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.

Keywords: Riemann zeta-function, simple zeros.
AMS subject classification numbers: 11M06.

1 Introduction and statement of results

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

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

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 nontrivial (non-real) zeros lie on the critical line $\text{Re } s = 1/2$. The number $N(T)$ of nontrivial zeros with ordinates in the interval $(0, T]$ is asymptotically given by the Riemann-von Mangoldt formula

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

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 zeta-function taken at simple zeros.

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

\[
S_k(T, \theta) = \sum_{\lambda_{n+1} - \lambda_n \leq 2\pi \theta / \log T} |\zeta'(1/2 + it_n)|^{2k},
\]

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 nontrivial 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 \( \lambda_n \) and \( \lambda_n + 1 \) and there is always a \( \lambda_n \) between \( t_n \) and \( t_{n+1} \) for sufficiently large \( n \) (see Edwards [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 zeros.

**Theorem 1** As \( T \to \infty \),

\[
S_1(T, \infty) \leq 0.02513 \ldots T(\log T)^4 + O\left(T(\log T)^3\right),
\]

\[
S_2(T, \infty) \leq (0.000030036 \ldots + o(1))T(\log T)^9.
\]

On the basis of random matrix theory, Hughes, Keating and O’Connell [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

\[
\sum_{\gamma \leq T} |\zeta'(1/2 + i\gamma)|^{2k} \sim \frac{G^2(k + 2)}{G(2k + 3)} a(k) \frac{T}{2\pi} (\log T)^{(k+1)^2}
\]

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

\[
G(z + 1) = (2\pi)^{z/2} \exp \left(-\frac{1}{2}(z(z + 1) + \gamma z^2)\right) \times
\]

\[
\times \prod_{n=1}^{\infty} \left(1 + \frac{z}{n}\right) \exp \left(-z + \frac{z^2}{n}\right),
\]

and \( \gamma \) 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 \( k = -1 \). 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

\[
S_1(T, \infty) = \frac{1}{24\pi} T(\log T)^4 + O\left(T(\log T)^3\right).
\]

(3)
The constant 0.02513... in the unconditional estimate of Theorem 1 does not fall much beyond $1/(24\pi) = 0.01326...$ in the asymptotic formula above. For the case $k = 2$ formula (2) gives (see Hughes, Keating and O’Connell [11] or Ng [15])

$$S_2(T, \infty) \sim \frac{1}{2880\pi^3} T (\log T)^9,$$

Note that $1/2880\pi^3 = 0.00001198...$. Recently, Ng [15] proved, under assumption of the truth of Riemann’s hypothesis,

$$(0.000002... + o(1)) T (\log T)^9 \leq S_2(T, \infty) \leq (0.000166... + o(1)) (\log T)^9.$$

Thus the unconditional constant 0.00003036... 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

$$S_{-1}(T, \infty) \gg T.$$

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

$$S_{1/2}(T, \infty) \ll T (\log T)^{9/4}.$$  \hfill (4)

Furthermore, we shall consider $S_k(T, \theta)$ with respect to small values of $\theta > 0$.

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

$$S_1(T, \theta) \leq \frac{\pi^3 \theta^3}{2688} T (\log T)^4 + O\left(T (\log T)^3\right),$$

$$S_2(T, \theta) \leq \left(\frac{\pi \theta^3}{73920} + o(1)\right) T (\log T)^9.$$

The estimates are uniform in $\theta$.

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 $\lambda_n$ is replaced by $t_{n+1} - t_n \leq 2\pi\theta / \log T$. For instance,

$$\sum_{n \leq N} \left|\zeta'(1/2 + it_n)\right|^4 \leq \left(\frac{17\pi \theta^3}{221760} + o(1)\right) T (\log T)^9.$$

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 [13] which claims under assumption of the Riemann hypothesis that, for fixed $\alpha, \beta$ satisfying $0 < \alpha < \beta$,

$$\lim_{T \to \infty} \frac{1}{N(T)} \# \left\{ 0 < \gamma, \gamma' < T : \alpha \leq \frac{(\gamma - \gamma') \log T}{2\pi} \leq \beta \right\} = \int_{\alpha}^{\beta} \left(1 - \left(\frac{\sin \pi u}{\pi u}\right)^2\right) du,$$
where $\gamma$ and $\gamma'$ are ordinates of zeros of $\zeta(s)$. This open conjecture implies that the number of $t_n$ with $n \leq N$ and $t_{n+1} - t_n \leq 2\pi \theta / \log T$ 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

$$S_k^-(T, \theta) = S_k(T, \theta) \quad \text{and} \quad S_k^+(T, \theta) = \sum_{\lambda_{n+1} \lambda_n \geq 2\pi \theta / \log T} |\zeta'(1/2 + it_n)|^{2k}.$$ 

Then

$$S_k(T, \infty) = S_k^-(T, \theta) + S_k^+(T, \theta).$$

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

$$S_k^+(T, \theta) \geq c(\theta) T (\log T)^4 + O\left( T (\log T)^3 \right), \quad (5)$$

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,

$$\limsup_{\lambda_{n+1} \lambda_n \geq 2\pi / \log \lambda_n} \lambda_{n+1} - \lambda_n \geq 1.04762 \ldots. \quad (6)$$

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, Ghosh and Gonek [3], and Hall [9]. However, here it follows that (6) holds for quite many zeros of the zeta-function. By the Cauchy-Schwarz inequality,

$$S_k^+(T, \theta)^2 \leq S_k^+ (T, \theta) S_k^+ (T, \theta).$$

The right hand side is bounded above by

$$S_0^+ (T, \theta) S_2 (T, \infty) \quad \text{and} \quad S_0(T, \infty) S_2^+ (T, \theta),$$

respectively. Note that $S_0^+$ 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 $T \to \infty$,

$$S_0^+ (T, \theta) \geq (33.292.8 \ldots + o(1)) \left(\frac{1}{24\pi} - \frac{\pi^3 \theta^3}{2688}\right)^2 \frac{T}{\log T},$$

$$S_2^+ (T, \theta) \geq (2\pi + o(1)) \left(\frac{1}{24\pi} - \frac{\pi^3 \theta^3}{2688}\right)^2 T (\log T)^7.$$
2 Preliminaries: mean values for Hardy’s $Z$-function

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

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

(7)

where

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

(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

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

(9)

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

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

(10)

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

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

(11)

and

$$\int_0^T Z'(t)^2 Z''(t)^2 dt = \frac{19}{604800 \pi^2} T (\log T)^{10} + O \left( T (\log T)^9 \right).$$

(12)

In addition, the second author [18] obtained

$$\int_0^T Z''(t)^4 dt \sim \frac{17}{1774080 \pi^2} T (\log T)^{12}. $$

(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,

$$\int_1^T |A_1A_2(1/2 + it)|^2 dt \sim c(P_1, P_2) \frac{6}{\pi^2} TL^4, $$

(14)
where
\[
c(P_1, P_2) := \int_{\mathcal{R}} \left( P_1(\alpha + \beta)P_2(\gamma + \delta)P_1(\alpha + \gamma)P_2(\beta + \delta) + P_1(1 - \alpha - \beta) \times P_2(1 - \gamma - \delta)P_1(1 - \alpha - \gamma)P_2(1 - \beta - \delta) \right) \, d\alpha d\beta d\gamma d\delta
\]
with
\[
\mathcal{R} = \{0 \leq \alpha, \beta, \gamma, \delta \leq 1 : \alpha + \beta + \gamma + \delta \leq 1\}.
\]
We apply this asymptotic formula to \( A_1 = Z'(t) \) and \( A_2 = Z'''(t) \).

In view of (9),
\[
Z'''(t) = \exp(i\vartheta(t)) \left\{ (i\vartheta'''(t) - 3\vartheta' \vartheta''(t) - i\vartheta'(t)^3)\zeta(1/2 + it) + 3(\vartheta''(t) + i\vartheta'(t)^2)\zeta'(1/2 + it) - 3i\vartheta(t)'\zeta''(1/2 + it) - i\zeta'''(1/2 + it) \right\}.
\]
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 \( t \leq T \), we may rewrite (9) and (15) as
\[
Z'(t) = i \exp(i\vartheta(t)) \left\{ \left( \frac{1}{2} L + O(1) \right) \zeta(1/2 + it) + \zeta'(1/2 + it) \right\},
\]
\[
Z'''(t) = -i \exp(i\vartheta(t)) \left\{ \left( \frac{1}{5} L^3 + O(L^2) \right) \zeta(1/2 + it) + \left( \frac{3}{4} L^2 + O(L) \right) \times \zeta'(1/2 + it) + \left( \frac{3}{2} L + O(1) \right) \zeta''(1/2 + it) + \zeta'''(1/2 + it) \right\}.
\]
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
\[
\int_0^T Z'(t)^2 Z'''(t)^2 \, dt \sim L^8 \int_0^T |A_1 A_2(1/2 + it)|^2 \, dt.
\]
After a short computation, Conrey’s asymptotic formula (14) implies
\[
\int_0^T Z'(t)^2 Z'''(t)^2 \, dt \sim \frac{19}{1774080\pi^2} T (\log T)^{12}.
\]
3 Proofs of the theorems

From (9) it follows that
\[ |Z'(t_n)| = |\zeta'(1/2 + it_n)|. \] (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 \( \lambda_m \) 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 \( \lambda_n \) 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
\[ S_k(T, \infty) = \sum_{n \leq N} |\zeta'(1/2 + it_n)|^{2k} \leq \sum_{m \leq M} F_m^{2k}, \]

where \( M \) is the number of zeros \( \tilde{\lambda}_m \) of \( Z'(t) \) not exceeding \( T \). Matsumoto and Tani-gawa [13] proved that the number of zeros of the \( k \)-th 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 \( N \leq M \leq N(T) + O(\log T) \), 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
\[ F^2 \leq \frac{\lambda^2 \mu^2 A + (\lambda^2 + \mu^2) B + C}{2(\mu^2 - \lambda^2)} \left( \frac{1}{\lambda} \tanh \frac{\lambda L}{2} - \frac{1}{\mu} \tanh \frac{\mu L}{2} \right), \]
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 \( \lambda = u \log T, \mu = v \log T, \ell_m = L = \tilde{\lambda}_{m+1} - \lambda_m \), 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 $y = \tilde{Z}'$, 

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

Summing up we obtain via (10) 

$$\sum_{m \leq M} F_m^2 w(u, v; \ell_m) \leq \int_0^T \left( u^2 v^2 (t)^2 \log T + \frac{1}{\log T} (u^2 + v^2) Z''(t)^2 + \frac{1}{(\log T)^3} Z'''(t)^2 \right) dt + F_M^2 w(u, v; \ell_M)$$ 

$$\leq \left( \frac{u^2 v^2}{12} + \frac{u^2 + v^2}{80} + \frac{1}{448} \right) (T \log T)^4 + O(T \log T^3). \tag{18}$$ 

The function $w(u, v; \ell)$ is decreasing in $\ell$ 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 $p \leq \frac{s^2}{4}$, 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 $p \leq s^2/4$ 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 

$$\frac{1}{6615000} (735 + 420 \sqrt{14})^{3/2} + \frac{11}{63000} \sqrt{735 + 420 \sqrt{14}} = 0.02513 \ldots.$$ 

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) 

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

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. \text{ The minimal value is }
\begin{align*}
&\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{align*}

This proves the upper bound for the fourth moment.

It remains to give the

**Proof of Theorem 2.** It follows from (18) that
\[
\sum_{m \leq M, \ell_m \leq 2\pi\theta/\log T} F_m^2 \leq w \left( u, u; \frac{2\pi\theta}{\log T} \right)^{-1} \left( \frac{u^4}{12} + \frac{u^2}{40} + \frac{1}{448} \right) T(\log T)^4 + \\
+ O \left( T(\log T)^3 \right).
\]

Putting } u = 0 \text{ we obtain the assertion on the second moment. In view of (19) we get
\[
\sum_{m \leq M, \ell_m \leq 2\pi\theta/\log T} F_m^4 \leq w \left( u, u; \frac{2\pi\theta}{\log T} \right)^{-1} \frac{1}{1120\pi^2} \left( u^4 + \frac{19u^2}{135} + \frac{1}{11} + o(1) \right) T(\log T)^9.
\]

Putting } u = 0 \text{ we obtain the estimate for the fourth moment. The uniformity in } \theta \text{ follows from Hall’s method.

**Acknowledgements.** The authors are grateful to Prof. R.R. Hall for pointing out an error in a previous version of the paper.

**References**


