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Simple zeros and discrete moments of the derivative of the Riemann zeta-function

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Abstract

We prove unconditional upper bounds for the second and fourth discrete moment of the first derivative of the zeta-function at its simple zeros on the critical line.

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Keywords: Riemann zeta-function; Simple zeros

1. Introduction and statement of results

The Riemann zeta-function $\zeta(s)$ is for $\mathrm{Re}\, s > 1$ defined by

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \prod_p \left(1 - \frac{1}{p^s}\right)^{-1},$$

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where the product is taken over all prime numbers p, and by analytic continuation elsewhere except for a simple pole at $s = 1$. The famous yet unsolved Riemann hypothesis states that all so-called non-trivial (non-real) zeros lie on the critical line $\operatorname{Re} s = 1/2$. The number $N(T)$ of non-trivial zeros with ordinates in the interval $(0, T]$ is asymptotically given by the Riemann–von Mangoldt formula

$$N(T) = \frac{T}{2\pi} \log \frac{T}{2\pi e} + O(\log T). \tag{1}$$

Conrey [2] proved (refining a method of Levinson) that more than two-fifths of the zeros are simple and on the critical line. It is conjectured that all or at least almost all zeros of the zeta-function are simple.

Hall [8] proved upper estimates for the second and fourth moment of the extreme values of the Riemann zeta-function between its zeros on the critical line with respect to the spacing of consecutive extrema. In this paper, we study the related discrete moments of the values of the derivative of the zeta-function taken at simple zeros.

Denote the positive roots of the function $\zeta(1/2 + it)$ in ascending order by t_n according to their multiplicities. Let λ_n be the least t in the interval (t_n, t_{n+1}) for which $|\zeta(\frac{1}{2} + it)|$ is maximal and let T and θ be positive parameters. Finally, for $k \geqslant 0$, define

$$\mathcal{S}_k(T, \theta) = \sum_{\substack{n \leqslant N \\ \lambda_{n+1} - \lambda_n \leqslant 2\pi\theta/\log T}} |\zeta'(1/2 + it_n)|^{2k},$$

where N is the number of ordinates t_n not exceeding T. Note that the Riemann hypothesis implies that the t_n correspond to the positive ordinates of non-trival zeros of the zeta-function, i.e., $N = N(T) \sim \frac{T}{2\pi} \log T$ by (1). If the Riemann hypothesis is true, there is always one ordinate t_n between λ_n and λ_{n+1} and there is always a λ_n between t_n and t_{n+1} for sufficiently large n (see [4]). The average spacing between consecutive zeros with ordinates of order T is $2\pi/\log T$, which tends to zero as $T \to \infty$. Since a positive proportion of the zeros lies on the critical line (by Conrey's result mentioned above), we have $N \gg N(T)$ unconditionally. We write $\theta = \infty$ when there is no restriction on the spacing of consecutive λ_n

Theorem 1. *As* $T \to \infty$,

$$\mathcal{S}_1(T, \infty) \leqslant 0.02513\ldots T(\log T)^4 + O(T(\log T)^3),$$
$$\mathcal{S}_2(T, \infty) \leqslant (0.00003\,0036\ldots + o(1))T(\log T)^9.$$

On the basis of random matrix theory, Hughes, et al. [11] stated an interesting conjecture on discrete moments of the zeta-function at its zeros subject to the truth of Riemann's hypothesis and the assumption that all zeros are simple. This conjecture includes that for fixed $k > -3/2$ the asymptotic formula

$$\sum_{0<\gamma\leqslant T} |\zeta'(1/2+i\gamma)|^{2k} \sim \frac{G^2(k+2)}{G(2k+3)} a(k) \frac{T}{2\pi} (\log T)^{(k+1)^2} \tag{2}$$

holds, where

$$a(k) = \prod_p \left(1 - \frac{1}{p^2}\right)^{k^2} \sum_{m=0}^{\infty} \left(\frac{\Gamma(m+k)}{m!\Gamma(k)}\right)^2 \frac{1}{p^m},$$

G is the Barnes G-functions, defined by

$$G(z+1) = (2\pi)^{z/2} \exp\left(-\frac{1}{2}(z(z+1)+\gamma z^2)\right) \times \prod_{n=1}^{\infty} \left(1+\frac{z}{n}\right)^n \exp\left(-z+\frac{z^2}{n}\right)$$

and γ is Euler's constant; note that in the above definition of the numbers $a(k)$, one must take an appropriate limit if $k = 0$ or -1. Conjecture (2) is known to be true only in the trivial case $k = 0$ and in the case of the second moment $k = 1$. Assuming the truth of the Riemann hypothesis Gonek [6] proved

$$\mathcal{S}_1(T, \infty) = \frac{1}{24\pi} T(\log T)^4 + O\left(T(\log T)^3\right). \tag{3}$$

The constant $0.02513\ldots$ in the unconditional estimate of Theorem 1 does not fall much beyond $1/(24\pi) = 0.01326\ldots$ in the asymptotic formula above. For the case $k = 2$ formula (2) gives (see [11] or [15])

$$\mathcal{S}_2(T, \infty) \sim \frac{1}{2880\pi^3} T(\log T)^9.$$

Note that $1/2880\pi^3 = 0.00001\,1198\ldots$. Recently, Ng [15] proved, under assumption of the truth of Riemann's hypothesis,

$$(0.00000\,2\ldots + o(1))T(\log\ T)^9 \leqslant \mathcal{S}_2(T, \infty) \leqslant (0.00016\,6\ldots + o(1))(\log\ T)^9.$$

Thus the unconditional constant $0.00003\,0036\ldots$ from Theorem 1 improves the upper bound in Ng's result.

Estimates of the predicted size are known for some more cases, most of them conditional to some unproved conjectures. Assuming the Riemann hypothesis and that all zeros of the zeta-function are simple, Gonek [7] obtained the lower bound

$$\mathcal{S}_{-1}(T,\infty) \gg T.$$

The only known unconditional estimate is due to Garaev [5] (implicitly) and Laurinčikas, Šleževičienė and the second author [12,17] (independently), namely

$$\mathcal{S}_{1/2}(T,\infty) \ll T(\log T)^{9/4}. \tag{4}$$

Furthermore, we shall consider $\mathcal{S}_k(T,\theta)$ with respect to small values of $\theta > 0$.

Theorem 2. *As* $T \to \infty$,

$$\mathcal{S}_1(T,\theta) \leqslant \frac{\pi^3\theta^3}{2688} T(\log T)^4 + O(T(\log T)^3),$$

$$\mathcal{S}_2(T,\theta) \leqslant \left(\frac{\pi\theta^3}{73920} + o(1)\right) T(\log T)^9.$$

The estimates are uniform in θ.

The above upper bounds can be compared with estimates due to the second author [18] (obtained with a different method) where the condition on gaps of consecutive λ_n is replaced by $t_{n+1} - t_n \leqslant 2\pi\theta/\log T$. For instance,

$$\sum_{\substack{n \leqslant N \\ t_{n+1}-t_n \leqslant 2\pi\theta/\log T}} |\zeta'(1/2 + it_n)|^4 \leqslant \left(\frac{17\pi\theta^3}{221\,760} + o(1)\right) T(\log T)^9.$$

As Hall [10] pointed out for his discrete moments on extremal values, estimates like those above give some numerical evidence for the truth of Montgomery's pair correlation conjecture [14] which claims under assumption of the Riemann hypothesis that, for fixed α, β satisfying $0 < \alpha < \beta$,

$$\lim_{T\to\infty} \frac{1}{N(T)} \sharp \left\{ 0 < \gamma, \gamma' < T \,:\, \alpha \leqslant \frac{(\gamma - \gamma')\log T}{2\pi} \leqslant \beta \right\} = \int_\alpha^\beta \left(1 - \left(\frac{\sin \pi u}{\pi u}\right)^2\right) du,$$

where γ and γ' are ordinates of zeros of $\zeta(s)$. This open conjecture implies that the number of t_n with $n \leqslant N$ and $t_{n+1} - t_n \leqslant 2\pi\theta/\log T$ is asymptotically equal to

$$\left(\frac{\pi^2\theta^3}{9} + O(\theta^4)\right) N(T).$$

The estimates of Theorem 2 provide information about large gaps between consecutive extreme values on the critical line. Define

$$\mathcal{S}_k^-(T,\theta)=\mathcal{S}_k(T,\theta) \quad \text{and} \quad \mathcal{S}_k^+(T,\theta)=\sum_{\substack{n\leqslant N\\ \lambda_{n+1}-\lambda_n>2\pi\theta/\log T}}|\zeta'(1/2+it_n)|^{2k}.$$

Then

$$\mathcal{S}_k(T,\infty)=\mathcal{S}_k^-(T,\theta)+\mathcal{S}_k^+(T,\theta).$$

In view of Gonek's asymptotic formula (3) and Theorem 2, under assumption of the Riemann hypothesis,

$$\mathcal{S}_1^+(T,\theta)\geqslant c(\theta)T(\log T)^4+O\left(T(\log T)^3\right), \tag{5}$$

where

$$c(\theta):=\frac{1}{24\pi}-\frac{\pi^3\theta^3}{2688}.$$

The quantity $c(\theta)$ is positive for $\theta<2\times 14^{1/3}/\pi^{4/3}=1.04762\ldots$. It follows that, assuming Riemann's hypothesis,

$$\limsup_{\substack{n\to\infty\\ \zeta'(1/2+it_n)\neq 0}}\frac{\lambda_{n+1}-\lambda_n}{2\pi/\log\lambda_n}\geqslant 1.04762\ldots\ . \tag{6}$$

With respect to the average spacing of consecutive zeros any value larger than one is non-trivial. A refined analysis would lead a lower bound $1.273\ldots$, however, methods designed for such estimates lead to much better lower bounds; e.g. Selberg [16], Conrey et al. [3], and Hall [9]. However, here it follows that (6) holds for quite many zeros of the zeta-function. By the Cauchy–Schwarz inequality,

$$\mathcal{S}_1^+(T,\theta)^2\leqslant\mathcal{S}_0^+(T,\theta)\,\mathcal{S}_2^+(T,\theta).$$

The right-hand side is bounded above by

$$\mathcal{S}_0^+(T,\theta)\,\mathcal{S}_2(T,\infty) \quad \text{and} \quad \mathcal{S}_0(T,\infty)\,\mathcal{S}_2^+(T,\theta),$$

respectively. Note that $\mathcal{S}_0^+$ counts simple zeros on the critical line with respect to the distance between consecutive extrema. Taking into account Theorems 1, 2, and inequality (5) we obtain

Corollary 3. *Assume the truth of the Riemann hypothesis. Then, for any* $\theta \in (0, 1.04762\ldots)$, *as* $T \to \infty$,

$$\mathcal{S}_0^+(T,\theta) \geqslant (33\,292.8\ldots + o(1)) \left(\frac{1}{24\pi} - \frac{\pi^3\theta^3}{2688} \right)^2 \frac{T}{\log T},$$

$$\mathcal{S}_2^+(T,\theta) \geqslant (2\pi + o(1)) \left(\frac{1}{24\pi} - \frac{\pi^3\theta^3}{2688} \right)^2 T(\log T)^7.$$

2. Preliminaries: mean values for Hardy's Z-function

Hardy's Z-function $Z(t)$ is defined by

$$Z(t) = \exp(i\vartheta(t))\zeta(1/2 + it), \tag{7}$$

where

$$\exp(i\vartheta(t)) := \pi^{-it/2} \frac{\Gamma(1/4 + it/2)}{|\Gamma(1/4 + it/2)|}. \tag{8}$$

The functional equation for the zeta-function implies that $Z(t)$ is an infinitely often differentiable function which is real for real t. Moreover,

$$|\zeta(1/2 + it)| = |Z(t)|.$$

Thus, the zeros and extrema of $Z(t)$ correspond to the zeros and extrema of the zeta-function on the critical line, respectively. Differentiation of (7) yields

$$Z'(t) = i\ \exp(i\vartheta(t)) \left\{ \vartheta'(t)\zeta(1/2 + it) + \zeta'(1/2 + it) \right\}. \tag{9}$$

In order to prove our results we shall use asymptotic formulae for derivatives of Hardy's Z-function. Hall [8] proved, for any $k \in \mathbb{N} \cup \{0\}$,

$$\int_0^T Z^{(k)}(t)^2\,dt = \frac{1}{2^{2k}(2k+1)} T P_{2k+1}\left(\log \frac{T}{2\pi} \right) + O\left(T^{3/4} (\log T)^{2k+1/2} \right), \tag{10}$$

where P_{2k+1} is a monic polynomial of degree $2k+1$,

$$\int_0^T Z'(t)^4\,dt = \frac{1}{1120\pi^2} T(\log T)^8 + O\left(T(\log T)^7 \right) \tag{11}$$

and

$$\int_0^T Z'(t)^2 Z''(t)^2\,dt = \frac{19}{604\,800\pi^2} T(\log T)^{10} + O\left(T(\log T)^9\right). \tag{12}$$

In addition, the second author [18] obtained

$$\int_0^T Z''(t)^4 dt \sim \frac{17}{1\,774\,080\pi^2} T(\log T)^{12}. \tag{13}$$

However, we will also need an asymptotic formula for the mean-square of $Z'(t)Z'''(t)$.

Conrey [1] proved an asymptotic formula for the fourth moment of derivatives of the zeta-function. For some polynomials P_j, $j = 1, 2$, let

$$A_j(s) = P_j\left(-\frac{1}{L}\frac{d}{ds}\right)\zeta(s),$$

where $L := \log(T/(2\pi))$. Then,

$$\int_1^T |A_1 A_2(1/2+it)|^2\,dt \sim c(P_1, P_2)\frac{6}{\pi^2} T L^4, \tag{14}$$

where

$$\begin{aligned} c(P_1, P_2) := \int_{\mathcal{R}} &(P_1(\alpha+\beta)P_2(\gamma+\delta)P_1(\alpha+\gamma)P_2(\beta+\delta) + P_1(1-\alpha-\beta) \\ &\times P_2(1-\gamma-\delta)P_1(1-\alpha-\gamma)P_2(1-\beta-\delta))\; d\alpha\, d\beta\, d\gamma\, d\delta \end{aligned}$$

with

$$\mathcal{R} = \{0 \leqslant \alpha, \beta, \gamma, \delta \leqslant 1 \;:\; \alpha+\beta+\gamma+\delta \leqslant 1\}.$$

We apply this asymptotic formula to $A_1 = Z'(t)$ and $A_2 = Z'''(t)$.

In view of (9),

$$\begin{aligned} Z'''(t) = \exp(i\vartheta(t)) \Big\{ &(i\vartheta'''(t) - 3\vartheta'\vartheta''(t) - i\vartheta'(t)^3)\zeta(1/2+it) \\ &-3(\vartheta''(t) + i\vartheta'(t)^2)\zeta'(1/2+it) \\ &- 3i\vartheta(t)'\zeta''(1/2+it) - i\zeta'''(1/2+it)\Big\}. \end{aligned} \tag{15}$$

By Stirling's formula,

$$\vartheta(t) = \frac{t}{2}\log\frac{t}{2\pi e} - \frac{\pi}{8} + O\left(\frac{1}{t}\right), \quad \vartheta'(t) = \frac{1}{2}\log\frac{t}{2\pi} + O\left(\frac{1}{t}\right)$$

and

$$\vartheta''(t),\ \ \vartheta'''(t) \ll \frac{1}{t},$$

all estimates valid for sufficiently large t. Then, for $t \leqslant T$, we may rewrite (9) and (15) as

$$\begin{aligned} Z'(t) &= i\ \exp(i\vartheta(t))\left\{\left(\frac{1}{2}L + O(1)\right)\zeta(1/2+it) + \zeta'(1/2+it)\right\}, \\ Z'''(t) &= -i\ \exp(i\vartheta(t))\left\{\left(\frac{1}{8}L^3 + O(L^2)\right)\zeta(1/2+it) + \left(\frac{3}{4}L^2 + O(L)\right)\right. \\ &\qquad \left. \times\zeta'(1/2+it) + \left(\frac{3}{2}L + O(1)\right)\zeta''(1/2+it) + \zeta'''(1/2+it)\right\}. \end{aligned}$$

Putting

$$P_1(X) = -X + \frac{1}{2} \quad \text{and} \quad P_2(X) = -X^3 + \frac{3}{2}X^2 - \frac{3}{4}X + \frac{1}{8},$$

we get

$$\int_0^T Z'(t)^2 Z'''(t)^2\,dt \sim L^8 \int_0^T |A_1A_2(1/2+it)|^2\,dt.$$

After a short computation, Conrey's asymptotic formula (14) implies

$$\int_0^T Z'(t)^2 Z'''(t)^2\,dt \sim \frac{19}{1\,774\,080\pi^2} T(\log T)^{12}. \tag{16}$$

3. Proofs of the theorems

From (9) it follows that

$$|Z'(t_n)| = |\zeta'(1/2+it_n)|. \tag{17}$$

Thus, if and only if the first derivative $Z'(t)$ does not vanish in the ordinate t_n of a zero of the zeta-function on the critical line, the zero $1/2+it_n$ is simple.

By definition, the λ_n are positive distinct zeros of $Z'(t)$. Denote by $\tilde{\lambda}_m$ the positive roots of the function $Z'(t)$ in ascending order (counting multiplicities); then for any λ_n there is a positive integer m such that $\lambda_n = \tilde{\lambda}_m$. Define

$$F_m = \max_{\tilde{\lambda}_m < t < \tilde{\lambda}_{m+1}} |Z'(t)|.$$

Then

$$\mathcal{S}_k(T, \infty) = \sum_{n \leqslant N} |\zeta'(1/2 + it_n)|^{2k} \leqslant \sum_{m \leqslant M} F_m^{2k},$$

where M is the number of zeros $\tilde{\lambda}_m$ of $Z'(t)$ not exceeding T. Matsumoto and Tanigawa [13] proved that the number of zeros of the kth derivative $Z^{(k)}(t)$ of Hardy's Z-function in the interval $(0, T)$ is less than or equal to

$$\frac{T}{2\pi} \log \frac{T}{2\pi e} + O_k(\log T).$$

In comparison with (1) it follows that $N \leqslant M \leqslant N(T) + O(\log T)$, so the above quantity is an upper bound for M too.

The heart of the proofs is the following lemma due to Hall [8].

Lemma 4. *Let $y(x)$ be real-valued on $[a, b]$, $y(a) = y(b) = 0$. Suppose that y is twice differentiable, $y'' \in L^2[a, b]$, and that*

$$\int_a^b y(x)^2\, dx = A, \quad \int_a^b y'(x)^2\, dx = B, \quad \int_a^b y''(x)^2\, dx = C.$$

Put $F = \max\{|y(x)| : a < x < b\}$. Then, for arbitrary $\mu > \lambda > 0$, we have

$$F^2 \leqslant \frac{\lambda^2 \mu^2 A + (\lambda^2 + \mu^2) B + C}{2(\mu^2 - \lambda^2)} \left(\frac{1}{\lambda} \tanh \frac{\lambda L}{2} - \frac{1}{\mu} \tanh \frac{\mu L}{2} \right)$$

in which $L = b - a$.

We start with the

Proof of Theorem 1. First we consider the second moment. As in Hall [8] we apply Lemma 4 with $\lambda = u \log T$, $\mu = v \log T$, $\ell_m = L = \tilde{\lambda}_{m+1} - \tilde{\lambda}_m$, and

$$w(u, v; \ell_m)^{-1} = \frac{1}{2(\mu^2 - \lambda^2)} \left(\frac{1}{\lambda} \tanh \frac{\lambda L}{2} - \frac{1}{\mu} \tanh \frac{\mu L}{2} \right).$$

Then by Lemma 4 with $y = Z'$,

$$F_m^2 w(u, v; \ell_m) \leqslant \int_{\tilde{\lambda}_m}^{\tilde{\lambda}_{m+1}} \left(u^2 v^2 Z'(t)^2 \log T + \frac{1}{\log T}(u^2 + v^2) Z''(t)^2 + \frac{1}{(\log T)^3} Z'''(t)^2 \right) dt.$$

Summing up we obtain via (10)

$$\begin{aligned} \sum_{m \leqslant M} F_m^2 w(u, v; \ell_m) &\leqslant \int_0^T \left(u^2 v^2 Z'(t)^2 \log T + \frac{1}{\log T}(u^2 + v^2) Z''(t)^2 \right. \\ &\quad \left. + \frac{1}{(\log T)^3} Z'''(t)^2 \right) dt + F_M^2 w(u, v; \ell_M) \\ &\leqslant \left(\frac{u^2 v^2}{12} + \frac{u^2 + v^2}{80} + \frac{1}{448} \right) T (\log T)^4 \\ &\quad + O\left(T (\log T)^3 \right). \end{aligned} \tag{18}$$

The function $w(u, v; \ell)$ is decreasing in ℓ and

$$w(u, v; \infty) = 2uv(u + v).$$

Thus we need to minimize the function

$$g(p, s) := \frac{1}{2ps} \left(\frac{p^2}{12} + \frac{s^2 - 2p}{80} + \frac{1}{448} \right),$$

where $p = uv$, $s = u + v$, and $p \leqslant \frac{s^2}{4}$, and this minimum will be the coefficient in our upper estimate.

It turns out that $g(p, s)$ has an extreme value for $p = 5/28$ and $s = \pm\sqrt{15}/21$, however, for these values the condition $p \leqslant s^2/4$ is not satisfied. Thus we look for the minimal value of $g(p, s)$ under the condition $p = s^2/4$. After a short computation we find that this value is equal to

$$\frac{1}{6\,615\,000}(735 + 420\sqrt{14})^{3/2} + \frac{11}{63\,000}\sqrt{735 + 420\sqrt{14}} = 0.02513\ \ldots.$$

This proves the upper bound for the second moment.

Next we consider the estimate for the fourth moment. For this purpose we apply Lemma 4 with $y = Z'^2$. In view of (11), (13), and (16)

$$\sum_{m \leqslant M} F_m^4 w(u, v; \ell_m) \leqslant \frac{1}{1120\pi^2} \left(u^2 v^2 + \frac{19(u^2+v^2)}{135} + \frac{1}{11} + o(1) \right) T(\log T)^9. \quad (19)$$

In this case we need to minimize the function

$$f(p,s) := \frac{1}{2240\pi^2 ps} \left(p^2 + \frac{19(s^2-2p)}{135} + \frac{1}{11} \right)$$

for $p = s^2/4$. The minimal value is

$$\begin{aligned} &\frac{19}{15\,004\,350\,900\,000\pi^2}(34\,485 + 165\sqrt{645\,106})^{3/2} \\ &+\frac{46\,733}{90\,935\,460\,000\pi^2}\sqrt{34\,485 + 165\sqrt{645\,106}} \\ &= 0.00003\,0036\ldots\ . \end{aligned}$$

This proves the upper bound for the fourth moment. □

It remains to give the

Proof of Theorem 2. It follows from (18) that

$$\sum_{\substack{m \leqslant M \\ \ell_m \leqslant 2\pi\theta/\log T}} F_m^2 \leqslant w\left(u, u; \frac{2\pi\theta}{\log T}\right)^{-1} \left(\frac{u^4}{12} + \frac{u^2}{40} + \frac{1}{448} \right) (T(\log T)^4$$
$$+ O(T(\log T)^3)).$$

Putting $u = 0$ we obtain the assertion on the second moment. In view of (19) we get

$$\sum_{\substack{m \leqslant M \\ \ell_m \leqslant 2\pi\theta/\log T}} F_m^4 \leqslant w\left(u, u; \frac{2\pi\theta}{\log T}\right)^{-1} \frac{1}{1120\pi^2} \left(u^4 + \frac{19u^2}{135} + \frac{1}{11} + o(1) \right) T(\log T)^9.$$

Putting $u = 0$ we obtain the estimate for the fourth moment. The uniformity in θ follows from Hall's method. □

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