From: Philippe.Flajolet@inria.fr
To: Linas Vepstas (linas@lians.org)
Subject: Differences of Zeta values
Date: January 6, 2006 $\rightsquigarrow$ Sun Jan 8 18:31:59 CET 2006

Dear Linas,

While googling around, I discovered earlier this year your startling note on the web:

> "*A series representation for the Riemann Zeta derived from the Gauss-Kuzmin-Wirsing Operator* is a less rambling, more tightly focused extract of the above, meant for publication."

As a matter of fact, I have a keen interest in difference calculus, special functions, summations, and such; see my web page easily found from Google: flajolet. In the context of the present discussion, you may also find some relevant work in my join paper with Brigitte Vallée:

> *Continued Fractions, Comparison Algorithms, and Fine Structure Constants.*

(The other earlier paper with a somewhat similar looking title is more introductory and less focussed on today's discussion: I believe these two papers paper and the earlier paper by Daudé-Flajolet-Vallée are related to the first part of your note and "behind" Keith Briggs' own notes on the subject, but I haven't had time to think much about these aspects in detail.)

I think I can prove a quantitative version of your conjectures relative to the asymptotic behaviour of finite differences of the Riemann zeta function. Perhaps, if you are interested, your calculations and empirical data could well be merged with my asymptotics, and we could then consider a joint submission to a journal like *Experimental Mathematics* or the *Ramanujan Journal*, or something similar. Else, no problem: I'll probably try to publish somewhere a suitably edited version of the quick note that follows.

I have enjoyed spending a few nights on your sequence, and, although I encountered a few unexpected difficulties, I am quite thrilled by your observations regarding differences of zeta values and their curious properties.

A happy new year to you,

Laimingų Naujųjų Metų!

Philippe

ASYMPTOTICS OF DIFFERENCES OF THE ZETA FUNCTION

Philippe Flajolet, January 6, 2005

§1. Introduction In web notes, Linas Vepstas considers the Newton series expansion of the Riemann zeta function. This leads him to investigate the finite differences of zeta values, taken here in the form:

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

Let H_n be the harmonic number $H_n := 1 + \frac{1}{2} + \cdots + \frac{1}{n}$ and let γ be Euler's constant. Amongst the striking observations made by Vepstas, we find (upon slightly rephrasing his numerical results) a collection of near identities. For instance, one has to more than 35D:

(1)
$$\left\{ \begin{array}{rcl} S(499) - H_{499} + 1 & = & 0.57\underline{\mathbf{8}}21\,56649\,01532\,86060\,65120\,90082\,40243\ldots \\ \gamma & = & 0.57\underline{\mathbf{7}}21\,56649\,01532\,86060\,65120\,90082\,40243\ldots, \end{array} \right.$$

where the sole discrepancy observed[1] is in the third decimal digit:

$$\gamma + \frac{1}{1000} \doteq -S(499).$$

Thus, Euler's constant γ appears to be expressible (to the stated precision at least) as a $\mathbb{Q}$-linear combination of 1 and the zeta values $\zeta(2), \ldots, \zeta(500)$. (Throughout this paper $\zeta(s) = \sum 1/n^s$ denotes the Riemann zeta function.)

Precisely, Vepstas investigates the Newton series expansion of a mildly regularized version of the zeta function. He takes as a starting point

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

The singularity at $s = 1$ has been eliminated, but, strangely enough, a new singularity at 0 is introduced[2]. By substituting $s = 1, 2, \ldots$ and solving successively for the t_n, we find

$$t_n = S(n) - H_n + 1 - \gamma.$$

Then, Vepstas goes on with a detailed numerical analysis of t_n, from which a clear numerical approximation emerges:

$$t_n \doteq \frac{1}{2(n+1)}.$$

The surprise is that the difference betwen the two terms above is extraordinarily small, and this "explains" (1), provided, of course, we can quantify the amount of smallness.

§2. The basic integral representation. Making use of the classical Nörlund-Rice complex integral representation of nth differences of an analytic function, we have

$$S(n) = (-1)^n \frac{n!}{2i\pi} \int_{1/2-i\infty}^{1/2+i\infty} \frac{\zeta(1+s)}{1+s} \, \frac{ds}{s(s-1)\cdots(s-n)}. \tag{2}$$

The direct verification by residues is easy: there is a pole at each $s = k$ (for $k \in [2\,..\,n]$), whose residue generates both $\binom{n}{k}$, the alternating sign, and a zeta value.

Equation (2) is the keystone of our analysis. First, we move the integration line to the left: poles at $s = 0$ and $s = -1$ are encountered. The residues of the double pole at $s = 0$ is

$$-H_n + 1 - \gamma,$$

[1] We use $\doteq$ in the loose sense of "numerically close"

[2] In the perspective of the present note, it'd be neater to operate directly with the *standard* Newton series of $\zeta(s) - 1/(s-1) - \gamma$. Changes are essentially notational.

while the residue at the simple pole $s=-1$ appears to be exactly

$$-\frac{1}{2(n+1)}.$$

Thus, we have

$$S(n)+\gamma-H_n+1-\frac{1}{2(n+1)}=I(n), \tag{3}$$

where $I(n)$, our main object of study from now on, is

$$I(n):=(-1)^n\frac{n!}{2i\pi}\int_{-3/2-i\infty}^{-3/2+i\infty}\frac{\zeta(1+s)}{1+s}\,\frac{ds}{s(s-1)\cdots(s-n)}. \tag{4}$$

(The integral $I(n)$ is what Vepstas denotes by a_n.)

§3. Numerical data. Experimentally, the quantity $I(n)$ exhibits two startling features. First, it is small, despite the fact that, in its definition, binomial coefficients can be almost as large as 2^n. Here is a table exemplifying smallness for some values of n:

(5)

$I(10)$	$I(20)$	$I(50)$	$I(100)$
$-0.11634\cdot 10^{-5}$	$-0.36536\cdot 10^{-8}$	$-0.34851\cdot 10^{-13}$	$-0.73084\cdot 10^{-17}$.

A rough fit proposed by Vepstas for the order of magnitude is of the form $e^{K\sqrt{n}}$.

Second, closer investigation of numerical values of the $I(n)$ reveals that they oscillate. For instance, there are sign changes after the following values of n:

$$1,\ 5,\ 11,\ 19,\ 27,\ 38,\ 50,\ 63,\ 78,\ 95,\ldots.$$

The sequence of sign changes was investigated with great precision by Vepstas who obtains an excellent fit with a quadratic function.

The last two observations, pushed till values of $n=2,000$, led Vepstas to conjecture for $I(n)$ the rough asymptotic formula:

$$I(n)\overset{??}{\approx}\exp\left(-3.6\sqrt{n+1}-3\right)\cdot\sin\pi\left(\sqrt{\frac{4}{\pi}(n-1.97)+\frac{289}{256}}-\frac{1}{16}\right), \tag{6}$$

though, in his words, "*a more precise fit is strangely difficult*". We are going to see that the *shape* conjectured by Vepstas is correct, though the actual values of the constants require modifications.

§4. The functional equation of ζ: main integral representation. The asymptotic behaviour of a Nörlund-Rice integral is usually dictated[3] by singularities in left half-planes. Here, no singularities are present to the left of $s=-1$. In such a case, the next recourse is often the saddle point method[4].

Greater clarity is obtained if values of s are brought back to a right half-plane, which corresponds to the change of variables $s\mapsto -s$. The factor $\zeta(1-s)$ calls for making use of the functional equation of the Riemann ζ function:

$$\zeta(1-s)=(2\pi)^{-s}2\cos\left(\frac{s\pi}{2}\right)\Gamma(s)\zeta(s).$$

[3]See, e.g., Flajolet-Sedgewick on Mellin & Rice.

[4]For another (simpler) isntance of such a situation, see Flajolet-Gerhold-Salvy, in preparation.

(Similar techniques serve in the elementary transformation theory of modular functions.) We then get the following alternative form of (4):

$$I(n) = \frac{n!}{2i\pi} \int_{3/2-i\infty}^{3/2+i\infty} \frac{\zeta(s)}{1-s} (2\pi)^{-s} 2\cos\left(\frac{s\pi}{2}\right) \Gamma(s) \frac{ds}{s(s+1)\cdots(s+n)}. \tag{7}$$

There the $(-1)^n$ factor has nicely disappeared.

§5. A crude saddle-point approximate model. A simplified version of the integrand, namely

$$\frac{1}{1-s}(2\pi)^{-s}\frac{\Gamma(s)}{s(s+1)\cdots(s+n)}$$

has its modulus that is infinite both at $s=1^+$ and at $+\infty$, with a minimum near $\sigma_0(n)=\sqrt{2\pi n}$. This suggests the possibility of integrating along the transverse line $\Re(s)=\sigma_0(n)$ and, at first, looks promising since then an estimate of the rough form

$$e^{K\sqrt{n}}\sin(L\sqrt{n}),$$

would result, with the cosine factor providing the desired oscillations. However, a quick numerical evaluation of the integrand at $\sigma_0(n)$ shows that it is "too small". when compared to the values of (5): the exponents implied by this heuristic turn out to be systematically about 1.5 times their actual values.

The preceding discussion still suggests that the scale of the geometry is according to the quantity $\sqrt{n}$, but now, the possibility of nonreal saddle points should be envisioned.

Let us re-examine the integral (7) when s lies in the upper plane $\Im(s)>0$. There, up to exponentially small terms, we can simplify the cosine:

$$2\cos\frac{\pi s}{2} = \exp\left(-i\frac{\pi}{2}s\right) + O\left(e^{-i\pi s/2}\right).$$

Next, we know that Stirling's formula is valid in the complete half-plane $\Re(s)>0$ (and even beyond!). Also, as $\Re(s)\to+\infty$, the zeta function is almost 1:

$$\zeta(s) = 1 + O\left(2^{-\Re(s)}\right).$$

Finally, experience teaches us that, in saddle point calulations, rational factors like $(1-s)^{-1}$ only introduce minor perturbations that can be accommodated *after* the main saddle point has been determined. Consequently, we examine the following function

$$\phi(s) = -s\log(2\pi) - i\frac{\pi s}{2} + \log\Gamma(s) + \log\frac{\Gamma(s)}{\Gamma(s+n+1)}. \tag{8}$$

This function is meant to be a fair approximation of the logarithm of the integrand of (7), when both $\Re(s)$ and $\Im(s)$ tend to infinity, with $\Im(s)\geq 0$.

In the regime

$$s = x\sqrt{n},$$

we can avail ourselves of Stirling's formula and the corresponding asymptotic approximation of the ψ function:

$$\psi(s) := \frac{d}{ds}\log\Gamma(s) \sim \log s - \frac{1}{2s} - \frac{1}{12s^2} + O(s^{-3}), \qquad s\to\infty.$$

Then, it is found[5] that

$$\phi'(x\sqrt{n}) = \left[-\log(2\pi) - i\frac{\pi}{2} + 2\log x\right] - \left(x + \frac{1}{x}\right)\frac{1}{\sqrt{n}} + O(n^{-1}). \tag{9}$$

Observe also that, at $s = x\sqrt{n}$, one has

$$\begin{aligned}\log\left(n!\phi(x\sqrt{n})\right) &= \sqrt{n}\left[2x\log x - 2x - x\log(2\pi) - \frac{1}{2}i\pi x\right] \\ &\quad - \log(x) - \log\sqrt{n} + \log(2\pi) - \frac{1}{2}x^2 + O(n^{-1/2}).\end{aligned} \tag{10}$$

This leads us to choose as an approximation to the saddle point the quantity

$$\sigma(n) = e^{i\pi/4}\sqrt{2\pi n} = (1+i)\sqrt{\pi n}.$$

Define

$$\eta(s) := n!\frac{\zeta(s)}{1-s}(2\pi)^{-s}2\cos\left(\frac{s\pi}{2}\right)\Gamma(s)\,\frac{ds}{s(s+1)\cdots(s+n)}, \tag{11}$$

which is the integrand of (7). A plot of the values of the ratio

$$\rho_1(n) := \left|\frac{\eta(\sigma(n))}{I(n))}\right| \tag{12}$$

in Figure 1 [left] exhibits spikes, corresponding to sign changes of $I(n)$: this indicates that we do not "catch the phase" by the crude approximation $|\eta(\sigma(n))|$. However, when the ratio is ceiled by 2.5, as in Figure 1 [right], we are led to optimism: the approximation does appear to capture the exponential decay of $I(n)$ in the form of the approximation

$$\exp\left(-2\sqrt{\pi n}\right) \doteq \exp\left(-3.54490\sqrt{n}\right).$$

Note that the coefficient $2\sqrt{\pi} \doteq -3.54490$ is close to the empirically estimated value of 3.6 in (6). Another encouraging fact is that our current crude estimate is consistent with the prediction of the fluctuations in (6), since it corresponds to an oscillating factor of the form

$$\sin\left(2\sqrt{\pi n} + O(1)\right).$$

§6. The actual saddle point analysis. In this section, we fix the integration contour to be the line

$$\Re(s) = \sqrt{\pi n},$$

which passes through an approximate saddle point in the upper half plane. Also, we shall split $I(n)$ as

$$I(n) = I^+(n) + I^-(n),$$

where $I^+(n)$ is the integral along the part $\Re(s) \geq 0$. Clearly, it suffices to estimate $I^+(n)$.

In what follows, I freely make use of the simplifications:

$$\zeta(s) \mapsto 1, \qquad 2\cos\frac{\pi s}{2} \mapsto e^{-i\pi s/2}.$$

Remember also that we have available the main estimates of (9) and (10) at $s = x\sqrt{n}$. Finally, simple asymptotic approximations show that, along the contour,

$$\phi''(s) \sim \frac{2}{s} - \frac{1}{s+n+1}, \qquad \phi'''(s) \sim -\frac{2}{s^2} + \frac{1}{(s+n+1)^2}. \tag{13}$$

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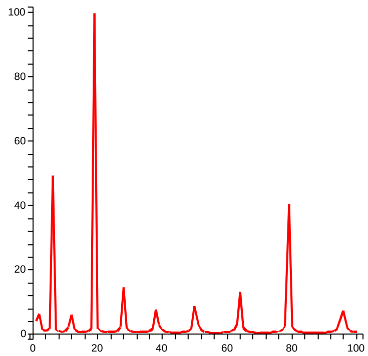
[5] Maple is a great help in all such calculations.



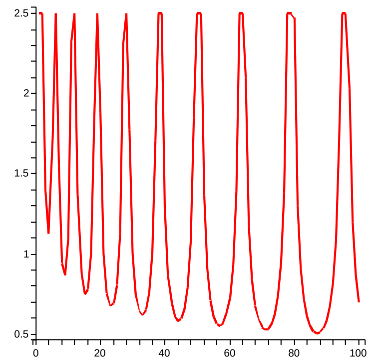


FIGURE 1. The approximations to $I(n)$ provided by the modulus of the integrand of $I(n)$ at the approximate saddle point $\sigma(n)$, as measured by $\rho_1(n)$ defined in Equation (12): [left] raw data; [right] data ceiled by 2.5.

The saddle point is, from previous considerations, close to

$$\Im(s) = \sqrt{\pi n}.$$

A closer examination of the available asymptotc approximations for ϕ and its derivative show the following facts.

— In the scale of $\sqrt{n}$, the integrand decreases fast[6] in modulus, away from the approximate saddle point $\sigma(n) = (1+i)\sqrt{\pi n}$. Precisely, up to $\exp(-O(\sqrt{n}))$ error terms, we can *a priori* limit ourselves to a segment

$$\left[\sqrt{\pi n}(1 + i(1 - \delta)), \sqrt{\pi n}(1 + i(1 + \delta)), \right]$$

for δ fixed, but taken as small as we need in order to guarantee good local convexity properties of expansions, as a function of x for x near $1 + i$.

— The estimate of the second derivative in (13) implies that the "range" of the saddle point is in the scale of $n^{1/4}$. Accordingly, we should set

$$s = \sqrt{\pi n}(1 + i + iwn^{-1/4}),$$

and let w vary in an interval:

$$w \in [\omega(n), +\omega(n)], \qquad \omega(n) = (\log n)^2,$$

for instance. The error arising from the tails is exponentially small, as usual. The error arising from neglecting the third derivatives and beyond are of the form $O(n^{-A})$ for some $A > 0$, i.e., they are polynomially small. (A full asymptotic expansion would then be possible. Not here!)

From now on, we dispense with writing explicitly error terms and only sketch the calculations (MAPLE's helping!).

[6]Note that we are not using a steepest descent in the strict sense since the axis of the saddle point is not vertical. But still, the method works because the vertical line crosses the saddle point from one valley to the next.

We find, with

$$s = x\sqrt{n}, \qquad x = \sqrt{\pi}(1 + i + in^{-1/4}w),$$

the following major approximation:

$$\log\left(n!e^{\phi}(s)\right) \underset{n\to\infty}{\sim} -2\sqrt{\pi n}(1+i) + \log\sqrt{\frac{2\pi}{n}} - \frac{5i\pi}{4} - \frac{1}{2}\sqrt{\pi}w^2(1-i).$$

In other words,we have:

$$n!e^{\phi}(s) \sim e^{-5i\pi/4}e^{-2\sqrt{\pi n}(1+i)}\sqrt{\frac{2\pi}{n}}\exp\left(-\frac{1}{2}\sqrt{\pi}w^2(1-i)\right). \tag{14}$$

This is truly beautiful!

Finally some trivial bookkeeping:

— We have "forgotten" the factor

$$\frac{1}{2i\pi}$$

that is in front of the complex integral.

— The differential element satisfies

$$ds \mapsto i\sqrt{\pi}n^{1/4}dw.$$

— The Gausian integral along a slanted line is given by

$$e^{-5i\pi/4}\int_{-\infty}^{+\infty}\exp\left(-\frac{1}{2}\sqrt{\pi}w^2(1-i)\right)dw = e^{7i\pi/8}\pi^{1/4}2^{1/4}.$$

— The factor $1/(1-s)$ (truly forgotten till the last minute!!) in the integrand brings in an extra contribution:

$$\frac{1}{1-s} \mapsto \frac{e^{3i\pi/4}}{\sqrt{2\pi n}}.$$

Thus, we find

$$I^{+}(n) \sim 2^{-3/4}\pi^{-1/4}n^{-3/4}e^{-3i\pi/8}e^{-\sqrt{2\pi n}(1+i)}.$$

Adding the conjugate contribution from $I^{-}(n)$ gives us finally:

Theorem. *The sequence $I(n)$ satisfies the estimate:*

$$I(n) = 2^{1/4}\pi^{-1/4}n^{-3/4}e^{-2\sqrt{\pi n}}\cos\left(2\sqrt{\pi n} + \frac{3\pi}{8}\right) + O\left(n^{-1}e^{-2\sqrt{\pi n}}\right). \tag{15}$$

The estimate of the error term is conservative. Further terms in the asymptotic expansion (in powers of $n^{-1/4}$ or, most probably, even $n^{-1/2}$) could be computed at will (with time and patience!).

Postscript: January 8, 2006. The last stages of the computation are **shaky** at the moment: I had forgotten some terms and had to do last minute hasty changes. There are certainly some trivial mistakes remaining in some of the details (e.g., the sign seems to be the opposite of what it should be?). Figure 2 shows what I obtain when I compare the main term to of the approximation in the Theorem to exact values.

A consequence of the estimate is, I believe, the fact that the Newton expansion of a suitably regularized ζ converges throughout the whole plane. It is amusing, but typical, that values of zeta at the integers can be used to compute numerically values

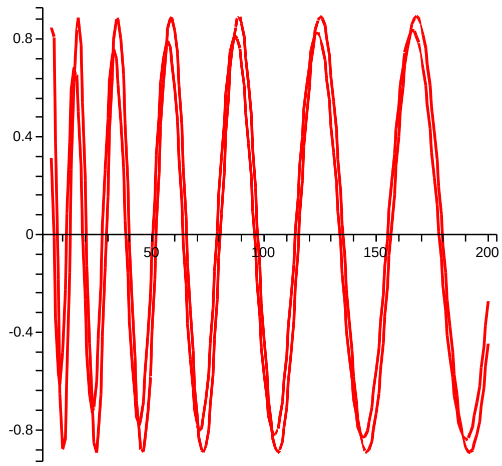


FIGURE 2. The values of $-I(n)$ compared to the approximation $\beta(n)$ provided by the Theorem, for $n = 5\,..\,200$. Both quantities are multiplied by $e^{2\sqrt{\pi n}} n^{3/4}$ before plotting, for readability.

of zeta at other points. (Due to large cancellations and high precision demand, I don't think this gives an efficient algorithms, though!).

Another thread could be investigated: After having used the functional equation, we can expand the zeta function. We get an infinite sum of differences that can be evaluated by residues on the left. We can also expand zeta inside the original combinatorial sum. Thus two combinatorial sums are equal, and, in a way, the fact that they are equal should be nonovious as it is implied by the functional equation of zeta. (See Pólya's elementary derivation of the theta transformation as a guide.) I don't expect anything shattering there, but perhaps it's worth having a quick look at it later. (This cryptic note is so that I won't forget!).

This looks great!