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Evidence of Random Matrix Corrections for the Large Deviations of Selberg's Central Limit Theorem

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ABSTRACT

Selberg's central limit theorem states that the values of $\log|\zeta(1/2+i\tau)|$, where τ is a uniform random variable on $[T, 2T]$, are asymptotically distributed like a Gaussian random variable of mean 0 and standard deviation $\sqrt{\frac{1}{2}\log\log T}$. It was conjectured by Radziwiłł that this distribution breaks down for values of order $\log\log T$, where a multiplicative correction C_k would be present at level $k\log\log T$, $k > 0$. This constant should be the same as the one conjectured by Keating and Snaith for the leading asymptotic of the $2k^{th}$ moment of ζ. In this paper, we provide numerical and theoretical evidence for this conjecture. We propose that this correction has a significant effect on the distribution of the maximum of $\log|\zeta|$ in intervals of size $(\log T)^\theta$, $\theta > 0$. The precision of the prediction enables the numerical detection of C_k even for low T's of order $T = 10^8$. A similar correction appears in the large deviations of the Keating–Snaith central limit theorem for the logarithm of the characteristic polynomial of a random unitary matrix, as first proved by Féray, Méliot and Nikeghbali.

KEYWORDS

Riemann zeta function; extreme value statistics; random matrix theory

1. Introduction and main results

1.1. Introduction

The large values of the Riemann zeta function $\zeta : \mathbb{C}\setminus\{1\} \to \mathbb{C}$ on the critical line $\mathrm{Re}(s) = 1/2$ play an important role in number theory. There are several conjectures describing its behavior. For example, the *moment conjecture* gives the leading order of the moments of the function on the interval $[0, T]$ (see, e.g., [26, 28, 35]):

Conjecture 1 (Moment Conjecture). *For $k \geq 0$, as $T \to \infty$, we have*

$$\frac{1}{T}\int_0^T |\zeta(1/2+it)|^{2k}dt \sim C_k(\log T)^{k^2}. \tag{1}$$

Lower bounds of the same order of magnitude are known unconditionally (see [24, 32] and the earlier works of [19, 31]). Consistent upper bounds on the level of the leading exponent are known unconditionally for $0 \leq k \leq 2$ (from the work of [23]), and for all $k \geq 0$ conditionally on the Riemann hypothesis [17, 34]. This article is predominantly about the constants C_k.

At the level of the constant, Conjecture 1 is only proved in the case $k = 1$, by Hardy and Littlewood with $C_1 = 1$, and the case $k = 2$ by Ingham with $C_2 = \frac{1}{(2\pi)^2}$ [21, 25]. The constants C_k, $k > 0$, have been conjectured in [28] using random matrix theory to be of the form

$$C_k = a_k \cdot f_k, \tag{2}$$

where

$$a_k = \prod_{p \text{ primes}} \left(1-\frac{1}{p}\right)^{k^2} \sum_{m=0}^{\infty}\left(\frac{\Gamma(k+m)}{m!\Gamma(k)}\right)^2 p^{-m}, \tag{3}$$

and

$$f_k = \frac{\mathcal{G}^2(1+k)}{\mathcal{G}(1+2k)}. \tag{4}$$

Here, $\mathcal{G}$ denotes the Barnes $\mathcal{G}-$function. An alternative approach using Dirichlet series yields the same conjecture [12].

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As pointed out in [30], the constants C_k should also appear in the large deviations of Selberg's central limit theorem. The original theorem asserts that if τ is sampled uniformly in the interval $[T, 2T]$, then for $\sigma_T^2 = \frac{1}{2}\log\log T$ and any fixed $V \in \mathbb{R}$,

$$\mathbf{P}\Big(\log|\zeta(1/2+\mathrm{i}\tau)| > \sigma_T \cdot V\Big) \sim \int_V^\infty \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}}\mathrm{d}x, \qquad \text{as } T \to \infty. \tag{5}$$

However, for V of the order of the variance, the proposed correction is

Conjecture 2 (Radziwiłł's Conjecture[1]). *If τ is uniformly distributed on $[T, 2T]$ and $\sigma_T^2 = \frac{1}{2}\log\log T$, then for $V = V(T) \sim k\sqrt{2\log\log T}$ with $k > 0$, we have*

$$\boldsymbol{P}\Big(\log|\zeta(1/2+i\tau)| > \sigma_T \cdot V\Big) \sim C_k \int_V^\infty \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}}dx, \qquad \textit{as } T \to \infty. \tag{6}$$

measure?

To see why the conjecture is plausible, one can weigh the choice of τ by the value $|\zeta(1/2+\mathrm{i}\tau)|^{2k}$ by defining the probability $\widetilde{\mathbf{P}}$ with $\frac{\mathrm{d}\widetilde{\mathbf{P}}}{\mathrm{d}\mathbf{P}} = \frac{|\zeta(1/2+\mathrm{i}\tau)|^{2k}}{\mathbf{E}[|\zeta(1/2+\mathrm{i}\tau)|^{2k}]}$ (and $\widetilde{\mathbf{E}}$ for the corresponding expectation). With this notation, the left-hand side of (6) becomes

$$\mathbf{P}\Big(\log|\zeta(1/2+\mathrm{i}\tau)| > \sigma_T \cdot V\Big) = \mathbf{E}[|\zeta(1/2+\mathrm{i}\tau)|^{2k}] \cdot (\log T)^{-2k^2} \cdot \widetilde{\mathbf{E}}[e^{-2kX_T}\mathbb{1}(X_T > 0)], \tag{7}$$

where $X_T = \log|\zeta(1/2+\mathrm{i}\tau)| - k\log\log T$. The limiting distribution of X_T/σ_T under $\widetilde{\mathbf{P}}$ (for integer k) has been recently proved by Fazzari to be standard Gaussian as in Selberg's theorem [13]. Together with the asymptotics (1), this would imply that as $T \to \infty$,

$$\begin{aligned}\mathbf{P}\Big(\log|\zeta(1/2+\mathrm{i}\tau)| > \sigma_T \cdot V\Big) &\sim C_k(\log T)^{-k^2}\int_0^\infty e^{-2k\sigma_T z}\frac{e^{-z^2/2}}{\sqrt{2\pi}}\mathrm{d}z \\ &\sim C_k(\log T)^{-k^2}\frac{1}{\sqrt{2\pi}\cdot k\sqrt{2\log\log T}},\end{aligned}$$

by taking $e^{-z^2/2} = 1 - \frac{z^2}{2} + \dots$ and integrating. The right-hand side is the same asymptotic as Equation (6) since a standard Gaussian estimate yields $\int_V^\infty \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}}\mathrm{d}x \sim \frac{1}{\sqrt{2\pi}}\frac{e^{-V^2/2}}{V}$ as $V \to \infty$.

1.2. Results

The main objective of this article is to provide more evidence that the moment correction C_k, predicted by random matrix theory, should be present in (6). On the theoretical side, it was proved by Féray, Méliot, and Nikeghbali that a similar correction naturally appears in the large deviations of the Keating–Snaith central limit theorem for the characteristic polynomial of the circular unitary ensemble (CUE):

Theorem 1.1 (Theorem 7.5.1 [16]). *Let $P_N(\theta) = \det(I - e^{i\theta}U)$ be the characteristic polynomial of an $N \times N$ random matrix U sampled under the Haar measure $\mathbb{P}_{\mathcal{U}(N)}$ on the unitary group $\mathcal{U}(N)$. Write $\sigma_N^2 = \frac{1}{2}\log N$. Then we have for $V = V(N) \sim k\sqrt{2\log N}$ as $N \to \infty$, $k \geq 0$, and any $\theta \in [0, 2\pi)$,*

$$\mathbb{P}_{\mathcal{U}(N)}\Big(\log|P_N(\theta)| > \sigma_N \cdot V\Big) \sim f_k \int_V^\infty \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}}dx, \quad \textit{as } N \to \infty,$$

where f_k is given in Equation (4).

The statement of Theorem 1.1 is precisely the random matrix analogue of (6). Using the usual dictionary (see, e.g., [7, 27, 28]), one compares the unitary characteristic polynomial $P_N(\theta)$ with $\zeta(1/2+\mathrm{i}t)$, and by comparing densities of eigenvalues and zeros of zeta, the matrix size N corresponds to a height $\log(t/2\pi)$.

Large deviations in different ranges were also considered by Hughes et al. [20]. In that paper, they show that $\log|P_N(\theta)|/A(N)$ satisfies a large deviation principle, for various ranges of $A(N)$. The appropriate range in the context of Theorem 1.1 is *moderate* deviations: $\sqrt{\log N} \ll A(N) \ll N$, and it is shown in [20] that the rate function is either quadratic or linear, depending on the precise growth of $A(N)$. Similar results have also been proved in the general context of β-ensembles and Wigner matrices in [10, 11]. Theorem 1.1 differs in that it examines a very particular form of $A(N)$ and derives the resulting precise constant multiple of the Gaussian. The proof of Theorem 1.1 was done in [16] in the general context for mod-ϕ convergence. For completeness, we provide the detailed computation following the result of Keating and Snaith in the appendix.

[1] There is a small typo in the statement of the conjecture in the original paper where $V \sim k\sqrt{\log\log T}$. A factor of 2 in the square root is missing.

The statement of Theorem 1.1 may be adapted for the imaginary part of $\log P_N(\theta)$[2]. Additionally, the statement of Theorem 1.1 can be generalized to other classical compact groups, where the distribution should again be Gaussian but with a different correction g_k (corresponding to the relevant matrix group moment), see, for example, Féray et al. [16]. From such calculations one could deduce conjectures akin to Conjecture 2 for symplectic and orthogonal families of L-functions (cf. [7]).

Beyond the theoretical evidence from Theorem 1.1, we also provide numerical evidence of the presence of the correction C_k. We choose to investigate its effect on the maximum of the real part of the logarithm of the zeta function in short intervals, instead of directly testing (6). The reason for this is that the presence of the correction leads to a very precise refinement of the Fyodorov-Hiary-Keating conjecture for the maximum of $\log|\zeta(1/2+\mathrm{i}\tau+\mathrm{i}h)|$ for h in a short interval, [14, 15]. The conjecture was originally stated for *mesoscopic* intervals, that is, intervals of size $2\pi(\log T)^\theta$ for $-1<\theta\le 0$. The statement was adapted in [5] (cf. Theorem 1.2) to *macroscopic* intervals of size $2\pi(\log T)^\theta$, for $\theta>0$, but fell short of capturing terms beyond the leading order. It turns out that the correction C_k has a measurable effect on the recentering of the maximum. More precisely, we propose the following refinement:

Conjecture 3. *Consider a fixed $\theta>0$. If τ is uniformly distributed on $[T,2T]$, then we have*

$$\max_{|h|\le\pi(\log T)^\theta}\log|\zeta(1/2+i(\tau+h))| = \sqrt{1+\theta}\log\log T - \frac{1}{4\sqrt{1+\theta}}\log\log\log T + \mathcal{G}_{\theta,T}, \tag{8}$$

where $(\mathcal{G}_{\theta,T}, T\ge 1)$ is a family of random variables converging in distribution to a Gumbel random variable $\mathcal{G}_\theta$ with $\mathbf{P}(\mathcal{G}_\theta\le x)=\exp(-e^{-\frac{1}{\beta}(x-m)})$ and parameters

$$\begin{aligned}\beta=\beta(\theta)&=\frac{1}{2\sqrt{1+\theta}}\\ m=m(\theta)&=(0.06537\ldots)+\beta^2\log C_{\sqrt{1+\theta}}-\frac{\beta^2}{2}\Big(\log(1+\theta)-\log(4\pi)\Big).\end{aligned} \tag{9}$$

As can be seen from the leading order of (8), the relevant regime of large deviation at a given θ is $\sqrt{1+\theta}\log\log T$. Together with Conjecture 2, this leads naturally to the choice $k=\sqrt{1+\theta}$ for C_k in (9). The precise numerical constant appearing in the definition of m in (9) is the Meissel-Mertens constant divided by 4, see Equation (14).

The upshot of Conjecture 3 is a very precise prediction to order one for the maximum of $\log|\zeta(1/2+\mathrm{i}(\tau+h))|$, including very good control of the finite-size effects, that can be compared to the numerical data. The high precision of the conjecture to order one is the saving grace here, as the factors $\log\log T$, $\log\log\log T$, and $\mathcal{G}_{\theta,T}$ in (8) remain essentially of the same order for all testable T's (around $T=10^{23}$ seems to be the current computational limit). In particular, this spares us some of the difficulty of testing the moment conjecture, see [22].

maybe truncated, conjectural

Table 1. Values of the leading order coefficient in the moment conjecture (1). The exact values for $k=1,2$ are due to Hardy and Littlewood, and Ingham respectively [21, 25]. The (truncated) numerical values for higher k can be found in [22].

k	$C_k=a_kf_k$
1	1
2	$\frac{1}{2\pi^2}\approx 5.066\times10^{-2}$
3	5.708×10^{-6}
4	2.465×10^{-13}

Table 2. The ratio of the empirical mean of $\max_{|h|\le\pi(\log T)^\theta}\log|\zeta(1/2+\mathrm{i}(\tau+h))|$ divided by the model prediction with no correction ($C\equiv1$) and with $C_{\sqrt{1+\theta}}$ at integer θ. From left to right, the data corresponds to $T=10^7$, $T=10^8$, and $T=10^9$.

θ	$C\equiv1$	$C_{\sqrt{1+\theta}}$
0	0.9441	1.0490
1	0.9143	1.0147
2	0.8343	0.9679
3	0.7569	0.9165

θ	$C\equiv1$	$C_{\sqrt{1+\theta}}$
0	0.9544	1.0454
1	0.9170	1.0099
2	0.8450	0.9708
3	0.7713	0.9225

θ	$C\equiv1$	$C_{\sqrt{1+\theta}}$
0	0.9540	1.0343
1	0.9174	1.0043
2	0.8510	0.9703
3	0.7795	0.9234

[2]The appropriate calculation yields $f_k=|\mathcal{G}(1+ik)|^2$.

We chose to test Equations (8) and (9) at $T = 10^7, 10^8$ and 10^9, where it is not costly to amass a good sample size for many θ's for $0 < \theta \leq 3$. A snapshot of the results for the empirical mean of the maximum are given in Table 2 and Figures 2, 3 and 4. The main conclusion there is that the correction C_k is necessary to fit the data. Details on the numerical experiments are given in Section 3.

The case $\theta = 0$ is special as Conjecture 3 is not expected to hold. It was proposed in [14, 15] that the subleading order should instead be $-\frac{3}{4}\log\log\log T$. One then would expect the empirical mean to lie *lower* than the prediction (8). In addition, the fluctuations should not be exactly Gumbel but a randomly shifted Gumbel. The effect of the random shift is such that the right tail of the distribution of the recentered maximum is not exponential, as for a pure Gumbel, but should be heavier: of the form $ye^{-\beta y}$. This would in effect *increase* the contribution of the fluctuations to the mean. The two above corrections seem hard to observe numerically. One problem is that they are competing effects, which may mutually cancel. Secondly, there is the systematic problem that the standard deviation of the maximum is fairly large at $\theta = 0$, as can be seen for example in Figure 4. Theoretical progress to settle the Fyodorov-Hiary-Keating conjecture has recently been made in [1, 3, 18, 29]. A continuous smoothing of the subleading order between $-\frac{1}{4\sqrt{1+\theta}}\log\log T$ to $-\frac{3}{4}\log\log T$ as $\theta \downarrow 0$ has been proposed in [4] by taking $\theta \sim (\log\log T)^{-\alpha}$, $0 < \alpha < 1$. This gives a subleading order of $-\frac{(1+2\alpha)}{4}\log\log T$. Again, this interpolation seems hard to capture numerically as the standard deviation of the maximum is large for small θ.

The paper is structured as follows. The details on how the theoretical prediction based on Conjecture 3 is generated are given in Section 2. The conjecture is derived in Section 2.1 using basic extremal value theory, assuming Conjecture 2 and reasonable properties of ζ. We comment on the control of the finite-size effects and on the numerical computations of the C_k's for all $0 \leq k \leq 2$ in Section 2.2. Numerical experiments are discussed in Section 3. The appendix contains a proof of Theorem 1.1 following the work of Keating and Snaith [28].

2. Derivation of prediction

2.1. Derivation of Conjecture 3

In this section, we derive Conjecture 3 based on the following assumptions:

Assumption. *For τ a uniform random variable on $[T, 2T]$ and $\theta > 0$, the stochastic process*

$$(|\zeta(1/2 + i(\tau + h))|, |h| \leq \pi(\log T)^{\theta})$$

satisfies the following:

1. *Discretization: the maximum over the interval $[-\pi(\log T)^{\theta}, \pi(\log T)^{\theta}]$ can be reduced to the maximum over a discrete set $\mathcal{H}_{\theta,T}$ corresponding to the midpoints between the zeros of $|\zeta(1/2 + i(\tau + h))|$ on the interval.*
2. *Independence: The variables $|\zeta(1/2 + i(\tau + h))|$, $h \in \mathcal{H}_{\theta,T}$, are independent.*
3. *Large deviations of Selberg's central limit theorem: Equation (6) holds with $k = \sqrt{1+\theta}$.*

Assumption 1 is reasonable as the maximum should be achieved between two zeros. The precise discretization can be rigorously established, see Proposition 2.7 in [5]. The idea there is simple. The approximate functional equation (see for example Theorem 1.8 in [26]) gives

$$\zeta(1/2 + \mathrm{i}\tau) = \sum_{n \leq T} n^{-1/2-\mathrm{i}\tau} + \mathcal{O}(T^{-1/2}).$$

Therefore, as far as the large values are concerned, ζ behaves like a trigonometric polynomial with frequency at most $\log T$. This implies that the spacing between local maxima (and the zeros) should be of the order of $1/\log T$. Similar reductions have been used in the study of large values of the characteristic polynomial of random matrices, see Lemma 4.3 in [9]. Assumption 2 cannot be exact, but it is likely a very good approximation. More precisely, it has been known since the work of Bourgade [6] that the correlation between $\log|\zeta(1/2 + \mathrm{i}(\tau + h))|$ and $\log|\zeta(1/2 + \mathrm{i}(\tau + h'))|$ should decay like $\log|h - h'|^{-1}$ whenever $|h - h'| \leq 1$. The values are then said to be log-correlated. These fairly strong correlations are responsible for the different behavior at $\theta = 0$ mentioned in the introduction. However, for $\theta > 0$, most pairs of points in the large interval now lie at a distance much larger than one. The correlations between the values at h and h' then should decay very fast with the distance: like $|h - h'|^{-1}$, see Equation 1.27 in [5] and Lemma 2.1 in [2]. Assumption 3 is the one to be tested. The choice of k comes from the expected leading order of the maximum being $\sqrt{1+\theta}\log\log T$.

From these assumptions, the derivation of the distribution of the maximum is a standard computation in extreme value theory. However, we shall need very good control of the finite-size effects to compare with numerics, so we include the details. The finite-size effects are discussed in the next section.

The number of zeros $\mathcal{N}(t)$ on $[0, t]$ is known to a very good level of precision thanks to the Riemann-von Mangoldt formula, see for example [26, 36],

$$\mathcal{N}(t) = \frac{t}{2\pi}\log\frac{t}{2\pi e} + \frac{1}{\pi}\mathrm{Im}\log\zeta(1/2 + \mathrm{i}t) + \mathcal{O}(1). \tag{10}$$

This implies that the number of zeros in the interval $[\tau - \pi(\log T)^\theta, \tau + \pi(\log T)^\theta]$ is

$$\begin{aligned} N_{\theta,T} &= \mathcal{N}(\tau + \pi(\log T)^\theta) - \mathcal{N}(\tau - \pi(\log T)^\theta) \\ &= (\log T)^\theta \log \frac{\tau}{2\pi e} + \mathcal{O}((\log T)^\theta) \\ &= (\log T)^{1+\theta} + \mathcal{O}((\log T)^\theta). \end{aligned} \tag{11}$$

This will be the approximation for the cardinality of the discrete set $\mathcal{H}_{\theta,T}$. The above implies

$$\log N_{\theta,T} = (1+\theta)\log\log T + \mathcal{O}((\log T)^{-1}). \tag{12}$$

Focussing on Assumption 3, the right tail of the distribution of $\log|\zeta(1/2 + \mathrm{i}\tau)|$ is expected to be Gaussian with multiplicative correction C_k and variance

$$\sigma_T^2 = \frac{1}{2}\sum_{p\le T}\frac{1}{p}. \tag{13}$$

In [30], Conjecture 2 is stated for $\sigma_T^2 = \frac{1}{2}\log\log T$. Whereas it is true that $\sum_{p\le T}\frac{1}{p} = (1 + \mathrm{o}(1))\log\log T$, the $\mathrm{o}(1)$-term is needed for precise numerics. Mertens' second theorem asserts that, see for example [37],

$$\sum_{p\le T}\frac{1}{p} = \log\log T + B + \mathcal{O}\left(\frac{1}{(\log T)^3}\right), \tag{14}$$

where $B = 0.26149\ldots$ is the Meissel-Mertens contant. Hence, from (13), the standard deviation is asymptotically

$$\sigma_T = \sqrt{\tfrac{1}{2}\log\log T} + \frac{B}{2\sqrt{2\log\log T}} + \mathcal{O}\left(\frac{1}{(\log T)^3}\right). \tag{15}$$

We are now ready to derive Conjecture 3. We use the shorthand notation $N = N_{\theta,T}$, $\sigma = \sigma_T$ and $C = C_{\sqrt{1+\theta}}$ (the moment coefficient). Under Assumptions 1, 2, and 3, we have for any $Y = Y(T)$ with $\sigma Y \sim \sqrt{1+\theta}\log\log T$ as $T \to \infty$,

$$\mathbf{P}\left(\max_{|h|\le\pi(\log T)^\theta}\log|\zeta(1/2 + \mathrm{i}(\tau+h))| \le \sigma\ Y\right) \sim \left(1 - \frac{NC\int_Y^\infty \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}}\mathrm{d}x}{N}\right)^N. \tag{16}$$

The correct level of the maximum is obtained by choosing Y for which the numerator in Equation (16) is of order one. With this mind, consider $Y^\star$ the solution to the equation

$$NC\int_{Y^\star}^\infty \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}}\mathrm{d}x = 1. \tag{17}$$

Since

$$\left(1 - \frac{a}{n}\right)^n = e^{-a}\cdot\left(1 - \mathcal{O}\left(\frac{a^2}{n}\right)\right), \tag{18}$$

Equations (17) and (16) then imply for $\sigma Y = \sigma\ Y^\star + y$, $y \in \mathbb{R}$, as $T \to \infty$,

$$\mathbf{P}\left(\max_{|h|\le\pi(\log T)^\theta}\log|\zeta(1/2 + \mathrm{i}(\tau+h))| \le \sigma\ Y^\star + y\right) \sim \exp\left(-G(y)\right), \tag{19}$$

where

$$G(y) = \frac{\int_{Y^\star + y/\sigma}^\infty e^{-\frac{x^2}{2}}\mathrm{d}x}{\int_{Y^\star}^\infty e^{-\frac{x^2}{2}}\mathrm{d}x}. \tag{20}$$

The quantity $\sigma Y^\star$ is the deterministic shift in Equation (9). To see this, recall that standard Gaussian estimates give the asymptotics

$$\int_Y^\infty \frac{e^{-\frac{y^2}{2}}}{\sqrt{2\pi}}\mathrm{d}y = \left(1 - \mathcal{O}\left(\frac{1}{Y^2}\right)\right)\frac{1}{Y}\frac{e^{-\frac{Y^2}{2}}}{\sqrt{2\pi}}. \tag{21}$$

Combining (17) and (21) gives the following equation for $Y^\star = Y^\star(T)$:

$$\frac{NC}{\sqrt{2\pi}} \frac{e^{-\frac{(Y^\star)^2}{2}}}{Y^\star} = 1 + \mathcal{O}\left(\frac{1}{(Y^\star)^2}\right). \tag{22}$$

The solution can be approximated recursively. A first approximation omitting $\frac{1}{Y^\star} = e^{-\log Y^\star}$ yields $Y^\star \approx \sqrt{2\log N}$. Writing $Y^\star = \sqrt{2\log N} + \delta$ in (22) gives an equation for δ:

$$\frac{\delta^2}{2} + \delta\sqrt{2\log N} + \frac{1}{2}\log\log N + \frac{1}{2}\log 2 + \log\left(1 + \frac{\delta}{\sqrt{2\log N}}\right) = \log C - \frac{1}{2}\log 2\pi. \tag{23}$$

It is straightforward to solve this by expanding the logarithm to get

$$Y^\star = \sqrt{2\log N} + \delta \tag{24}$$

$$= \sqrt{2\log N} - \frac{1}{2\sqrt{2\log N}}\Big(\log\log N + \log 4\pi - 2\log C\Big) + \mathcal{O}\left(\frac{\log\log N}{\log N}\right). \tag{25}$$

It remains to note that Equation (11) and Equation (15) imply as $T \to \infty$

$$\sigma\sqrt{2\log N} = \sqrt{1+\theta}\,\log\log T + \sqrt{1+\theta}\,\frac{B}{2} + \mathrm{o}(1), \tag{26}$$

$$\frac{\sigma}{2\sqrt{2\log N}} = \frac{1}{4\sqrt{1+\theta}}\left(1 + \mathcal{O}((\log\log T)^{-1})\right). \tag{27}$$

After multiplication by σ, the first two terms in Equation (25) give the leading correction for the maximum of $\log|\zeta|$:

$$\sqrt{1+\theta}\log\log T - \frac{1}{4\sqrt{1+\theta}}\log\log\log T.$$

The remaining terms with $\log C$, B, $\log(1+\theta)$ and $\log 4\pi$ amount to the deterministic shift m in Equation (9).

It remains to study the fluctuations around $Y^\star$. This is done by computing the asymptotics of the function G, defined by (20). Using the Gaussian estimate (21) again yields

$$G(y) \sim e^{-\frac{Y^\star}{\sigma}y} \cdot \frac{e^{-\frac{y^2}{(2\sigma^2)}}}{1 + \frac{y}{\sigma Y^\star}}, \qquad \text{as } T \to \infty. \tag{28}$$

Equation (9) follows by noting that $e^{-y^2/(2\sigma^2)} \sim 1$ by (15), and $1 + \frac{y}{\sigma Y^\star} \sim 1$ for any fixed y by (25). Moreover, Equations (11), (15) and (25) imply

$$\frac{Y^\star}{\sigma} \sim 2\sqrt{1+\theta}, \qquad \text{as } T \to \infty. \tag{29}$$

Putting this back in (28) gives the parameter β of the Gumbel distribution in Equation (9).

2.2. Discussion of the Finite-Size Effects

In this section, we explain how the numerical predictions of Conjecture 3 are obtained, including the computations of the coefficients C_k.

According to Conjecture 3, the mean of $\max_{|h|\le\pi(\log T)^\theta} \log|\zeta(1/2+\mathrm{i}(\tau+h))|$ consists of two terms: the deterministic recentering

$$\sqrt{1+\theta}\log\log T - \frac{1}{4\sqrt{1+\theta}}\log\log\log T, \tag{30}$$

and the expectation of the Gumbel random variable $\mathcal{G}_{\theta,T}$. In the limit $T \to \infty$, this variable should converge to a Gumbel random variable $\mathcal{G}_\theta$ with parameters m and β given in Equation (9) so that

$$\mathbf{E}[\mathcal{G}_\theta] = m + \beta\gamma, \tag{31}$$

where γ is the Euler constant $\gamma = 0.577\ldots$.

To give an idea of the orders of magnitude in the problem considered, note that for $T = 10^8$, we have

$$\log\log 10^8 = 2.78\ldots, \quad \log\log\log 10^8 = 1.07\ldots. \tag{32}$$

this is correct

$\log\log 10^8 = 2.91\ldots$ $\log\log 10^7 = 2.78\ldots$

Scaling the simulations up to to $T = 10^{23}$ wouldn't result in much additional precision, since there

$$\log\log 10^{23} = 3.97\ldots, \quad \log\log\log 10^{23} = 1.39\ldots. \tag{33}$$

This modest gain would come at a substantial computational time cost. Despite the curse of iterated logarithms, it is possible to derive accurate numerical predictions thanks to a precise control of the lower order terms and their finite-size corrections.

The computation of the deterministic shift $\sigma Y^\star$ follows the treatment in the last section. More precisely, for the number of zeros $N_{\theta,T}$, we rely on Equation (11) and take

$$N_{\theta,T} \approx (\log T)^\theta \log \frac{T}{2\pi e}. \tag{34}$$

The error term in (11) is of order $(\log T)^{-1}$, which is comparatively small. For the variance σ_T^2, note that the constant $B = 0.26149\ldots$ is fairly close to the value of $\log\log T$ in view of (32). For this reason, we use Equation (15) in the computation. One might expect a quadratic correction to $\sum_{p\le T}\frac{1}{p}$ of the form $\sum_{p\le T}\frac{1}{8p^2} \approx \frac{1}{32}$, due to the expansion of the Euler product. However, this only leads to a change of approximately 0.01 in the prediction at $\theta = 3$ and $T = 10^9$ that we choose to neglect. The approximation of the product by the exponential in Equation 18 also comes at a low cost, since the multiplicative error $(1 - \mathcal{O}(a^2/n))$ is evaluated at $a = 1$, by design in (17), and at $n = N_{\theta,T} \approx (\log T)^\theta \ge 18.4$. This multiplicative error becomes of small shift in the exponential, allowing us to discard it. The Gaussian estimate (22) is not quite precise enough for these fine numerics. Indeed, this leads to Equation (25), with an error $\mathcal{O}\left(\frac{\log\log N_{\theta,T}}{\log N_{\theta,T}}\right)$. This error remains substantial at any T's that are computationally reachable. For this reason, we approximate $Y^\star$ directly by numerically solving Equation (17) [3]. This takes care of all finite-size corrections to $\sigma Y^\star$.

It remains to evaluate the mean of the Gumbel random variable $\mathcal{G}_{\theta,T}$. As can be seen from Equation (28), the function G converges to $e^{-2\sqrt{1+\theta}y}$, albeit very slowly. The term $e^{-y^2/2\sigma^2}$ could be particularly problematic since σ is of the order $\sqrt{\log\log T}$. To take care of this, instead of using $\beta\gamma$ in the mean of a Gumbel (cf. Equation (31)), we simply evaluate the mean by working directly with the function $G(y)$ in Equation (20). The mean of the recentered random variable $\max_{|h|\le\pi(\log T)^\theta}\log|\zeta(1/2+\mathrm{i}(\tau+h))| - \sigma Y^\star$ can then be evaluated using the cumulative distribution function $1 - \exp(-G(y))$. This may be over cautious as this procedure yields a value that differs from the limiting mean by only 0.03 at $T = 10^9$ and $\theta = 3$. In Equation (29), we also use $\frac{\sigma^2}{\sigma Y^\star}$ for β instead of the limiting value $(2\sqrt{1+\theta})^{-1}$. For $\theta = 3$, these considerations yield a mean of $0.17\ldots$ for $\mathcal{G}_{\theta,T}$ compared to $0.14\ldots$ for the limiting function $e^{-2\sqrt{1+\theta}y}$. In the same way, the variance of $\max_{|h|\le\pi(\log T)^\theta}\log|\zeta(1/2+\mathrm{i}(\tau+h))|$ in the limit should be the one of a Gumbel with parameter β, i.e.,

$$\mathrm{Var}(\mathcal{G}_\theta) = \frac{\beta^2\pi^2}{6}. \tag{35}$$

The finite-size effects of computing the variance with the CDF $1 - \exp(-G(y))$ are small compared to using Equation (35), so we use the latter for simplicity. (The difference for the standard deviation between the two values is around 0.05 for $T = 10^9$ at $\theta = 3$, which is relatively small compared to the gap between the prediction and the numerical value, cf. Figure 6.)

Finally, we turn to computing the moment coefficient C_k (which recall appears in the definition of m, see (9)). For our purpose, we are interested in the value of $C_k = a_k f_k$ given by Equation (2) for $k \in (1,2)$, since $k = \sqrt{1+\theta}$ and for our numerics we take $\theta \in (0,3)$. Certain evaluations of a_k and f_k appear in the literature: see for example [22], where they compute C_k for the first few integers k:

The numerical values of $C_k = a_k f_k$ presented in Section 3 were computed[4] by evaluating (3) and (4). Figure 1 plots C_k for $\theta \in (0,3)$ (i.e. $k \in (1,2)$).

3. Numerical Experiments

3.1. About the Experiments

Thanks to the precision of Conjecture 3, the prediction can be tested using fairly rudimentary numerical experiments. The datasets were generated using Python 3.8. We employ SageMath's *lcalc* function [33], which uses Michael Rubinstein's *L*-function calculator. We also implement multiprocessing to expedite the run-time for large simulations. Samples were constructed at $T = 10^7, 10^8$ and 10^9 over the interval $0 \le \theta \le 3$ for each 0.1 increment for $T = 10^7, 10^8$ and for each 0.25 increment for $T = 10^9$.

For each height, T, the method consisted on generating $\mathcal{S}$ evaluations of τ, for τ uniformly distributed on $[T, 2T]$. Hence, the interval $[\tau - \pi(\log T)^\theta, \tau + \pi(\log T)^\theta]$ was discretized at every $\frac{2\pi}{\log(T/2\pi)}$, and the maximum over this discrete set of points computed. The sample sizes $\mathcal{S}$ at each θ were 500, 400, 300 for $T = 10^7$, 10^8 and 10^9 respectively.

[3] We use the numerical solver *NSolve* of Mathematica 11.3 which gives a precision of 16 digits.
[4] Computations were completed in SageMath [33], version 9.1, using Python 3.8.

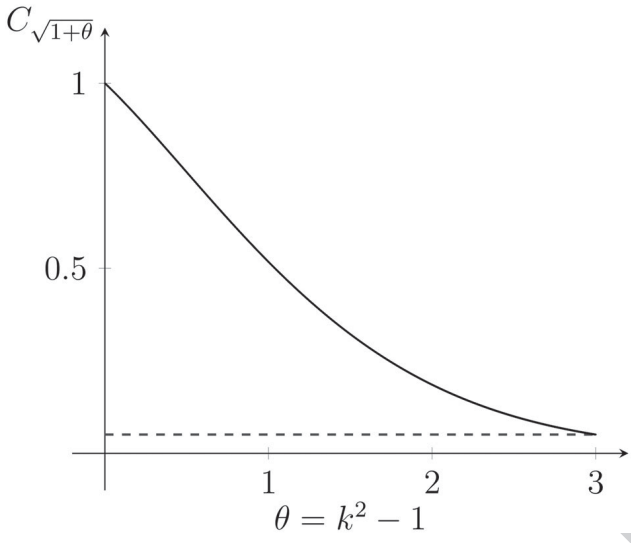

Figure 1. Graph of the conjectured leading order coefficient C_k of the $2k^{th}$ moment of $|\zeta(1/2+it)|$, for $k = \sqrt{1+\theta}$. The horizontal dashed line is at the value $C_2 = \frac{1}{2\pi^2}$ corresponding to $\theta = 3$.

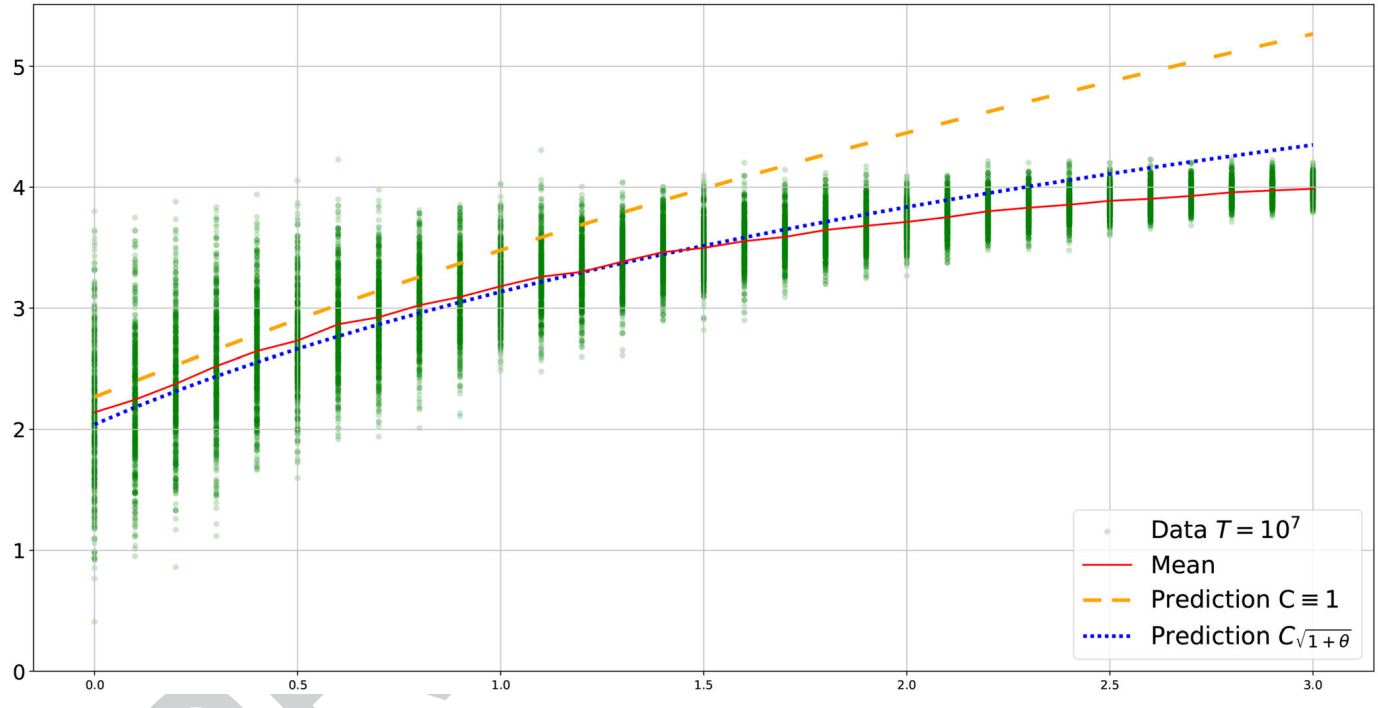

Figure 2. The empirical mean of the samples of $\max_{|h|\leq\pi(\log T)^\theta} \log|\zeta(1/2+\mathrm{i}(\tau+h))|$ as a function of θ, $0 \leq \theta \leq 3$, with step size 0.1 at $T = 10^7$. The dotted lines correspond to the theoretical predictions for $C \equiv 1$ and for $C_{\sqrt{1+\theta}}$.

3.2. Results

The main numerical results concern the empirical mean of $\max_{|h|\leq\pi(\log T)^\theta} \log|\zeta(1/2+\mathrm{i}(\tau+h))|$ as a function of $0 \leq \theta \leq 3$. These are plotted in Figures 2, 3 and 4. The results are compared with the theoretical predictions of Conjecture 3 (as detailed in Section 2), both including the correction $C_{\sqrt{1+\theta}}$ and without, i.e., $C \equiv 1$. We observe that the prediction line for $C \equiv 1$ exhibits greater divergence from the mean as θ grows, when compared to the corrected $C_{\sqrt{1+\theta}}$ prediction. This is despite the drastic reduction in the variance. This reduction in variance is consistent with the prediction of the parameter β of the Gumbel distribution in Equation (9), which decreases with θ. There is a small discrepancy for large θ, where the prediction is slightly outside the intervals given by the sample values. Indeed, the prediction is above the maximum of the sample at $\theta = 3$ by 0.144 for $T = 10^7$ (a relative error of 3%), for $T = 10^8$ by 0.082 (a relative error of 1.8%), and for $T = 10^9$ by 0.076 (a relative error of 1.6%). The discrepancy seems to get worse as θ grows. This may be the trace of lower order terms of $\mathbf{E}[|\zeta(1/2+\mathrm{i}\tau))|^{2k}]$. Such terms were studied in [8]. There, a refinement of Equation (1) is given where $\mathbf{E}[|\zeta(1/2+\mathrm{i}\tau))|^{2k}]$ is proposed to be a polynomial in $\log T$ of degree k^2. They do observe that for larger k's the leading coefficient C_k in Equation (1) is much smaller than the coefficients of lower order powers, see p.29 in [8]. This could potentially have a detectable effect for T of the order of 10^8.

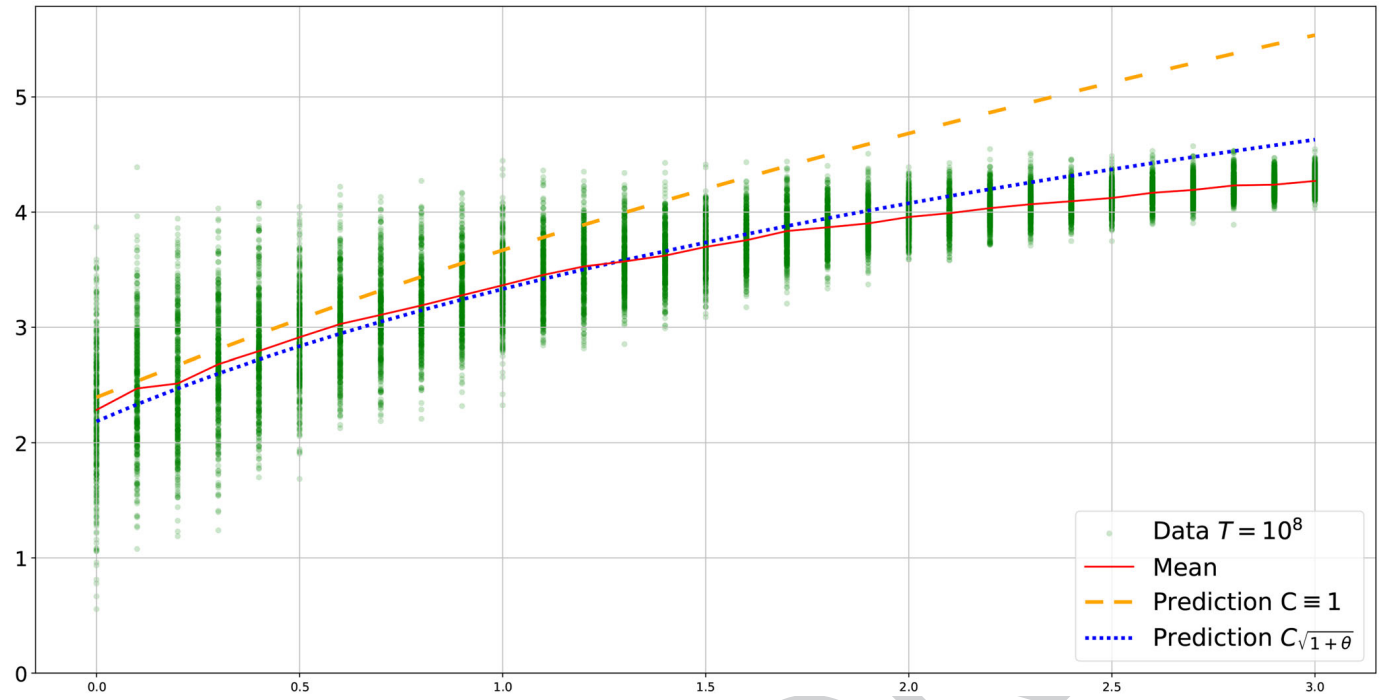

Figure 3. The empirical mean of the samples of $\max_{|h|\le\pi(\log T)^\theta} \log|\zeta(1/2+\mathrm{i}(\tau+h))|$ as a function of θ, $0 \le \theta \le 3$, with step size 0.1 at $T = 10^8$. The dotted lines correspond to the theoretical predictions for $C \equiv 1$ and for $C_{\sqrt{1+\theta}}$.

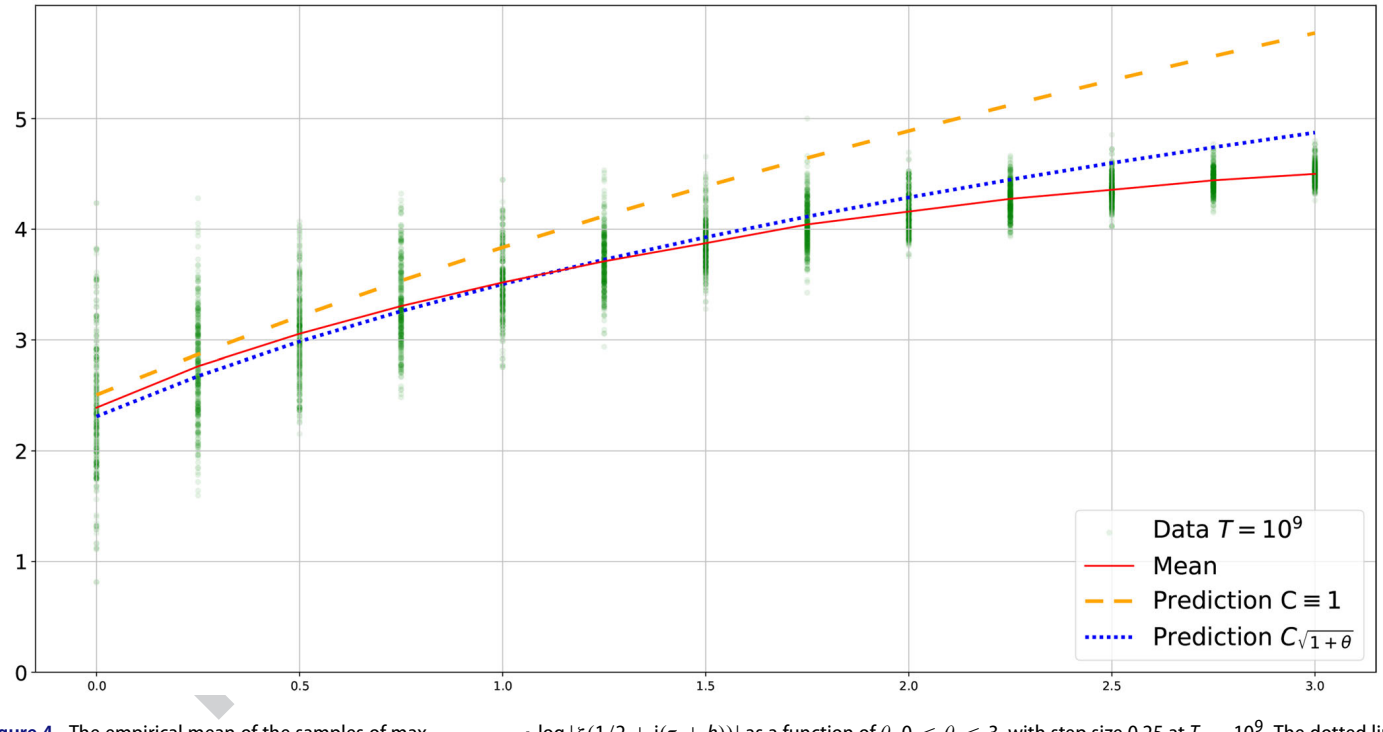

Figure 4. The empirical mean of the samples of $\max_{|h|\le\pi(\log T)^\theta} \log|\zeta(1/2+\mathrm{i}(\tau+h))|$ as a function of θ, $0 \le \theta \le 3$, with step size 0.25 at $T = 10^9$. The dotted lines correspond to the theoretical predictions for $C \equiv 1$ and for $C_{\sqrt{1+\theta}}$.

Table 2 gives the ratio of the empirical mean over the two predictions ($C \equiv 1$ and $C_{\sqrt{1+\theta}}$) for $T = 10^7$, $T = 10^8$ and $T = 10^9$. Again, the ratios suggest that $C_{\sqrt{1+\theta}}$ is the correct prediction. Note that the ratios are improving as T increases.

We also examine the convergence of the empirical mean by computing the relative displacement for the predictions from the empirical means, and by calculating the normalized kernel density estimator as shown in Figure 5. We see that as T grows the relative displacements exhibit smaller deviation centered around 0, with the most pronounced effect occurring for $C_{\sqrt{1+\theta}}$ at $T = 10^9$.

The estimate of the standard deviation of $\max_{|h|\le\pi(\log T)^\theta} \log|\zeta(1/2+\mathrm{i}(\tau+h))|$ turned out to be trickier, see Figure 6. The method to obtain the theoretical prediction is explained after Equation (35). There is a significant discrepancy between the prediction and the numerical results. We do observe a reduction of the variance as predicted by Equation (35) and the definition of β in Equation

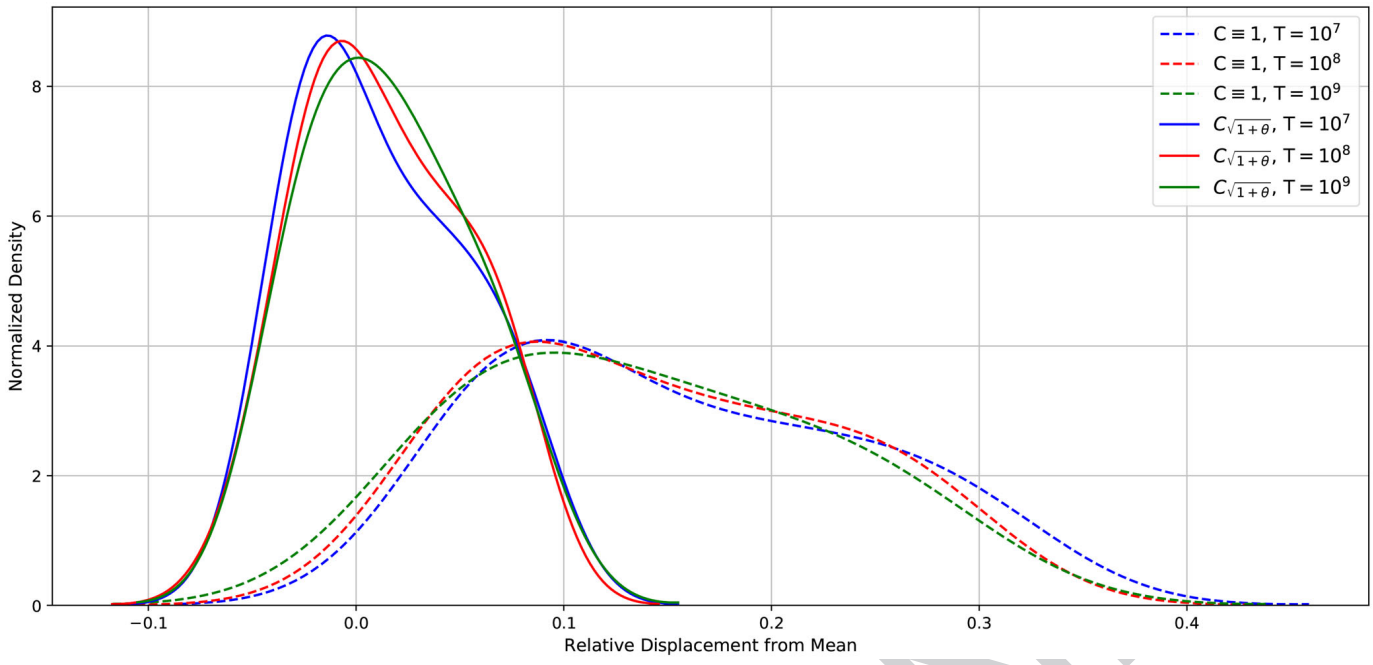

Figure 5. The relative displacement of the samples of $\max_{|h|\leq\pi(\log T)^\theta} \log|\zeta(1/2+\mathrm{i}(\tau+h))|$ from the mean.

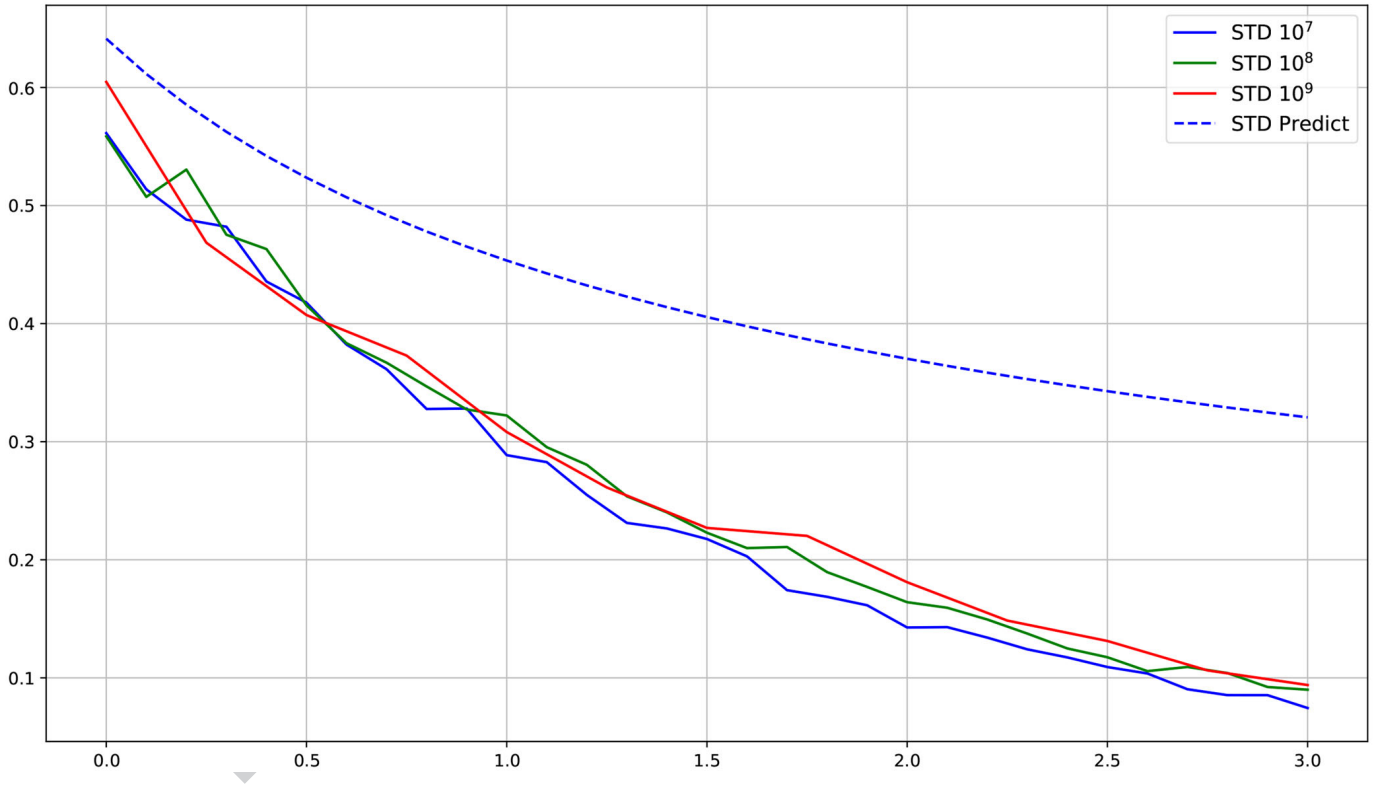

Figure 6. The standard deviation of the samples of $\max_{|h|\leq\pi(\log T)^\theta} \log|\zeta(1/2+\mathrm{i}(\tau+h))|$ as a function of $\theta, 0 \leq \theta \leq 3$.

(9). Note that the standard deviation is fairly small on the whole range of θ. In fact, it is of the order of $1/\sqrt{\mathcal{S}}$, where $\mathcal{S}$ is the size of the sample. This might complicate the detection of a signal. The discrepancy seems to be the same for all range of T's. It is also increasing in θ. We currently have no convincing explanations for this phenomenon.

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Declaration of Interest

No potential conflict of interest was reported by the author(s).

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Appendix A: Proof of Theorem 1.1

For completeness, we provide the proof of Theorem 1.1 based on the work of Keating and Snaith [28]. Recall that we write $P_N(\theta) = \det(I - e^{i\theta}U)$ for the characteristic polynomial of a random $N \times N$ unitary matrix. Let $\sigma_N^2 = \frac{1}{2}\log N$ and $V = V(N) \sim k\sqrt{2\log N}$ as $N \to \infty$. We will show that as $N \to \infty$

$$\mathbb{P}_{\mathcal{U}(N)}\left(\frac{\log|P_N(\theta)|}{\sigma_N} > V\right) \sim f_k \int_V^\infty \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}}\mathrm{d}x, \tag{A1}$$

where f_k is given in (4).

First, consider the Laplace-Fourier transform of $\log|P_N(\theta)|$:

$$M_N(s) = \mathbb{E}_{\mathcal{U}(N)}[|P_N(\theta)|^s] = \sum_{j=0}^\infty \frac{\mathbb{E}_{\mathcal{U}(N)}\left[(\log|P_N(\theta)|)^j\right]}{j!}s^j, \qquad s \in \mathbb{C}, \tag{A2}$$

where the average is taken over the unitary group with respect to Haar measure. Due to the rotational invariance of the Haar measure on $\mathcal{U}(N)$, $M_N(s)$ is independent of θ. Using the Selberg integral, Keating and Snaith [28] (cf. [28], Equation (6)) determined a finite N formula for $M_N(s)$, valid for all real θ and $\mathrm{Re}(s) > -1$

$$M_N(s) = \mathbb{E}_{\mathcal{U}(N)}[|P_N(\theta)|^s] = \prod_{j=1}^N \frac{\Gamma(j)\Gamma(j+s)}{\Gamma^2(j+s/2)}. \tag{A3}$$

From (A3), one deduces that, as $N \to \infty$, $M_N(2k) \sim f_k N^{k^2}$.

The quantity $M_N(s)$ can be written in terms of the *cumulants* $Q_j(N)$ as follows

$$M_N(s) = \exp\left(\sum_{j=1}^\infty \frac{Q_j(N)}{j!}s^j\right). \tag{A4}$$

The cumulants are simply the Taylor coefficients of $\log M_N(s)$. By differentiating the logarithm of (A3), Keating and Snaith calculated the asymptotic form of the cumulants $Q_j(N)$ (see Section 2.2 in [28])

$$Q_1(N) = 0 \tag{A5}$$

$$Q_2(N) = \frac{1}{2}\log N + \frac{1}{2}(\gamma+1) + \frac{1}{24N^2} - \frac{1}{80N^4} + \mathcal{O}\left(\frac{1}{N^6}\right) \tag{A6}$$

$$Q_m(N) = (-1)^m \frac{2^{m-1}-1}{2^{m-1}}\left(\Gamma(m)\zeta(m-1) - \frac{(m-3)!}{N^{m-2}}\right) + \mathcal{O}\left(\frac{1}{N^{m-1}}\right), \tag{A7}$$

for $m \geq 3$. Note that $Q_2(N) = \sigma_N^2(1 + \mathrm{o}(1))$. So we can prove (A1) with σ_N^2 replaced by $Q_2(N)$.

Now, let $\rho_N(x)$ be the probability density function of $\log|P_N(\theta)|$:

$$\rho_N(x) = \frac{\mathrm{d}}{\mathrm{d}x}\mathbb{E}_{\mathcal{U}(N)}[\mathbb{1}\{\log|P_N(\theta)| \leq x\}], \tag{A8}$$

and its rescaled version

$$\tilde{\rho}_N(x) = \sqrt{Q_2(N)}\rho_N(\sqrt{Q_2(N)}x). \tag{A9}$$

Note that $\tilde{\rho}_N$ is the derivative with respect to V of the left-hand side of (A1). Using the relation $\rho_n(x) = \frac{1}{2\pi}\int_{\mathbb{R}} e^{-\mathrm{i}yx}M_N(iy)\mathrm{d}y$, Keating and Snaith determined (cf. [28], Equation (53)) that

$$\tilde{\rho}_N(x) = \frac{1}{\sqrt{2\pi}}e^{-\frac{x^2}{2}}\left(1 + \sum_{m=3}^\infty \frac{A_m(N)}{Q_2(N)^{\frac{m}{2}}}\sum_{p=0}^m \binom{m}{p}x^p\mathcal{E}(m,p)\right), \tag{A10}$$

where

$$\mathcal{E}(m,p)=\begin{cases}\mathrm{i}^{m-p}(m-p-1)!!, & m-p \text{ even}\\ 0, & m-p \text{ odd}\end{cases}, \tag{A11}$$

and where the terms $A_m(N)$ are determined combinatorially from the cumulants and Equation (A9). For example, we have

$$\begin{aligned}A_3(N)&=\frac{Q_3(N)}{3!}\\ A_4(N)&=\frac{Q_4(N)}{4!}\\ A_5(N)&=\frac{Q_5(N)}{5!}\\ A_6(N)&=\frac{Q_6(N)}{6!}+\frac{1}{2!}\frac{Q_3(N)^2}{(3!)^2}.\end{aligned}$$

The sum over p in Equation (A10) is a monic polynomial in x of degree m. The right-hand side of Equation (A10) is rapidly convergent as x grows, which is the regime of interest.

As $N\to\infty$, $A_m(N)$ approaches a constant, see [28]. Evaluating Equation (A10) at $x=\frac{k\log N}{\sqrt{Q_2(N)}}$ then gives

$$\tilde{\rho}_N\left(\frac{k\log N}{\sqrt{Q_2(N)}}\right)=\frac{1}{\sqrt{2\pi}}e^{-\frac{1}{2}\frac{k^2\log^2 N}{Q_2(N)}}\left(1+\sum_{m=3}^{\infty}\frac{A_m(N)}{Q_2(N)^{\frac{m}{2}}}\sum_{p=0}^{m}\binom{m}{p}\left(\frac{k\log N}{\sqrt{Q_2(N)}}\right)^p\mathcal{E}(m,p)\right). \tag{A12}$$

Note that $x\sim k\sqrt{2\log N}$ as $N\to\infty$, ensuring the convergence of Equation (A12). For large N (hence large x), the leading term corresponding to $p=m$ dominates in the sum over p, hence

$$\tilde{\rho}_N\left(\frac{k\log N}{\sqrt{Q_2(N)}}\right)\sim\frac{1}{\sqrt{2\pi}}e^{-\frac{1}{2}\frac{k^2\log^2 N}{Q_2(N)}}\left(1+\sum_{m=3}^{\infty}A_m(N)\left(\frac{k\log N}{Q_2(N)}\right)^m\right) \tag{A13}$$

$$\sim\frac{1}{\sqrt{2\pi}}N^{-k^2}e^{k^2(\gamma+1)}\left(1+\sum_{m=3}^{\infty}A_m(N)(2k)^m\right), \tag{A14}$$

using Equation (A6).

To prove the theorem, it remains to express the term in the parenthesis in terms of f_k. Recall from the comment following Equation (A3) that

$$f_k=\lim_{N\to\infty}\frac{M_N(2k)}{N^{k^2}}. \tag{A15}$$

Then, we have as $N\to\infty$ using (A6),

$$\frac{M_N(2k)}{N^{k^2}}=\exp\left(2k^2Q_2(N)-k^2\log N+\sum_{m=3}^{\infty}\frac{Q_m(N)}{m!}(2k)^m\right) \tag{A16}$$

$$\sim\exp\left(k^2(\gamma+1)+\sum_{m=3}^{\infty}\frac{Q_m(N)}{m!}(2k)^m\right) \tag{A17}$$

$$=\exp\left(k^2(\gamma+1)\right)\left(1+\sum_{m=3}^{\infty}A_m(N)(2k)^m\right). \tag{A18}$$

The final line follows by expanding the exponential with the infinite sum in the exponent in the Taylor series, and then grouping terms according to power of $2k$. The fact that this results in the weights $A_m(N)$ follows immediately from the combinatorial definition, see the discussion following (A11) and [28]. Hence f_k is given by Equation (A18), and the result follows by substituting the expression into (A14).

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