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ASYMPTOTIC ESTIMATION OF $\xi^{(2n)}(1/2)$: ON A CONJECTURE OF FARMER AND RHOADES

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ABSTRACT. We verify a very recent conjecture of Farmer and Rhoades on the asymptotic rate of growth of the derivatives of the Riemann xi function at $s = 1/2$. We give two separate proofs of this result, with the more general method not restricted to $s = 1/2$. We briefly describe other approaches to our results, give a heuristic argument, and mention supporting numerical evidence.

INTRODUCTION

Let ξ be the Riemann xi function, given by $\xi(s) = \frac{1}{2}s(s-1)\pi^{-s/2}\Gamma(s/2)\zeta(s)$, where Γ is the Gamma function and ζ is the Riemann zeta function [7, 17]. It satisfies the functional equation $\xi(s) = \xi(1-s)$ and is entire of order 1. The functional equation implies that all odd order derivatives of ξ vanish at $s = 1/2$. On the other hand, estimation of the even order derivatives there has been an open problem and of interest from many points of view. Our main results are Propositions 1 and 2.

Proposition 1. *Let ξ be the Riemann xi function and n a positive integer. Then as $n \to \infty$ we have*

$$\ln \xi^{(2n)}\left(\frac{1}{2}\right) = 2n\ln(\ln n) - 2\left(\ln 2 + \frac{1}{\ln n}\right)n + \frac{9}{4}\ln(2n) - \frac{3}{4}\ln(\ln n) + O(1). \tag{1}$$

Proposition 2. *For real s and $j \to \infty$ we have*

$$\xi^{(j)}(s) = \frac{j(j-1)}{2^{j-1}}\frac{(j-2)^{(s-1)/2}}{\ln^{s/2}(j-2)}\left\{1 + (-1)^j\left[\frac{\ln(j-2)}{j-2}\right]^{s-1/2}\right\}$$
$$\times\left[\ln\left(\frac{j-2}{\pi}\right) - \ln\left(\ln\left(\frac{j-2}{\pi}\right)\right) + o(1)\right]^{j-3/2}\exp\left[-\frac{(j-2)}{\ln(j-2)}\right]. \tag{2}$$

Proposition 1 is in response to a conjecture of Farmer and Rhoades [8] that $\ln\xi^{(2n)}(1/2)$ should increase very regularly and not too much faster than linearly as $n \to \infty$. They made this conjecture in the course of a study of the effect of repeated differentiation upon the zero spacings of a real entire function of order 1. Current limited numerical evidence due to Kreminski [15] supports the conjecture and equation (1). The conjecture of Farmer and Rhoades was based upon the zero count $n_\pm(r)$ of the function $\Xi(z) = \xi(1/2 + iz)$ in the intervals $(0, r]$ and $[-r, 0)$,

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respectively. On the Riemann hypothesis, Ξ has only real zeros and $n_\pm(r) = (r/2\pi)\ln(r/2\pi e) + O(\ln r)$. We note that simply the leading term of (1) suffices to verify the conjecture of Farmer and Rhoades.

An initial set of values $\left\{\ln \xi^{(2n)}(1/2)\right\}_{n=0}^{20}$ is effectively given in Table 4.1 of [6] or Table 3.1 of [18]. However, these values are not yet in the asymptotic regime and indeed show a decrease rather than an increase with n.

Proposition 2 is separately proved from Proposition 1 and obviously subsumes the latter. Neither result is contingent upon the Riemann hypothesis. Proposition 2 is strong enough to imply a very recent result of Ki [14] that demonstrated another conjecture stated by Farmer and Rhoades. The asymptotic result (2) exhibits the property $\xi^{(j)}(1-s) = (-1)^j \xi^{(j)}(s)$.

After describing the proofs of (1) and (2) we provide further discussion, application, and context of these derivatives of the xi function. In particular, we briefly elaborate on important earlier numerical calculations.

Proof of Proposition 1

The result (1) uses estimates of Grosswald [9, 10] and Hayman [13] and the notation here essentially follows that of Grosswald. The function $\Xi(t)$ is even and the coefficients of t^2 alternate in sign. Putting

$$\xi(1/2+it) \equiv \Xi(t) = \sum_{n=0}^{\infty} c_n t^n = f(-t^2) = f(z) = \sum_{n=0}^{\infty} \alpha_n z^n, \tag{3}$$

we have $\xi(1/2+it) = \sum_{n=0}^{\infty}(-1)^n \alpha_n t^{2n}$, so that

$$\alpha_n = \frac{1}{(2n)!}\xi^{(2n)}\left(\frac{1}{2}\right). \tag{4}$$

We are interested in estimating the coefficients α_n, and for this we introduce the functions [9]

$$a_1(z) = \frac{1}{4}z^{1/2}\ln\frac{z^{1/2}}{2\pi} + \frac{7}{8} - \frac{1}{12}(z^{-1/2} - z^{-1}) + O(z^{-3/2}), \tag{5a}$$

$$a_2(z) = \frac{1}{8}z^{1/2}\ln\frac{ez^{1/2}}{2\pi} + \frac{1}{24}(z^{-1/2} - 2z^{-1}) + O(z^{-3/2}), \tag{5b}$$

and

$$\ln f(z) = \frac{1}{2}z^{1/2}\ln\frac{z^{1/2}}{2\pi e} + \frac{7}{8}\ln z + \frac{1}{4}\ln\frac{\pi}{2} + o(1) \tag{6}$$

$$= \frac{1}{2}z^{1/2}\ln\frac{z^{1/2}}{2\pi e} + \frac{7}{8}\ln z + \frac{1}{4}\ln\frac{\pi}{2} + \frac{1}{6z^{1/2}} + O\left(\frac{1}{z^{3/2}}\right),\ |z| \to \infty. \tag{7}$$

These functions are related by way of $a_2(z) = za_1'(z)$ and $a_1(z) = zf'(z)/f(z)$. The expression (6) due to Hayman [13] was refined by Grosswald [9, 10]. Equation (7) containing the first improvements to Hayman's result suffices for our purposes. We let r_n be the unique root of the equation $a_1(r) = n$ that approaches infinity as $n \to \infty$. We then have [9]

$$r_n^{1/2} = \frac{4n}{\ln n}\left[1 + O\left(\frac{\log_2 n}{\ln n}\right)\right], \tag{8a}$$

$$r_n^{1/2}\ln(r_n^{1/2}/2\pi) = 4(n - 7/8) + (r_n^{-1/2} - r_n^{-1})/3 + O(r_n^{-3/2}), \tag{8b}$$

and

$$\alpha_n = r_n^{-n}[2\pi a_2(r_n)]^{-1/2} f(r_n)\left[1-\frac{1}{24n}+O\left(\frac{1}{n\ln n}\right)\right]. \tag{9}$$

As seen from (8) we also need the estimate [9]

$$\frac{1}{a_2(z)} = \frac{2}{z}\left[1-\frac{1}{\ln z}+O\left(\frac{\log_2 z}{\ln^2 z}\right)\right]. \tag{10}$$

From (4) we have $\ln \xi^{(2n)}\left(\frac{1}{2}\right) = \ln \alpha_n + \ln(2n)!$, and we estimate this asymptotically in n, applying Stirling's formula to the second term on the right. In estimating $\ln f(r_n)$ coming from (9) we make use of (8b). The ordering of terms in powers or logarithms of r_n in terms of n is provided by (8a). We omit the further details that lead to (1). However, we note that the candidate leading term in $\ln \xi^{(2n)}\left(\frac{1}{2}\right)$ coming from $-n\ln r_n$ of $-2n\ln(2n)$ is cancelled by a contribution from $\ln(2n)!$.

Remarks. (i) The result (1) is improvable, as indeed Proposition 2 shows explicitly.

(ii) Grosswald [9] investigated the differences $D_n \equiv n\alpha_n^2 - (n+1)\alpha_{n-1}\alpha_{n+1}$ and found that $D_n = \alpha_n^2[1+O(1/\ln n)]$. Our explicit result (1) in terms of n now gives

Corollary 1.

$$\ln D_n = 4[1-\ln(4n)+\ln(\ln n)]n - \frac{4n}{\ln n} + \frac{7}{2}\ln(2n) - \frac{3}{2}\ln(\ln n) + O(1),\ n\to\infty. \tag{11}$$

Again, Proposition 2 offers refinements to this result.

Proof of Proposition 2

We have for all complex s [1]

$$\xi^{(j)}(s) = \frac{1}{2^{j-1}}\int_1^\infty [x^{3/2}\omega'(x)]'[x^{s/2-1/2}+(-1)^j x^{-s/2}]\ln^j x\; dx, \tag{12}$$

where the theta function $\omega(x) \equiv \sum_{n=1}^\infty \exp(-\pi n^2 x)$ [7]. We put, for $a>1$, $a+b\neq 1$, and $b\neq 0$,

$$I_j(a,b) \equiv \int_1^\infty [x^a\omega'(x)]' x^b \ln^{f(j)} x\; dx, \tag{13}$$

(14)
$$= \int_1^\infty x^{a+b-2}\omega(x)\ln^{f(j)-2} x[(a+b-1)b\ln^2 x + f(a+2b-1)\ln x + f(f-1)]dx,$$

(15)
$$= \int_0^\infty e^{(a+b-1)y}\omega(e^y)y^{f(j)-2}[(a+b-1)by^2x + f(a+2b-1)y + f(f-1)]dy,$$

where $f(j)>2$ is assumed to be monotonically increasing in j. We also impose the condition: if $b<0$ (respectively $b>0$), then $a>1-b$ (respectively $a<1-b$). We apply the method of steepest descent [21]. We write $I_j = \int_0^\infty e^{g(y)}dy$ and $\omega(x) = e^{-\pi x}[1+\omega_2(x)] = e^{-\pi x}[1+O(e^{-3\pi x})]$. Define y^* as the solution of the equation $dg/dy = 0$. We have

$$\frac{dg}{dy} = a+b-1+\frac{f(j)-2}{y}+\frac{2(a+b-1)by+f(a+2b-1)}{(a+b-1)by^2+f(a+2b-1)y+f(f-1)}-\pi e^y$$

$$+\frac{1}{1+\omega_2(e^y)}\frac{d}{dy}\omega_2(e^y), \tag{16a}$$

$$\frac{d^2g}{dy^2} = -\frac{[f(j)-2]}{y^2}-\pi e^y++\frac{d^2}{dy^2}\ln[1+\omega_2(e^y)]$$

$$+\frac{-2b^2(a+b-1)^2y^2-2b(a+b-1)(a+2b-1)y-2b^2(1+f)-2(a-1)b(f+1)-f^2(a-1)^2}{[(a+b-1)by^2+f(a+2b-1)y+f(f-1)]^2}. \tag{16b}$$

Under the conditions placed upon a and b, the quadratic expression in y in the denominator of the third term on the right side of (16a) will have real and distinct roots $y_\pm$ for large values of f. Furthermore, we then have $dg/dy \to \infty$ as $y \to 0$, $dg/dy \to -\infty$ as $y \to y_+$ from the left, and $d^2g/dy^2 < 0$ on $(0, y_+)$. This ensures that there is a unique solution y^* of $dg/dy = 0$. The approximate equation $[f(j)-2]/y = \pi \exp(y)$ is asymptotically solved as $f \to \infty$ by (e.g., [5])

$$y^* = \left[\ln\left(\frac{f(j)-2}{\pi}\right) - \ln\ln\left(\frac{f(j)-2}{\pi}\right)\right] + o(1). \tag{17}$$

This equation follows since $y^* = W[(f(j)-2)/\pi]$, where W is Lambert's W function [5]. To leading order in large f we have $|d^2g/dy^2|_{y=y^*} = (f-2)(1+1/y^*)/y^*$. We then find the asymptotic evaluation

$$I_j(a,b) \sim \frac{\sqrt{2\pi}\exp g(y^*)}{\left|\frac{d^2g}{dy^2}(y^*)\right|^{1/2}}$$

$$\sim \frac{f(f-1)(f-2)^{a+b-3/2}}{\ln^{a+b-1}(f-2)}\left[\ln\left(\frac{f-2}{\pi}\right)-\ln\left(\ln\left(\frac{f-2}{\pi}\right)\right)\right]^{f-3/2}\exp\left[-\frac{(f-2)}{\ln(f-2)}\right]. \tag{18}$$

The combination of (12), (13), and (18) then gives (2).

In particular, we have as $j \to \infty$:

Corollary 2.

$$\xi^{(j)}(1) \sim \frac{j(j-1)}{2^{j-1}\ln^{1/2}(j-2)}\left\{1+(-1)^j\left[\frac{\ln(j-2)}{j-2}\right]^{1/2}\right\}$$

$$\times\left[\ln\left(\frac{j-2}{\pi}\right)-\ln\left(\ln\left(\frac{j-2}{\pi}\right)\right)\right]^{j-3/2}\exp\left[-\frac{(j-2)}{\ln(j-2)}\right]. \tag{19}$$

Discussion: Other approaches and a heuristic

We first supply some remarks on the asymptotic results that we applied for equation (1). In a second paper, Grosswald [10] provided more details on his method, including specifically uniform estimates for his $a_\nu(z)$ functions that include a_1 and a_2 of (5). Grosswald's approach can sometimes provide stronger results than Hayman's [13] for "admissible" functions, since he further restricts the allowable functions. Very related work on asymptotic expansions for the coefficients of analytic functions was performed by Harris and Schoenfeld [11], wherein they invoke weaker hypotheses than Grosswald. Pertinent results on the maximum modulus and Fourier transform of the Riemann xi function are given by Haviland [12] and Wintner [19, 20].

The authors of [6], while investigating the Turán inequalities, used the moments

$$\hat{b}_m \equiv \int_0^\infty t^{2m}\Phi(t)dt, \tag{20}$$

where

$$\Phi(t) \equiv \sum_{n=0}^\infty (2n^4\pi^2 e^{9t} - 3n^2\pi e^{5t})\exp(-n^2\pi e^{4t}). \tag{21}$$

Given the power series

$$\frac{1}{8}\Xi\left(\frac{x}{2}\right) = \sum_{m=0}^\infty (-1)^m \frac{\hat{b}_m x^{2m}}{(2m)!}, \tag{22}$$

in view of (3) and (4) we identify

$$\hat{b}_m = \frac{(2m)!}{2^{2m+3}}\alpha_m = \frac{\xi^{(2m)}(1/2)}{2^{2m+3}}. \tag{23}$$

From Proposition 1 or 2 we therefore obtain

Corollary 3.

$$\ln \hat{b}_n = 2n\ln(\ln n) - 2\left(2\ln 2 + \frac{1}{\ln n}\right)n + \frac{9}{4}\ln(2n) - \frac{3}{4}\ln(\ln n) + O(1),\ \ n \to \infty. \tag{24}$$

The value of $\hat{b}_0$ is given exactly by $\hat{b}_0 = \xi(1/2)/8 = -\Gamma(1/4)\zeta(1/2)/64\pi^{1/2}$, where $\Gamma(1/4) = -\gamma - \pi/2 - 3\ln 2$, $\gamma = -\psi(1)$ is Euler's constant, ψ is the digamma function, and $\zeta(1/2) = (1+\sqrt{2})\sum_{n=1}^\infty (-1)^n/\sqrt{n}$, so that $\hat{b}_0 \simeq 0.0621401$. As alluded to in the Introduction, examining only the first 42 or so derivatives of ξ at $s = 1/2$ would give a misleading impression, as there is a minimum value after the initial decrease. Indeed, the initial decrease of $\xi^{(j)}(1/2)$ implies the monotonic decrease of the moments $\hat{b}_m$ until $m = 339$. Based upon the minimum numerical value of $\hat{b}_{339}$ [18, 16], we know that approximately $\xi^{(678)}(1/2) \simeq 2.19259386 \times 10^{134}$. The numerical result of Kreminski [15] agrees with this value. It turns out that all of the moments $\{\hat{b}_m\}_{m=0}^{1000}$ were numerically determined in [16] and Appendix A there gives their values to approximately 16 decimal digits. These calculations were done with FORTRAN using floating point precision of 360 decimal places. From the value of $\hat{b}_{1000}$ we then know that $\xi^{(2000)}(1/2) \simeq 3.993042456301144 \times 10^{600}$. To our knowledge, this remains the highest order derivative of the xi function at $s = 1/2$ numerically calculated and reported.

Very recently Ki [14] proved another conjecture of Farmer and Rhoades, that there are sequences $\{A_n\}$ and $\{C_n\}$, with $C_n \to 0$ slowly with n, such that

$$\lim_{n\to\infty} A_n \Xi^{(2n)}(C_n z) = \cos z \tag{25}$$

uniformly on compacts subsets of $\mathbb{C}$. Ki's proof employed a kind of saddle point method when differentiating the Fourier transform representation of the Ξ function. His result holds more generally for functions with a Fourier transform of a certain polynomial-times-exponential form. Ki's result (25) directly gives a heuristic for

(1). For by comparing Maclaurin series coefficients on both sides of (25) we would have for large values of n,

$$A_n \alpha_n \sim \frac{1}{(2n)!} \left(\frac{1}{C_n}\right)^{2n}, \tag{26}$$

where asymptotically

$$C_n^{-1} \sim \frac{1}{2} \left[\ln\left(\frac{2n}{\pi}\right) - \ln\ln\left(\frac{2n}{\pi}\right)\right], \tag{27}$$

$A_n = v_n(-1)^n C_n^{2n+1}/2$, and $\{v_n\}$ is another sequence. Then we could expect that as $n \to \infty$, $\ln A_n + \ln \alpha_n \sim -2n \ln C_n - \ln(2n)!$. Our Proposition 1 shows that indeed this relation holds. In fact, we now know that $v_n \sim 2(-1)^n/(2n)! \alpha_n C_n^{4n+1}$, so that $\ln|v_n| \sim 2n \ln(\ln n) + 2(\ln 2 + 1/\ln n)n + O(\ln n)$, giving the sequence $\{A_n\}$ explicitly to leading order also. As our method for Proposition 2 can provide the constant term in the asymptotic expansion of $\xi^{(2n)}(1/2)$, it gives another way to verify the conjecture (25) confirmed by Ki. Since Ki's result extends to other Ξ functions, including those for Hecke L-functions, we may similarly expect that asymptotic derivative results analogous to Propositions 1 and 2 are possible.

The relation (27) arises as the approximate solution for large n of the equation $aw_n \exp(w_n) = bw_n + 2n$, where $w_n = 1/C_n$ [14]. Assuming the slow variation of w_n with n, the simplified equation $w_n \exp(w_n) \simeq 2n/a$ is just that for the well-known Lambert W-function (e.g., [5]) that arises so often in asymptotic analysis and perturbation theory. The upshot is that the asymptotic expressions for w_n and C_n are improvable.

We mention some equivalent asymptotic estimation problems for Proposition 1 or 2. A frontal assault on computing $\xi^{(2j)}(1/2)$ can be made by using the definition of the xi function together with the product rule. Differentiating j times on the factor $\pi^{-s/2}$ simply gives $(-1/2)^j \pi^{-s/2} \ln^j \pi$ and differentiating m times on the factor $\Gamma(s/2)$ or $m-1$ times on $(1/2)\Gamma(s/2)\psi(s/2)$ gives a sum of terms of products of Gamma and polygamma functions. Within this approach, estimation of the values of $\zeta^{(n)}(1/2)$ are required and the expected difficulty is proper estimation of the significant cancellation occurring in the various summations.

From equation (12) we have for even integers j,

$$\xi^{(j)}\left(\frac{1}{2}\right) = \frac{1}{2^{j-2}} \int_1^\infty [x^{3/2}\omega'(x)]' x^{-1/4} \ln^j x \, dx > 0, \tag{28}$$

and equivalent forms by integration by parts. In addition, it has been described in [1] how to obtain $\xi^{(2m)}(1/2)$ as an infinite series using special functions. For the theta function in (12) and (28) one has the bound

$$\omega(x) \le \exp(-\pi x) \sum_{n=1}^\infty \exp[-\pi(n^2-1)] < 1.000081 \exp(-\pi x) \text{ for } x > 1.$$

From (3) we may alternatively write

$$\xi(s) = \sum_{n=0}^\infty \alpha_n \left(s - \frac{1}{2}\right)^{2n}. \tag{29}$$

By introducing a binomial expansion in this equation, we may expand the xi function for other points of the complex plane, thereby expressing the derivatives there in terms of the constants α_n. For instance, we have

$$\xi(s) = \sum_{j=0}^{\infty} c_j (s-1)^j, \tag{30}$$

where $c_j = \sum_{n=j/2}^{\infty} \binom{2n}{j} \alpha_n / 2^{2n-j} = \xi^{(j)}(1)/j!$. This permits estimation of the growth of xi function derivatives at other locations based upon Proposition 1. For $s = 1$, one method to express c_j is in terms of the well-known Stieltjes constants γ_k (e.g., [2, 3]). In particular, for (30), the values $\xi^{(j)}(1)$ (cf. Corollary 2) precisely enter the Li criterion for the validity of the Riemann hypothesis [1, 4].

Our Proposition 2 is strong enough to provide an alternative proof of the conjecture (25) confirmed by Ki [14]. It also gives asymptotic information on many other important constants. In particular, it has implications for the Stieltjes constants.

In concluding, we have demonstrated the validity of a very recent conjecture of Farmer and Rhoades [8] on the near-linear rate of growth of $\ln \xi^{(2j)}(1/2)$. This result is consistent with the known count of the number of nontrivial zeros of the xi function lying in the critical strip to a given height. Proposition 1 has been numerically examined elsewhere for $n \leq 400$ [15]. We have described connections of $\xi^{(2j)}(1/2)$ to the Turán differences for the Ξ function and other quantities. While it does not appear that the growth rate of these derivatives has a direct impact to the validity of the Riemann hypothesis, their behaviour is linked to the coefficients c_j of (30) and therefore to the Li/Keiper constants [1, 4].

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