ratios of the $(2m+1)$-th over the $(2m)$-th are monotone increasing. Note that various of our convergent series for ζ admit of internal differentiation. For example, one might invoke either series (30) or (32) and differentiate with respect to s inside the summations. This will entail derivatives of the incomplete gamma function; thus if one uses the integral representation following series 30, powers of logarithms of the integration variable will appear in the formalism, yet we know from the works of Karatsuba (see [68] for example) how to calculate such log-power integrals rapidly from series. What may also work is the differentiation of a sufficiently deep rational polynomial expression as such arises from the continued fraction formalism for incomplete gamma. It goes without saying that if a single negative $(2m)$-th derivative could be found—say to within rigorously bounded numerical error—then the Riemann hypothesis would perforce be broken.

Seemingly reminiscent results in recent times are that of Li [79] [19] to the effect that the Riemann hypothesis is equivalent to the positivity property:

$$\lambda_n = \sum_\rho \left(1 - \left(1 - \frac{1}{\rho}\right)^n\right) > 0$$

holding for each $n = 1, 2, 3, \ldots$, with the sum over critical-strip zeros being interpreted in the usual limit sense. Interestingly, the λ_n constants can be cast in terms of derivatives of $\log \xi(s)$, but this time all such evaluated at $s = 1$. Yet another criterion equivalent to the Riemann hypothesis is that of Lagarias [74]:

$$\Re\left(\frac{\xi'(s)}{\xi(s)}\right) > 0$$

whenever $\Re(s) > 1/2$. Furthermore it may well be that the infimum of the real part always occurs for a given $\Re(s)$ at $\Re(s) + 0i$, that is on the real axis.

We close this somewhat recreational section with "interdisciplinary" observations, some highly speculative but some revealing connections between ζ-function theory and other scientific fields.

Let us briefly touch upon experiments that have been performed in the matter of "listening" to the Riemann ζ function, by which we mean hearing a sound signal created as the real part of $\zeta(\sigma + it)$, with imaginary part t taken to be time. One can easily hear qualitative differences between sounds for say $\sigma = 0, 1/2, 1$ and so on. We expect this on the basis of differing growth behavior of ζ along these lines of the s-plane. An heuristic can be forwarded [42], to the effect that along the critical line $\sigma = 1/2$ the resulting sound is "whitest" in the sense of white (flat) spectrum. One can argue that, in view of the formal sum:

$$\zeta(\sigma + it) = \sum_{n=1}^{\infty} \frac{e^{-it \log n}}{n^{\sigma}},$$

the ζ function is a certain superposition of oscillators, with a scaling law that comes down to the estimate

$$P(\omega) \sim e^{-\omega(2\sigma - 1)}$$

for the power present at frequency ω. Indeed if this formula be continued—shall we say heuristically—over to the critical strip, the power spectrum would be white on the critical line. Actually, when one "hears" the critical-line signal, it is not random noise as we know it, but the signal does sound like a roughly equal-strength mix of many oscillators. To achieve rigor in these heuristics, one would have to analyze integrals such as (for large T):

$$\frac{1}{T} \int_{-T/2}^{T/2} \zeta(1/2 + it) e^{-i\omega t} dt,$$

whose absolute square is essentially the power $P(\omega)$. Due to the existence of such as the van der Pol integral representation earlier in this section, such delicate spectral analysis may well be possible (and may have been performed elsewhere, unbeknownst to the present authors).

More serious (less recreational) is the Hilbert-Pólya conjecture, saying in essence that the behavior of the Riemann zeta function on the critical line $\Re(s) = 1/2$ depends somehow on a mysterious (complex) Hermitian operator, of which the critical zeros would be eigenvalues. There is interesting literature, of both theoretical and computational flavors, in this regard. In particular, the pioneering work of Montgomery and Dyson [84] on the statistical correlations amongst consecutive critical zeros now has numerical supporting evidence; and it is widely conjectured that the mysterious Hilbert-Pólya operator is of the GUE (Gaussian unitary ensemble) class. A relevant n-by-n matrix G in such a theory has $G_{aa} = x_{aa}\sqrt{2}$ and for $a > b$, $G_{ab} = x_{ab} + iy_{ab}$, together with the Hermiticity condition $G_{ab} = G^*_{ba}$; where every x_{ab}, y_{ab} is a Gaussian random variable with unit variance, mean zero. The computations of Odlyzko [83] [85] show that the statistics of consecutive critical zeros are in many ways equivalent—experimentally speaking—to the theoretical distribution of eigenvalues of a large such matrix G. (Actually, there is evidence that a more refined class, namely that of unitary symplectic operators, may be more reasonable as the basis of such conjectures [95].) In these connections, a great deal of fascinating work—by M. V. Berry and colleagues—under the rubric of "quantum chaology" has arisen [17] [16]. In some of this work [16], there even appears an asymptotic expansion, reminiscent of the Riemann-Siegel expansion, motivated by semiclassical ideas yet suitable perhaps for high-accuracy calculations on the critical line.

In another connection with quantum chaology, A. Connes [41] has recently given a spectral interpretation of the critical zeros, as comprising an "absorption spectrum," with noncritical zeros appearing as "resonances." His work connects quantum chaology, algebraic geometry and field theory, yielding interesting equivalent forms of the Riemann hypothesis. There has also appeared an actual, claimed proof of the Riemann hypotheses by de Branges [27], although the present authors are at the time of this writing unaware of any confirmation of that proof.

It is intriguing that many of the various new expansion and associated observations relevant to the critical zeros arise from the field of quantum theory, feeding back, as it were, into the study of the Riemann zeta function. But the feedback of which we speak can move in the other direction, as techniques attendant on the Riemann ζ apply to quantum studies. There is the so-called "quantum zeta function," which is a sum (when it exists)

$$z(s) = \sum_n \frac{1}{{E_n}^s}$$

over eigenvalues $\{E_0, E_1, \ldots\}$ of a specified quantum system. For such as the quantum oscillator with potential x^2, so that energies are evenly spaced, the quantum z is essentially a scaled form of the Riemann ζ. But—and this is quite the fascinating thing—it turns out that for some quantum systems and certain s, we can evaluate $z(s)$ exactly, even when not a *single* eigenvalue E_n be known. Voros [104] showed that for the so-called power-law oscillator, in which the system potential is x^m for an integer $m > 0$, one has the exact evaluation:

$$z(1) = \left(\frac{2}{(m+2)^2}\right)^{m/(m+2)} \frac{\Gamma^2(\frac{2}{m+2})\Gamma(\frac{3}{m+2})}{\Gamma(\frac{4}{m+2})\Gamma(\frac{m+1}{m+2})} \left(1 + \sec\frac{2\pi}{m+2}\right).$$

Later, Crandall [48] showed that this relation holds for an arbitrary power-law (i.e. $m > 0$ need only be real), and conjectured that this relation for $z(1)$ is correct as an analytic continuation in some scenarios for which the literal sum $\sum 1/E_n$ diverges. This is very much like the fact of $\zeta(0) = -1/2$ even though the literal Riemann sum is, of course, divergent at $s = 0$. The point is, machinery developed over the years on behalf of the Riemann ζ may well apply to the problem of evaluating the quantum z. What is more, the *zeros* of $z(s)$ may signal, by way of their distribution, the level of quantum chaos inherent to the system. For this intriguing connection, see [48] and references therein.

But in a somewhat different vein there is a precise—in nature neither statistical nor asymptotic—connection between quantum-theoretical operators and the critical zeros. In 1991 it was observed by Crandall [44] that, in the standard formulation of quantum theory there exists a wave function (smooth, devoid of zeros) which, after a finite evolution time under an harmonic-oscillator Schroedinger equation, possesses infinitely many zeros; furthermore these zeros coincide precisely with the Riemann critical zeros. Specifically, define an initial wave function

$$\psi(x,0) = 2\pi \sum_{n=1}^{\infty} n^2 \exp(-\pi n^2 e^{2|x|})(2\pi n^2 e^{9|x|/2} - 3e^{5|x|/2}),$$

which appears in the standard theory of the critical zeros [100] [83], and amounts to the Fourier transform of the Ξ function defined in (18). When plotted graphically this initial wave function looks essentially like a "bell curve," certainly innocent, if you will, on casual inspection. However, evolution of a wave function $\psi(x,\tau)$ under a Schroedinger oscillator equation (where a is any positive real constant):

$$i\frac{\partial \psi}{\partial \tau} = -\frac{1}{a^2}\frac{\partial^2 \psi}{\partial x^2} + a^2 x^2 \psi$$

for a precise time interval $0 \le \tau \le \pi/4$ yields a very complicated wave function $\psi(x, \pi/4)$ whose zeros on the x-axis are the zeros of $\zeta(1/2 + ix)$, said zeros being therefore infinite in number. All of this is not hard to show from standard ζ function theory [100] and the theory of quantum harmonic oscillators. For within the latter formalism one can show that after one-quarter of a classical period of the oscillator evolution, a wave packet becomes essentially its own Fourier transform. However, one also knows that basis expansions of wave functions can be useful, so we might contemplate an eigenfunction expansion:

$$\psi(x/a, 0) = \sum_{n=2}^{\infty} c_n H_{2n}(x) \exp(-x^2/2),$$

where H_k denotes the Hermite polynomial of degree k, with the coefficients c_n computable in terms of the initial wave packet, via:

$$c_n = \frac{\sqrt{\pi}}{2^{2m-1}(2m)!} \int_0^{\infty} \psi(x/a, 0) H_{2m}(x) \exp(-x^2/2)\, dx,$$

with the parameter a free to be chosen for computational efficency ($a = 4$ is a good choice in practice, as below). The result of quantum evolution of a Hermite-basis expansion is particularly simple, and we obtain:

$$\Xi(x) = f(x)\zeta(\tfrac{1}{2} + ix) = a^{-1}\sqrt{2\pi} \exp(-x^2/(2a^2)) \sum_{n=0}^{\infty} c_n (-1)^n H_{2n}(x/a), \tag{71}$$

where we recall, as in the definition (18), that the function $\Xi(x) = f(x)\zeta(1/2 + ix)$ where f has no real zeros. It is a fascinating thing that the Hermite expansion of the initial wave function only needs these alternating $(-1)^n$ factors to change from a simple-looking wave packet to one with all the complications relevant to the critical line. These observations, albeit recreational, are not entirely specious. For one can perform an actual experiment, taking $a = 4$ and the sum in (71) to say $n = N = 27$ inclusive. In this way there will be 28 of the c coefficients—obtained via numerical integration of the initial packet—and we end up with a degree-54 polynomial in x as an approximation to $\Xi(x)$. This stated experiment yields the specific approximation:

$$\begin{aligned}\Xi(x) \quad \sim \quad & \exp(-x^2/32)(0.497120778225837245 + 0.00404905216049614136 x^2 \\ & + 0.00000725014346774865092 x^4 \cdots - 1.39799726436057536 \cdot 10^{-71} x^{54}),\end{aligned}$$

and real zeros of this degree-54 polynomial are located at 14.13472514, 21.022039, 25.01086, 30.4248, 32.93, 37.6, 40.9, and their negatives, where we have indicated the good digits in comparison with established critical zeros—i.e., only good digits have been provided. Incidentally, one does not forget that the degree-54 polynomial must have 54 complex zeros. It turns out that the 40 zeros remaining all have significant imaginary argument. The general picture seems to be this: if one adopts a large-degree-N polynomial, and plots its zeros on the complex ($s = 1/2 + ix$)-plane, then some number—increasing somehow with N itself—of said zeros lie on the critical line, the rest forming a kind of oval that circumscribes the collection of these real zeros. If the Riemann hypothesis were to be cast in terms of the asymptotic behavior of the zeros of the polynomial

$$\sum_{n=0}^{N} c_n (-1)^n H_{2n}(x/a),$$

the relevant statement would have to involve the eventual expulsion of all the nonreal zeros, away from, in some appropriate asymptotic sense, the Riemann critical strip. It is likewise intriguing that, as with any polynomial-root problem, the relevant zeros can in principle be described as eigenvalues of a Hessenberg matrix involving the polynomial coefficients.

Incidentally Hermite polynomials figure into the theory of the Riemann zeta function in at least three other ways. They figure into the Berry-Keating expansion, which we have said is an alternative to the Riemann-Siegel formula [16]. The polynomials have also been used in Motohashi's spectral theory pertinent to ζ [82]. Recently, Bump et al. have analyzed a "local Riemann hyopthesis" into which theory the zeros of Mellin transforms of orthogonal polynomials—including the Hermite variety—figure strongly [38].

Recreational aspects aside, an open issue is whether there is any computational benefit here. We observe that even though a differential equation would be solved numerically, there exist a great many techniques for value recycling—including fast Fourier transform analysis of the Schroedinger equation—in this case meaning simultaneous computation of many wave function values at once. And there is yet another intriguing, interdisciplinary connection. There has been some research on whether solutions to differential equations need be computable. Indeed in [90] it is shown that one can have computable boundary conditions and yet suffer from incomputable solutions. In turn, one recalls Bombieri's suggestion that the Riemann ζ on the critical line is not computable in polynomial (in $\log t$) time. This is all speculative, yes, but speculation has been a common activity over the long history of the Riemann zeta function.

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