

ON DIFFERENCES OF ZETA VALUES

PHILIPPE FLAJOLET AND LINAS VEPSTAS

ABSTRACT. Finite differences of the Riemann zeta function at the integers are explored. Such quantities, which occur as coefficients in Newton series representations, have surfaced in works of Mařlanka, Coffey, Báez-Duarte, Voros and others. We apply the theory of Nörlund-Rice integrals in conjunction with the saddle point method and derive precise asymptotic estimates. The method extends to Dirichlet L -functions, in which case our estimates appear to be partly related to earlier investigations surrounding Li's criterion for the Riemann hypothesis.

INTRODUCTION

In recent times, a variety of authors have, for a variety of reasons, been led to considering properties of representations of the Riemann zeta function $\zeta(s) = \sum 1/n^s$ as a *Newton interpolation series*. Amongst the many possible forms, we single out the one relative to a regularized version of Riemann zeta, namely,

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

where $\binom{s}{n}$ is a binomial coefficient:

$$\binom{s}{n} := \frac{s(s-1) \cdots (s-n+1)}{n!}.$$

Corollary 1 in Section 5 establishes that the representation (1) is valid throughout the complex plane, its coefficients being determined by a general formula in the calculus of finite differences [11, 17, 18]:

$$(2) \quad b_n = n(1 - \gamma - H_{n-1}) - \frac{1}{2} + \sum_{k=2}^n \binom{n}{k} (-1)^k \zeta(k),$$

(Here, $H_n = 1 + \frac{1}{2} + \cdots + \frac{1}{n}$ are the harmonic numbers.) Although the terms in the sum defining b_n become exponentially large, the values of the b_n are exponentially small, while exhibiting a curious oscillatory behavior. We shall indeed prove the estimate (Theorem 1 of Section 4)

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

A prime reason for interest in the representation (1) and the companion coefficients (2) is *Li's criterion* [13] for the Riemann Hypothesis (RH). Let ρ range over the nontrivial zeros

of $\zeta(s)$. Li's theorem asserts that RH is true if and only if all members of the sequence

$$\lambda_n = \sum_{\rho} \left[1 - \left(1 - \frac{1}{\rho} \right) \right], \quad n \geq 0,$$

are nonnegative. (Bombieri and Lagarias offer an insightful discussion of Li's criterion in [3].) Coffey [4] has shown that the λ_n can be alternatively expressed as a sum of two terms, one of which (the easier one, though) is an elementary variant \hat{b}_n of b_n . Theorem 2 of [4] amounts to the property that the coefficients \hat{b}_n decrease to 0. As we shall see in Section 6, the methods originally developed for estimating b_n yield precise asymptotic information on \hat{b}_n as well.

The zeta function has also received attention in physics, for its role in regularization and renormalization in quantum field theory. Motivated by such connections, Mařlanka introduced in [14] what amounts to a Newton series representation of $(1 - 2s)\zeta(2s)$. Further numerical observations relative to the corresponding coefficients are presented in [15], which have been subsequently vindicated by Báez-Duarte in [2]. In particular, Báez-Duarte's estimates imply that the coefficients in the Newton series of a regularized version of $(1 - 2s)\zeta(2s)$ decrease to 0 faster than any power of $1/n$.

A third independent reason was an attempt by one of us (Linus) around 2003 to obtain alternative tractable expressions for the Gauss-Kuzmin-Wirsing operator of continued fraction theory [unpublished; see <http://linas.org/math/poch-zeta.pdf>]

In this essay, we approach the problem of asymptotically estimating differences of zeta values by means of a combination of two well established techniques. We start from a contour integral representation of these differences as defined by (2) (for this technique, see especially Nörlund's treatise [18] and the study [7]), then proceed to estimate the corresponding complex integral by means of the classical saddle point method of asymptotic analysis [5, 19]. Our approach parallels a recent preprint of Voros [22] (motivated by Li's criterion), which our results supplement by providing a fairly detailed asymptotic analysis of differences of zeta values.

The next section (§1) will review the Newton series for the zeta function, and give some generating functions for its coefficients. This is followed by a brief review of some numerical results in §2. Section 3 gives the Nörlund integral representation for the series, while the Section 4 provides a careful saddle-point analysis of the resulting integrand. Section 6 develops the corresponding analysis for the Dirichlet L -functions. We end with a conclusion outlining other applications of Nörlund integrals in the realm of finite differences and zeta functions.

1. NEWTON SERIES AND ZETA VALUES

This section defines the Newton series for the Riemann zeta that is to be studied, demonstrates some of its simple properties, and gives some generating functions for its coefficients. In this paper, a Newton series will be taken to be defined as

$$(4) \quad \Phi(s) = \sum_{n=0}^{\infty} (-1)^n c_n \binom{s}{n}.$$

Given a function $\phi(s)$, one may attempt to represent it in some region of the complex plane by means of such a series. Since the series $\Phi(s)$ terminates at $s = 0, 1, 2, \dots$, the

conditions $\phi(m) = \Phi(m)$ at the nonnegative integers imply that the candidate sequence $\{c_n\}$ is linearly related to the sequence of values $\{\phi(m)\}$ by

$$\phi(m) = \sum_{n=0}^m (-1)^n c_n \binom{m}{n}.$$

The triangular system can then be inverted to give (by the binomial transform [9] or by direct elimination)

$$(5) \quad c_n = \sum_{k=0}^n \binom{n}{k} (-1)^k \phi(k), \quad n = 0, 1, 2, \dots$$

This choice of coefficients for (4) determines the Newton series *associated* to ϕ . The coincidence of the function ϕ and its associated series Φ is, by construction, granted at least at all the nonnegative integers. The validity of $\Phi(s) = \phi(s)$ is often found to extend to large parts of the complex plane, but this fact requires specific properties much beyond the mere convergence of the series in (4).

In the case of the Newton series for $\zeta(s) - 1/(s-1)$, the general relation (5) provides the coefficients in the form

$$(6) \quad b_n = s_0 - ns_1 + \sum_{k=2}^n \binom{n}{k} (-1)^k \left[\zeta(k) - \frac{1}{k-1} \right],$$

where

$$(7) \quad s_0 = \left[\zeta(s) - \frac{1}{s-1} \right]_{s=0} = \frac{1}{2}, \quad s_1 = \lim_{s \rightarrow 1} \left[\zeta(s) - \frac{1}{s-1} \right] = \gamma.$$

The harmonic numbers appear as

$$(8) \quad \sum_{k=2}^n \binom{n}{k} \frac{(-1)^k}{k-1} = 1 - n + nH_{n-1}.$$

Equations (6), (7), (8) then entail that the b_n , as defined by (2), are indeed the coefficients of the Newton series associated to $\zeta(s) - 1/(s-1)$. A proof of that the equality $\Phi(s) = \zeta(s) - 1/(s-1)$ holds for all complex s is given in Section 5, following the asymptotic analysis of the coefficients b_n and based on a Theorem of Carlson.

Before engaging in a detailed study of the b_n , we note a few simple facts regarding their elementary properties. Set

$$(9) \quad \delta_n := \sum_{k=2}^n \binom{n}{k} (-1)^k \zeta(k),$$

which are, up to minor adjustments, differences of zeta values at the integers. Defining the forward difference $\Delta f(x) := f(x+1) - f(x)$, one has

$$\delta_n = (-1)^n \Delta^n Z(x) \Big|_{x=0},$$

where $Z(k) = \zeta(k)$ for $k \geq 2$ and $Z(0) = Z(1) = 0$. Expanding the zeta function according to its definition and exchanging the order of summations in the resulting double sum shows that

$$(10) \quad \delta_n = \sum_{\ell \geq 1} \left[\left(1 - \frac{1}{\ell} \right)^n - 1 + \frac{n}{\ell} \right].$$

This rather simple sum shows a remarkably complex behavior; elucidating its behavior is one of the principal topics of this paper.

The ordinary generating function for the sequence $\{\delta_n\}$ is also of interest. Given the classical expansion [23] of the logarithmic derivative $\psi(z)$ of the Gamma function,

$$\psi(1+z) + \gamma = \zeta(2)z - \zeta(3)z^2 + \zeta(4)z^3 - \dots,$$

one finds

$$(11) \quad \sum_{n \geq 2} \delta_n z^n = \frac{z}{(1-z)^2} \left[\psi\left(\frac{1}{1-z}\right) + \gamma \right].$$

The exponential generating function for the sequence $\{\delta_n\}$ reflects (10) and is even simpler:

$$(12) \quad \sum_{n \geq 2} \delta_n \frac{z^n}{n!} = e^z \sum_{n \geq 2} \zeta(n) \frac{(-z)^n}{n!} = e^z \sum_{\ell \geq 1} \left[e^{-z/\ell} - 1 + \frac{z}{\ell} \right].$$

2. EXPERIMENTAL ANALYSIS

Detailed experiments on the b_n coefficients conducted by one of us are at the origin of the present paper. As it is usual when dealing with finite differences, the alternating binomial sums giving the b_n involve exponential cancellation since the binomial coefficients get almost as large as 2^n . We conducted evaluations of the b_n up to $n \approx 5000$, which requires computing zeta values up to several thousand digits of precision. (Note that the zeta values can be computed rapidly to extremely high precision using several efficient algorithms, which are available in several symbolic computation packages and numerical libraries.)

A quick inspection of numerical data immediately reveals two features of the constants b_n : they are oscillatory with slowly increasing period and their absolute values are very rapidly decreasing. For instance¹:

$$\begin{aligned} b_1 &\doteq -0.07721, & b_2 &\doteq -0.00949, & b_5 &\doteq 0.00071, \\ b_{10} &\doteq -0.00002, & b_{20} &\doteq 2.15965 \cdot 10^{-9}, & b_{50} &\doteq -1.08802 \cdot 10^{-11}. \end{aligned}$$

A numeric fit of the oscillatory behavior of the function may be made. There are sign changes in the sequence $\{b_n\}$ at

$$n = 3, 7, 13, 21, 29, 40, 52, 65, 80, 97, 115, 135, 157, 180, \dots,$$

the values growing roughly quadratically. A good fit for the k th zero is provided by

$$q(k) = \frac{\pi}{4}k^2 + \frac{9\pi}{16}k + 1,$$

rounded at the nearest integer. (The precise values of the first two constants were inferred from values of n well in the range of several thousands.) The quadratic polynomial is easily inverted to give the approximate oscillatory behavior of the b_n :

$$s(n) = \sin \pi \left(2\sqrt{\frac{n}{\pi}} - \frac{9}{8} \right).$$

¹The notation $x \doteq y$ designates a numerical approximation of x by y to the last decimal digit stated.

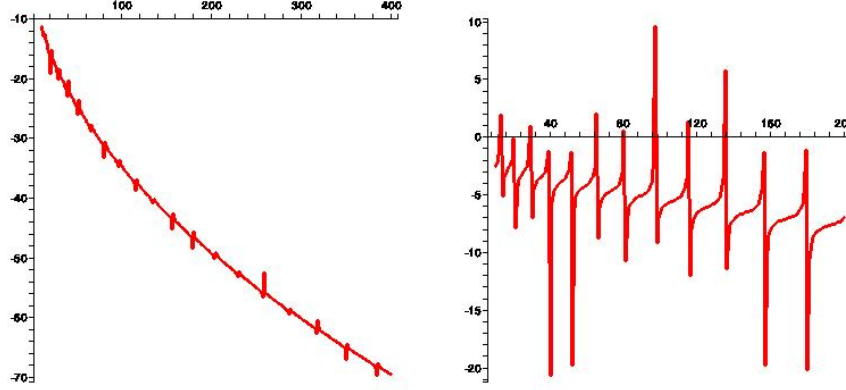


FIGURE 1. Numerical experiments with b_n . Left: a plot of $\log |b_n/s(n)|$. Right: a plot of $b_n/\beta(n)$.

Once the oscillatory behavior has been disposed of, the task of quantifying the general trend in the decrease becomes easier. A plot of the values of $\log |b_n/s(n)|$ displayed in Figure 1 (left) has a parabolic aspect, which suggests that

$$b_n \approx s(n)e^{-K\sqrt{n}} \quad \text{with } K \approx 3.6,$$

but a more precise fit is difficult.

In summary, this together with similar experiments led us to conjecture

$$(13) \quad \beta(n) := \sin \pi \left(2\sqrt{\frac{n}{\pi}} - \frac{9}{8} \right) e^{-K\sqrt{n}}, \quad K = 3.6 \pm 0.1.$$

as a rough approximation to b_n . Figure 1 (right) displays the ratios $b_n/\beta(n)$ for $n = 10 \dots 200$. The trend is compatible furthermore with the presence of an extra factor of the form $-n^\kappa$ for some $\kappa \in (0, 1)$. (The spikes correspond to occasional inaccuracies of our sign-change function, $s(n)$.) As we shall see, these empirical observations match reality quite well.

3. THE NÖRLUND INTEGRAL REPRESENTATION

Our approach to the asymptotic estimation of the b_n relies on a complex integral representation of finite differences of an analytic function, to be found in Nörlund's classic treatise [18, §VIII.5] first published in 1924. In computer science, this representation was popularized by Knuth [12], who attributed it to S.O. Rice, so that it also came to be known as "Rice's method"; see [7] for a review.

Lemma 1. *Let $\phi(s)$ be holomorphic in the half-plane $\Re(s) \geq n_0 - \frac{1}{2}$. Then the finite differences of the sequence $(\phi(k))$ admit the integral representation*

$$(14) \quad \sum_{k=n_0}^n \binom{n}{k} (-1)^k \phi(k) = \frac{(-1)^n}{2\pi i} \int_C \phi(s) \frac{n!}{s(s-1)\cdots(s-n)} ds,$$

where the contour of integration C encircles the integers $\{n_0, \dots, n\}$ in a positive direction and is contained in $\Re(s) \geq n_0 - \frac{1}{2}$.

Proof. The integral on the right of (14) is the sum of its residues at $s = n_0, \dots, n$, which precisely equals the sum on the left. \square

An immediate consequence is the following representation for the differences of zeta values (δ_n in (9)):

$$(15) \quad \delta_n \equiv \sum_{k=2}^n \binom{n}{k} (-1)^k \zeta(k) = \frac{(-1)^{n-1}}{2\pi i} \int_{3/2-i\infty}^{3/2+i\infty} \zeta(s) \frac{n!}{s(s-1)\cdots(s-n)} ds.$$

(Start from a small rectangle encircling $\{2, \dots, n\}$, then extend it to a long rectangle with horizontal sides at $\pm i\infty$, and finally push the right vertical side to $+\infty$. The contributions relative to all but the left vertical side vanish, since $\zeta(s)$ remains bounded in modulus by $\zeta(\frac{3}{2})$.)

Since b_n is δ_n plus a correction term (see Equation (2)), the first step is to move the line of integration further to the left. It is well known that the Riemann zeta function is of finite order in any right half-plane, that is, $|\zeta(s)| = O(|s|^A)$ uniformly as $|s| \rightarrow \infty$, for some A depending on the half-plane under consideration [21]. As a consequence, the integral of (15) remains convergent, when taken along any vertical line left of 0, as soon as n is large enough. Under these conditions, it is possible to replace the line of integration $\Re(s) = \frac{3}{2}$ by the line $\Re(s) = -\frac{1}{2}$, upon taking into account the residues of a double pole at $s = 1$ and a simple pole at $s = 0$. We find in this way

$$\delta_n = (-1)^{n-1} (R_1 + R_0) + \frac{(-1)^{n-1}}{2\pi i} \int_{-1/2-i\infty}^{-1/2+i\infty} \zeta(s) \frac{n!}{s(s-1)\cdots(s-n)} ds,$$

where, as shown by a routine calculation:

$$(-1)^n R_0 = -\frac{1}{2}, \quad (-1)^n R_1 = -n(1 - \gamma - H_{n-1}).$$

The residues thus compensate exactly for the difference between δ_n and b_n , so that

$$(16) \quad b_n = \frac{(-1)^{n-1}}{2\pi i} \int_{-1/2-i\infty}^{-1/2+i\infty} \zeta(s) \frac{n!}{s(s-1)\cdots(s-n)} ds.$$

4. SADDLE POINT ANALYSIS OF ZETA DIFFERENCES

The integrand in (4) is free of singularities on the left-hand side, and is thus amenable to evaluation by the saddle point (or steepest-descent) method. This evaluation is the main topic of this section, and culminates with the derivation of one of the principal results of this paper, equation (3).

It is convenient to perform a change of variables $s \mapsto -s$. The new integrand involves $\zeta(-s)$, which transforms by virtue of the functional equation of the zeta function,

$$(17) \quad \zeta(1-s) = (2\pi)^{-s} 2 \cos\left(\frac{s\pi}{2}\right) \Gamma(s) \zeta(s).$$

A combination of (16) and (17) then gives

$$(18) \quad b_n = -\frac{1}{\pi i} \int_{1/2-i\infty}^{1/2+i\infty} (2\pi)^{-s-1} \sin\left(\frac{\pi s}{2}\right) \zeta(1+s) \frac{n! \Gamma(1+s)}{s(s+1)\cdots(s+n)} ds,$$

which is the starting point of our asymptotic analysis.

The integral representation (18) has several noticeable features. First, the integrand has no singularity at all in $\Re(s) \geq \frac{1}{2}$ and it decays fast enough towards $\pm i\infty$, which means that one can freely choose the abscissa c (with $c \geq \frac{1}{2}$) in the representation

$$(19) \quad b_n = -\frac{1}{\pi i} \int_{c-i\infty}^{c+i\infty} (2\pi)^{-s-1} \sin\left(\frac{\pi s}{2}\right) \zeta(1+s) \frac{n! \Gamma(s+1)}{s(s+1) \cdots (s+n)} ds.$$

The very absence of singularities calls for an application of the saddle point method.

The factor $\zeta(1+s)$ remains bounded in modulus by a constant, and is in fact barely distinguishable from 1, as $\Re(s)$ increases, since

$$(20) \quad \zeta(s) = 1 + \mathcal{O}\left(2^{-\Re(s)}\right), \quad \Re(s) \geq \frac{3}{2}.$$

Also, for large $|s|$, the complex version of Stirling's formula applies:

$$(21) \quad \Gamma(1+s) = s^s e^{-s} \sqrt{2\pi s} \left(1 + \mathcal{O}(|s|^{-1})\right), \quad \Re(s) \geq 0.$$

Finally, the sine factor increases exponentially along vertical lines: one has

$$(22) \quad 2i \sin \frac{\pi s}{2} = -\exp\left(-i \frac{\pi s}{2}\right) + \mathcal{O}\left(e^{-\pi \Im(s)/2}\right), \quad \Im(s) \geq 0,$$

with a conjugate approximation holding for $\Im(s) < 0$.

In anticipation of applying saddle-point methods, the approximations (20), (21), and (22) then suggest the function $e^{\omega(s)}$ as a simplified model of the integrand in the upper half-plane, where

$$(23) \quad \omega(s) = -s \log(2\pi) - i \frac{\pi s}{2} + \log \frac{n! \Gamma(s)^2}{\Gamma(s+n)}.$$

We shall demonstrate shortly that the location of the appropriate saddle points in the complex plane scale as \sqrt{n} , which may be confirmed by numerical experiments. Therefore, in performing an asymptotic analysis, it is appropriate to perform a change of variable $s = x\sqrt{n}$, and expand in descending powers of n , presuming x to be approximately constant. We find, uniformly for x in any compact region of $\Re(x) > 0$, $\Im(x) > 0$:

$$(24) \quad \begin{cases} \omega(x\sqrt{n}) &= x\sqrt{n} \left[2 \log x - 2 - \log(2\pi) - \frac{1}{2} i\pi \right] + \frac{1}{2} \log n \\ &\quad - \log x + \log(2\pi) - \frac{1}{2} x^2 + \mathcal{O}(n^{-1/2}) \\ \omega'(x\sqrt{n}) &= \left[-\log(2\pi) - i \frac{\pi}{2} + 2 \log x \right] - \left(x + \frac{1}{x} \right) \frac{1}{\sqrt{n}} + \mathcal{O}(n^{-1}). \\ \omega''(x\sqrt{n}) &= \frac{2}{x\sqrt{n}} + \mathcal{O}(n^{-1}). \end{cases}$$

(The symbolic manipulation system MAPLE is a great help in such computations.)

From the second line of (24), an approximate root of $\omega'(s)$ is obtained by choosing the particular value x_0 of x that cancels ω' to main asymptotic order:

$$(25) \quad x_0 = e^{i\pi/4} \sqrt{2\pi}.$$

This corresponds to the following value for s ,

$$(26) \quad \sigma \equiv \sigma(n) = x_0 \sqrt{n} = (1+i) \sqrt{\pi n},$$

which is thus also an approximate saddle point for $e^{\omega(s)}$. The substitution of this value given the first line of (24) then leads to

$$(27) \quad \exp(\omega(\sigma(n))) = \exp(2i\sqrt{\pi n}) \cdot \exp(-2\sqrt{\pi n}) \cdot \Pi(n),$$

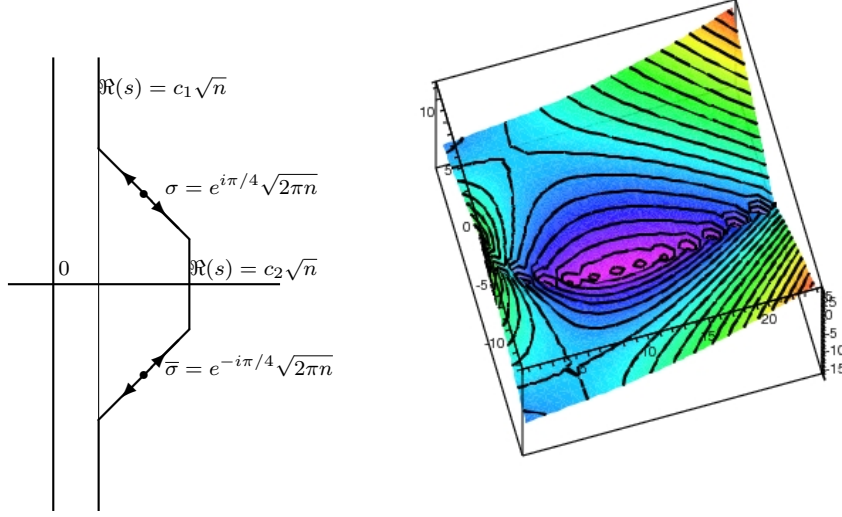


FIGURE 2. Left: The saddle point contour used for estimating b_n . The arrows point at the directions of steepest descent from the saddle points. Right: the landscape of the logarithm of the modulus of the integrand in the representation of b_n for $n = 10$.

where Π is an unspecified factor of at most polynomial growth. By using a suitable contour that passes through $\sigma(n)$, we thus expect the quantity in (27) to be an approximation (up to polynomial factors again) of b_n . This back-of-the-envelope calculation does predict the exponential decay of b_n as $\exp(-3.54490\sqrt{n})$, in a way consistent with numerical data, while the fluctuations, $\sin(2\sqrt{\pi n} + \mathcal{O}(1))$, are seen to be in stunning agreement with the empirically obtained formula (13).

We must now fix the contour of integration and provide final approximations. The contour adopted (Figure 2) goes through the saddle point $\sigma = \sigma(n)$ and symmetrically through its complex conjugate $\bar{\sigma} = \bar{\sigma}(n)$. In the upper half-plane, it traverses $\sigma(n)$ along a line of steepest descent whose direction, as determined from the argument of $\omega''(\sigma)$, is at an angle of $\frac{5\pi}{8}$ with the horizontal axis. The contour also includes parts of two vertical lines of respective abscissae $\Re(s) = c_1\sqrt{n}$ and $c_2\sqrt{n}$, where

$$0 < c_1 < \sqrt{\pi} < c_2 < 2\sqrt{\pi}.$$

The choice of the abscissae, c_1 and c_2 , is not critical (it is even possible to adapt the analysis to $c_1 = c_2 = \sqrt{\pi}$). One verifies easily, from crude approximations, that the contributions arising from the vertical parts of the contour are $\mathcal{O}(e^{-L_0\sqrt{n}})$, for some $L_0 > 2\sqrt{\pi}$, i.e., they are exponentially small in the scale of the problem:

$$(28) \quad \int_{\text{vertical}} = \mathcal{O}(e^{-L_0\sqrt{n}}) \quad L_0 > 2\sqrt{\pi}.$$

The slanted part of the contour is such that all the estimates of (24) apply. The scale of the problem is dictated by the value of $\omega''(\sigma)$, which is of order $\mathcal{O}(n^{-1/2})$. This indicates

that the “second order” scaling to be adopted is $n^{1/4}$. Accordingly, we set

$$(29) \quad s = (1 + i)\sqrt{\pi n} + e^{5i\pi/8}yn^{1/4}.$$

Define the *central region* of the slanted part of the contour by the condition that $|y| \leq \log^2 n$. Upon slightly varying the value of x around x_0 , one verifies from (24) that, for large n , the quantity

$$\Re \left(\frac{1}{\sqrt{n}} \omega \left(x_0 \sqrt{n} + e^{5i\pi/8} t \sqrt{n} \right) \right)$$

is an upward concave function of t near $t = 0$. There results, in the complement of the central part, $|y| \geq \log^2 n$, the approximation

$$\left| \exp \left(\omega \left(x_0 \sqrt{n} + e^{5i\pi/8} yn^{1/4} \right) \right) \right| < e^{\omega(x_0 \sqrt{n})} \cdot \exp(-L_1 \log^2 n), \quad L_1 > 0.$$

Figuratively:

$$(30) \quad \int_{\text{slanted}} = \int_{\text{central}} + \mathcal{O}(\exp(-L_1 \log^2 n)).$$

Thus, from (28) and (30), only the central part of the slanted region matters asymptotically. This applies to $e^{\omega(s)}$ but also to the full integrand of the representation (19) of b_n , given the approximations (20)–(24).

We are finally ready to reap the crop. Take the integral representation of (19) with the contour deformed as indicated in Figure 2 and let b_n^+ be the contribution arising from the upper half-plane, to the effect that

$$(31) \quad b_n = 2\Re(b_n^+),$$

by conjugacy. In the central region,

$$s = x_0 \sqrt{n} + e^{5i\pi/8} yn^{1/4},$$

the integrand of (19) becomes

$$(32) \quad \left(-\frac{1}{\pi i} \right) \cdot (2\pi)^{-1} \cdot \left(-\frac{1}{2i} \right) \cdot \left(1 + \mathcal{O}(2^{-\sqrt{n}}) \right) \cdot \frac{x_0}{n} \cdot e^{\omega(x_0 \sqrt{n})} \cdot e^{-y^2/\sqrt{2\pi}} \left(1 + \mathcal{O}\left(\frac{1}{\sqrt{n}}\right) \right).$$

The various factors found there (compare (19) to $e^{\omega(s)}$ with $\omega(s)$ defined in (23)) are in sequence: the Cauchy integral prefactor; the correction $(2\pi)^{-1}$ to the functional equation of Riemann zeta; the factor $-1/(2i)$ relating the sine to its exponential approximation; the approximation of Riemann zeta; the correction $s/(s+n)$ of the Gamma factors; the main term $e^{\omega(s)}$; the anticipated local Gaussian approximation; the errors resulting from approximations (20)–(24), which are of relative order $O(n^{-1/2})$. Upon completing the tails of the integral and neglecting exponentially small corrections, we get

$$(33) \quad b_n^+ = K_0 e^{\omega(x_0 \sqrt{n})} \frac{x_0}{\sqrt{n}} \int_{-\infty}^{+\infty} e^{-y^2/\sqrt{2\pi}} dy \cdot \left(e^{5i\pi/8} n^{1/4} \right) \left(1 + \mathcal{O}\left(\frac{1}{\sqrt{n}}\right) \right),$$

where K_0 is the constant factor of (32), while the factor following the integral translates the change of variables: $ds = e^{5i\pi/8} n^{1/4} dy$.

The asymptotic form of b_n is now completely determined by (31) and (33). We have obtained:

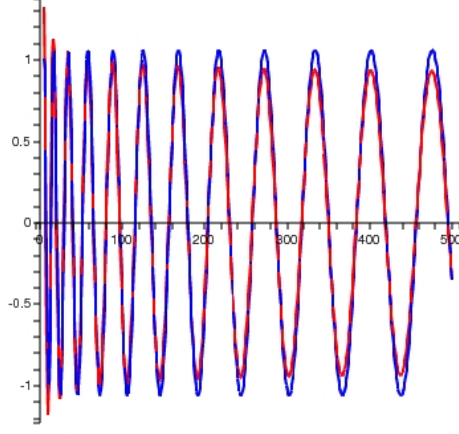


FIGURE 3. A comparative plot of b_n and the main term of its approximation (34), both multiplied by $e^{-2\sqrt{\pi n}} n^{-1/4}$, for $n = 5 \dots 500$.

Theorem 1. *The Newton coefficient b_n of $\zeta(s) - 1/(s-1)$ defined in (2) satisfies*

$$(34) \quad b_n = \left(\frac{2n}{\pi}\right)^{1/4} e^{-2\sqrt{\pi n}} \cos\left(2\sqrt{\pi n} - \frac{5\pi}{8}\right) + \mathcal{O}\left(e^{-2\sqrt{\pi n}} n^{-1/4}\right).$$

The agreement between asymptotic and exact values is quite good, even for small values of n (Figure 3).

The foregoing developments justify a posteriori the application of the saddle point formula to the Nörlund Rice integral representation (19) of zeta value differences. This formula reads

$$(35) \quad \int e^{-Nf(x)} dx = \sqrt{\frac{2\pi}{N|f''(x_0)|}} e^{-Nf(x_0)} \left(1 + \mathcal{O}\left(\frac{1}{N}\right)\right).$$

Here the analytic function $f(x)$ should be such that $|f(x)|$ has a saddle-point at x_0 , that is, $f'(x_0) = 0$ and $f''(x_0)$ is the second derivative of f at the saddle point. In the case of differences of zeta values, the appropriate scaling parameter is $s = x\sqrt{n}$ corresponding to $N = \sqrt{n}$, and the the function f is

$$f(x) = \lim_{n \rightarrow \infty} \frac{1}{\sqrt{n}} \omega(x\sqrt{n}),$$

up to smaller order corrections that can be treated as constants in the range of the saddle point.

5. CONVERGENCE OF THE NEWTON SERIES OF ZETA

The fact that the coefficients b_n decay to zero faster than any polynomial in $1/n$ implies that the Newton series

$$(36) \quad \Phi(s) = \sum_{n=0}^{\infty} (-1)^n b_n \binom{s}{n},$$

with b_n given by (2), converges throughout the complex plane, and consequently defines an entire function. Set $Z(s) := \zeta(s) - 1/(s-1)$ with $Z(1) = \gamma$. We have, by construction $\Phi(s) = Z(s)$ at $s = 0, 1, 2, \dots$, but the relation between Φ and Z at other points is still unclear.

Corollary 1. *The Newton series of (36) is a convergent representation of the function $\zeta(s) - 1/(s-1)$ valid at all points $s \in \mathbb{C}$.*

Proof. Here is our favorite proof. A classic theorem of Carlson (for a discussion and a proof, see, e.g., Hardy's Lectures [10, pp. 188-191] or Titchmarsh's treatise [20, §5.81]) says the following: Assume that (i) $g(s)$ is analytic and such that

$$|g(s)| < C^{A|s|},$$

where $A < \pi$, in the right half-plane of complex values of s , and (ii) $g(0) = g(1) = \dots = 0$. Then $g(s)$ vanishes identically.

To complete the proof, it suffices to apply Carlson's theorem to the difference $g(s) = \Phi(s+2) - Z(s+2)$. Condition (ii) is satisfied by construction of the Newton series. Condition (i) results from the fact that $Z(s+2)$ is $\mathcal{O}(1)$ while a general bound due to Nörlund (Equation (58) of [18, p. 228]) and valid for all convergent Newton series asserts that $|\Phi(s+2)|$ is of growth at most $e^{\frac{\pi}{2}|s|}$, throughout $\Re(s) > -\frac{1}{2}$. \square

An alternative proof can be given starting from a contour integral representation for the remainder of a general Newton series given [18, p. 223]. In a short note, Báez-Duarte [2] justified a similar looking Newton series representation of the zeta function due to Maślanka—however his bounds on the Newton coefficients are less precise than ours and his arguments (based on a doubly indexed sequence of polynomials) seem to be somewhat problem-specific.

6. DIRICHLET L -FUNCTIONS

The methods employed to deal with differences of zeta values have a more general scope, and we may reasonably expect them to be applicable to other kinds of Dirichlet series. Such is indeed the case for any Dirichlet L -function,

$$L(\chi, s) = \sum_{n=1}^{\infty} \frac{\chi(n)}{n^s},$$

where χ is a multiplicative character of some period k , that is, for all integers m, n , one has: $\chi(n+k) = \chi(n)$, $\chi(mn) = \chi(m)\chi(n)$, $\chi(1) = 1$, and $\chi(n) = 0$ whenever $\gcd(n, k) \neq 1$.

Let $\zeta(s, q)$ be the Hurwitz zeta function defined by

$$(37) \quad \zeta(s, q) = \sum_{n=0}^{\infty} \frac{1}{(n+q)^s}$$

Any L -function may be represented as a combination of Hurwitz zeta

$$(38) \quad L(\chi, s) = \frac{1}{k^s} \sum_{m=1}^k \chi(m) \zeta\left(s, \frac{m}{k}\right)$$

where k is the period of χ . In particular, the coefficients of the Newton series for $L(\chi, s)$ are simple linear combinations of the quantities

$$(39) \quad A_n(m, k) = \sum_{\ell=2}^n \binom{n}{\ell} (-1)^\ell \frac{\zeta\left(\ell, \frac{m}{k}\right)}{k^\ell},$$

which we adopt as our fundamental object of study.

Theorem 2. *The differences of Hurwitz zeta values, $A_n(m, k)$ defined by (39), satisfy the estimate*

$$(40) \quad A_n(m, k) = \left(\frac{m}{k} - \frac{1}{2}\right) - \frac{n}{k} \left[\psi\left(\frac{m}{k}\right) + \ln k + 1 - H_{n-1}\right] + a_n(m, k)$$

where the $a_n(m, k)$ are exponentially small:

$$(41) \quad a_n(m, k) = \frac{1}{k} \left(\frac{2n}{\pi k}\right)^{1/4} \exp\left(-\sqrt{\frac{4\pi n}{k}}\right) \cos\left(\sqrt{\frac{4\pi n}{k}} - \frac{5\pi}{8} - \frac{2\pi m}{k}\right) + \mathcal{O}\left(n^{-1/4} e^{-2\sqrt{\pi n/k}}\right).$$

The previous results for Riemann zeta may be regained by setting $m = k = 1$, so that $\delta_n = A_n(1, 1)$ and $b_n = a_n(1, 1)$.

Proof. Converting the sum to the Nörlund-Rice integral, and extending the contour to infinity, one obtains

$$(42) \quad A_n(m, k) = \frac{(-1)^n}{2\pi i} n! \int_{\frac{3}{2}-i\infty}^{\frac{3}{2}+i\infty} \frac{\zeta\left(s, \frac{m}{k}\right)}{k^s s(s-1)\cdots(s-n)} ds$$

Moving the contour to the left, one encounters a single pole at $s = 0$ and a double pole at $s = 1$. The residue of the pole at $s = 0$ is

$$\text{Res}(s=0) = \zeta\left(0, \frac{m}{k}\right) = \frac{1}{2} - \frac{m}{k}.$$

(See [23, p. 271] for this evaluation.) The double pole at $s = 1$ evaluates to

$$\text{Res}(s=1) = \frac{n}{k} \left[\psi\left(\frac{m}{k}\right) + \ln k + 1 - H_{n-1}\right]$$

Combining these, one obtains (40) where the a_n are given by

$$(43) \quad a_n(m, k) = \frac{(-1)^n}{2\pi i} n! \int_{-\frac{1}{2}-i\infty}^{-\frac{1}{2}+i\infty} \frac{\zeta\left(s, \frac{m}{k}\right)}{k^s s(s-1)\cdots(s-n)} ds.$$

As before, the $a_n(m, k)$ have the remarkable property of being exponentially small; that is, $a_n(m, k) = \mathcal{O}\left(e^{-\sqrt{Kn}}\right)$, for a constant K that only depends on k . The precise behavior of the exponentially small term may be obtained by using the same saddle-point analysis given in the previous sections. Again, its application here is abbreviated, as there are no substantial differences in the course of the derivations.

The term $a_n(m, k)$ is represented by the integral of (43). At this point, the functional equation for the Hurwitz zeta may be applied. This equation is

$$(44) \quad \zeta\left(1-s, \frac{m}{k}\right) = \frac{2\Gamma(s)}{(2\pi k)^s} \sum_{p=1}^k \cos\left(\frac{\pi s}{2} - \frac{2\pi pm}{k}\right) \zeta\left(s, \frac{p}{k}\right)$$

This allows the integral to be expressed as a sum:

$$a_n(m, k) = -\frac{2n!}{k\pi i} \sum_{p=1}^k \int_{\frac{3}{2}-i\infty}^{\frac{3}{2}+i\infty} \frac{1}{(2\pi)^s} \frac{\Gamma(s)\Gamma(s-1)}{\Gamma(s+n)} \cos\left(\frac{\pi s}{2} - \frac{2\pi pm}{k}\right) \zeta\left(s, \frac{p}{k}\right) ds$$

It proves convenient to pull the phase factor out of the cosine part and write the integral as

$$a_n(m, k) = -\frac{n!}{k\pi i} \sum_{p=1}^k \exp\left(i\frac{2\pi pm}{k}\right) \int_{\frac{3}{2}-i\infty}^{\frac{3}{2}+i\infty} \frac{1}{(2\pi)^s} \frac{\Gamma(s)\Gamma(s-1)}{\Gamma(s+n)} \exp\left(-i\frac{\pi s}{2}\right) \zeta\left(s, \frac{p}{k}\right) ds + \text{c.c.},$$

where *c.c.* (“*complex conjugate*”) means that i should be replaced by $-i$ in the two exp parts.

To recast the equation (6) into the form needed for the saddle point method, an asymptotic expansion of the integrands needs to be made for large n . As before, the appropriate scaling parameter is $x = s/\sqrt{n}$, and so one may perform a change of variable from s to x . The asymptotic expansion is then performed by holding x constant, and taking n large. Thus, one writes

$$(45) \quad a_n(m, k) = -\frac{1}{k\pi i} \sum_{p=1}^k \left[e^{i2\pi pm/k} \int_{\sigma_0-i\infty}^{\sigma_0+i\infty} e^{\omega(x\sqrt{n})} dx + e^{-i2\pi pm/k} \int_{\sigma_0-i\infty}^{\sigma_0+i\infty} e^{\bar{\omega}(x\sqrt{n})} dx \right].$$

Proceeding, one finds

$$\omega(s) = \log n! + \frac{1}{2} \log n - s \log\left(\frac{2\pi p}{k}\right) - i\frac{\pi s}{2} + \log \frac{\Gamma(s)\Gamma(s-1)}{\Gamma(s+n)} + \mathcal{O}\left(\left(\frac{p}{k+p}\right)^s\right)$$

where the approximation that $\log \zeta(s, p/k) = (k/p)^s + \mathcal{O}((p/(k+p))^s)$ for large s has been made. Expanding to $\mathcal{O}(1/\sqrt{n})$ and collecting terms, one obtains

$$(46) \quad \begin{aligned} \omega(x\sqrt{n}) &= \frac{1}{2} \log n - x\sqrt{n} \left[\log \frac{2\pi p}{k} + i\frac{\pi}{2} + 2 - 2 \log x \right] \\ &\quad + \log 2\pi - 2 \log x - \frac{x^2}{2} + \mathcal{O}(n^{-1/2}) \end{aligned}$$

The saddle point is obtained by solving $\omega'(x\sqrt{n}) = 0$. To lowest order, one obtains $x_0 = (1+i)\sqrt{\pi p/k}$. To use the saddle-point formula, one needs $\omega''(x\sqrt{n}) = 2/x\sqrt{n} + \mathcal{O}(n^{-1})$. Substituting, one directly obtains

$$(47) \quad \int_{\sigma_0-i\infty}^{\sigma_0+i\infty} e^{\omega(x\sqrt{n})} dx = \left(\frac{2\pi^3 pn}{k}\right)^{1/4} e^{i\pi/8} \exp\left(-(1+i)\sqrt{\frac{4\pi pn}{k}}\right) + \mathcal{O}\left(n^{-1/4} e^{-2\sqrt{\pi pn/k}}\right)$$

while the integral for $\bar{\omega}$ is the complex conjugate quantity (having a saddle point at the complex conjugate location). Inserting this into equation (45) gives a sum of contributions for $p = 1, \dots, k$, of which, for large n , only the $p = 1$ term contributes significantly. So, one has obtained the estimation (41) of the statement. \square

7. PERSPECTIVE

The previous results serve to unify and make precise a number of estimates carried out in the literature by a diversity of methods. For instance, the study of quantities arising in connection with Li's criterion calls for estimating, in the notations of (39),

$$(48) \quad A_n(2, 2) = \sum_{k=2}^n \binom{n}{k} (-1)^k (1 - 2^{-k}) \zeta(k).$$

Coffey encountered this quantity (his $S_1(n)$ in [4]), and proved, by means of series rearrangements akin to (10) used in conjunction with Euler-Maclaurin summation:

$$(49) \quad A_n(2, 2) \geq \frac{n}{2} \log n + (\gamma - 1) \frac{n}{2} + \frac{1}{2}.$$

Our analysis quantifies the difference between the two quantities above as being exponentially small and oscillating:

$$(50) \quad a_n(2, 2) = \frac{1}{2} \left(\frac{n}{\pi} \right)^{1/4} \exp \left(-\sqrt{2\pi n} \right) \cos \left(\sqrt{2\pi n} - \frac{5\pi}{8} \right) + \mathcal{O} \left(n^{-1/4} e^{-\sqrt{2\pi n}} \right)$$

Another observation is that the combination of Nörlund-Rice integrals and saddle point estimates applies to many “desingularized” versions of the Riemann zeta function, like

$$(1 - 2^{1-s})\zeta(s), \quad (s-1)\zeta(s), \quad \zeta(2s) - \frac{1}{2s-1}, \quad (2s-1)\zeta(2s).$$

The first one is directly amenable to Theorem 2. The Newton series involving $\zeta(2s)$ include Maślanka's expansion [14] (relative to $(2s-1)\zeta(2s)$) and have a striking feature—their Newton coefficients are polynomials in π with rational coefficients. For a function like $\zeta(2s) - 1/(2s-1)$ where the polar part is subtracted, the exponential smallness of the coefficients then has the peculiar feature of providing near identities that connect π and Euler's constant γ .

The Nörlund integrals are also of interest in the context of differences of inverse zeta values, for which curious relations with the Riemann hypothesis have been noticed by Flajolet–Vallée [8] and independently by Báez-Duarte [1]. Consider the typical quantity

$$(51) \quad d_n = \sum_{k=2}^n \binom{n}{k} (-1)^k \frac{1}{\zeta(k)},$$

which arises as coefficient in the Newton series representation of $1/\zeta(s)$. Its asymptotic analysis can be approached by means of a Nörlund-Rice representation as noted by the authors of [8] and more recently by Maślanka in [16], in related contexts. We have:

Theorem 3. *The differences of inverse zeta values d_n defined by (51) are such that the following two assertions are equivalent:*

FVBD Hypothesis (akin to [1, 8]). *For any $\epsilon > 0$, there exists a constant $C_\epsilon > 0$ such that*

$$|d_n| < C_\epsilon k^{1/2+\epsilon}.$$

RH (Riemann hypothesis). *The Riemann zeta function $\zeta(s)$ is free of zeros in the half-plane $\Re(s) > \frac{1}{2}$.*

Proof. (i) Assume **RH**. Under RH, it is known that, given any $\sigma_0 > \frac{1}{2}$ and any $\epsilon > 0$, one has $1/\zeta(s) = O(|t|^\epsilon)$ for $\Re(s) = \sigma_0$, where $t = \Im(s)$ (see Equation (14.2.6) of [21, p. 337]). Then, apply the Nörlund integral representation (valid unconditionally for $c > 1$):

$$(52) \quad d_n = \frac{(-1)^{n-1}}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{1}{\zeta(s)} \frac{n!}{(s(s-1)\cdots(s-n))} ds,$$

with $c = \sigma_0$. A simple majorization concludes the proof that $d_n = O(n^{\sigma_0})$.

(ii) Assume **FVBD**. First, a reorganization similar to the one leading to (10) but based on the expansion of $1/\zeta(s)$ shows that

$$d_n = \sum_{\ell=1}^{\infty} \mu(\ell) \left[\left(1 - \frac{1}{\ell}\right) - 1 + \frac{n}{\ell} \right],$$

with $\mu(\ell)$ the Möbius function. The general term of the sum decreases like n/ℓ^2 , which ensures absolute convergence. Next, introduce the function

$$D(x) = \sum_{\ell \geq 1} \mu(\ell) \left[e^{-x/\ell} - 1 + \frac{x}{\ell} \right],$$

whose general term decreases like x/ℓ^2 .

Fix any small $\delta > 0$ ($\delta = \frac{1}{10}$ is suitable) and define $\ell_0 = \lfloor x^{1-\delta} \rfloor$. The difference $d_n - D(n)$ satisfies

$$(53) \quad \begin{aligned} d_n - D(n) &= \sum_{\ell=1}^{\infty} \mu(\ell) \left[\left(1 - \frac{1}{\ell}\right)^n - e^{-n/\ell} \right] \\ &= \left(\sum_{\ell < \ell_0} + \sum_{\ell \geq \ell_0} \right) \mu(\ell) e^{-n/\ell} \left[e^{n/\ell + n \log(1-1/\ell)} - 1 \right] \\ &= \mathcal{O}\left(\ell_0 e^{-n/\ell_0}\right) + \sum_{\ell \geq \ell_0} \mathcal{O}\left(\frac{n}{\ell^2}\right) = \mathcal{O}(n^\delta), \end{aligned}$$

by series reorganization, a split of the sum according to $\ell \gtrless \ell_0$, and trivial majorizations.

Given (53), the FVBD Hypothesis implies that $D(x) = \mathcal{O}(x^{1/2+\epsilon})$, at least when x is a positive *integer*. To extend this estimate to real values of x , it suffices to note that $D(x)$ is differentiable on $\mathbb{R}_{>0}$ and

$$D'(x) = \sum_{\ell=1}^{\infty} \frac{\mu(\ell)}{\ell} \left[e^{-x/\ell} - 1 \right],$$

is proved to be $\mathcal{O}(1)$ by bounding techniques similar to (53). Thus, assuming the FVBD Hypothesis, the estimate

$$D(x) = \mathcal{O}\left(x^{1/2+\epsilon}\right), \quad x \rightarrow +\infty$$

holds for *real* values of x .

Regarding the behaviour of $D(x)$ at 0, the general term of $D(x)$ is asymptotic to $x^2/(2\ell^2)$, so that $D(x) = \mathcal{O}(x^2)$, as $x \rightarrow 0^+$. This, combined with the estimate of $D(x)$ at infinity, implies that the Mellin transform

$$(54) \quad D^*(s) := \int_0^\infty D(x) x^{s-1} dx,$$

exists and is an analytic function of s for all s in the strip $-2 < \Re(s) < -\frac{1}{2} - \epsilon$. On the other hand, the usual properties of Mellin transforms (see, e.g., the survey [6]) imply that

$$(55) \quad D^*(s) = \left(\sum_{\ell=1}^{\infty} \mu(\ell) \ell^s \right) \cdot \int_0^{\infty} e^{-x} x^{s-1} dx = \frac{\Gamma(s)}{\zeta(-s)},$$

at least for s such that $-2 < \Re(s) < 1$, which ensures that the expansion of $1/\zeta(-s)$ is absolutely convergent. The comparison of the analytic character of (54) in $-2 < \Re(s) < -\frac{1}{2} - \epsilon$ (implied by the FVBD Hypothesis) and of the explicit form of (55) shows that the Riemann Hypothesis is a consequence of the FVBD Hypothesis. \square

Regarding the numerical properties of the sequence d_n , it appears that there are complicated oscillations, and these can to some extent be understood by a residue evaluation of (52), as we now explain. Assuming for notational convenience the simplicity of the nontrivial zeros of $\zeta(s)$, one has (unconditionally)

$$(56) \quad d_n = \sum_{\rho}^* \frac{1}{\zeta'(\rho)} \frac{\Gamma(n+1)\Gamma(-\rho)}{\Gamma(n+1-\rho)},$$

where the summation extends to all nontrivial zeros ρ of $\zeta(s)$ with $0 < \Re(\rho) < 1$, while the starred sum (\sum^*) means that zeros should be suitably grouped (see the discussion in §9.8 of Titchmarsh's treatise [21, p. 219], in relation to a formula of Ramanujan). A heuristic model of the sequence d_n then follows from the fact that, for large n , any individual term of the sum in (56) corresponding to a zeta zero $\rho = \sigma + i\tau$ is asymptotically

$$\frac{\Gamma(-\rho)}{\zeta'(\rho)} n^{\sigma} e^{i\tau \log n}.$$

Such a term involves a logarithmically oscillating component, a slowly growing component n^{σ} ($n^{\frac{1}{2}}$ under RH), as well as a multiplier that is likely to be extremely small, since it involves the quantity $\Gamma(-\rho) \asymp e^{-\pi|\tau|/2}$. The resulting oscillations then have the curious feature of being numerically detectable only for rather large values of n , and a possible failure of RH is exponentially offset—a similar fact was observed in [8, 16]. It is finally of interest to note that such phenomena do occur in nature, specifically, in the determination by [8] of *the expected number of continued fraction digits that are necessary to sort n real numbers drawn uniformly at random from the unit interval*.

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