On the sign of the real part of the Riemann zeta function

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Joint work with

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In memory of Alf van der Poorten

Abstract

The real part of the Riemann zeta function $\zeta(s)$ is "usually positive" in the half-plane to the right of the critical line $\Re(s) = 1/2$. We make this statement precise and show how the density of positive values can be computed on vertical lines with fixed real part $\sigma = \Re(s) > 1/2$. Closely related results apply to $\arg\zeta(s)$.

This is a longer version of a 25-minute talk given in Newcastle[1] last week. It describes joint work with Juan Arias de Reyna and Jan van de Lune.

[1] International Number Theory Conference in Memory of Alf van der Poorten, Newcastle, 12–16 March 2012.
http://carmamaths.org/alfcon/

Alf van der Poorten

Like almost all number theorists, Alf van der Poorten was interested in the Riemann zeta function. For example, Alf gave a very clear exposition of Apéry's proof of the irrationality of $\zeta(3)$, in his 1979 paper *A proof that Euler missed . . . Apéry's proof of the irrationality of* $\zeta(3)$.

Thus, although my only joint work with Alf was on continued fractions of algebraic numbers, I decided to talk today on a topic related to the Riemann zeta function.

Summary

- Notation and definitions.
- Motivation – $\Re\zeta(s)$ is "usually" positive.
- The densities $d_+(\sigma)$, $d_-(\sigma)$ and $d(\sigma)$.
- A theorem of Bohr and Jessen.
- The characteristic function $\psi_\sigma(x)$ as an infinite product.
- The function $I(b,x)$.
- $\log I(b,x)$ and related polynomials $Q_n(x)$.
- Computation of $\psi_\sigma(x)$, $d(\sigma)$ and $d_-(\sigma)$.
- Numerical results.
- Asymptotics.
- Other L-functions.

Some notation and definitions

P is the set of primes and $p \in P$ is a prime.

We always have $s = \sigma + it \in \mathbb{C}$.

$\log \zeta(s)$ denotes the main branch defined in the usual way on the open set G equal to the complex plane $\mathbb{C}$ with cuts along the half-lines $(-\infty + i\gamma, \beta + i\gamma]$ for each zero or pole $\beta + i\gamma$ of $\zeta(s)$ with $\beta \geq 1/2$. Thus $\log \zeta(s)$ is real and positive in $(1, +\infty)$.

For $s \in G$, we can define $\arg \zeta(s)$ by

$$\log \zeta(s) = \log |\zeta(s)| + i \cdot \arg \zeta(s).$$

$|B|$ denotes the Lebesgue measure of a set B.

Usually $\sigma > 1/2$ is fixed, $t \in \mathbb{R}$ is regarded as the independent variable, and $b = p^\sigma$.

Motivation

Several authors (Gram, Titchmarsh, Edwards, ...) have observed that $\Re\zeta(s)$ is "usually" positive, at least for $\sigma \geq 1/2$. This is plausible because the Dirichlet series

$$\zeta(s) = 1 + 2^{-s} + 3^{-s} + 4^{-s} + \cdots$$

starts with a positive term, and the other terms n^{-s} may have positive or negative real part, depending on the sign of $\cos(t \log n)$.

Our aim is to quantify this observation.

The Euler product

Recall the *Euler product* formula

$$\zeta(s) = \prod_p \left(1 - p^{-s}\right)^{-1} \; ,$$

valid for $\sigma > 1$.

Taking logarithms, we get

$$\log \zeta(s) = -\sum_p \log\left(1 - p^{-s}\right) = \sum_p p^{-s} + O(1).$$

There is a sense in which $\log \zeta(s)$ can be approximated by a "short Dirichlet series" $\sum_{p \le x} p^{-s}$ in the region $1/2 \le \sigma \le 1$, but we won't discuss this today.

Remarks

Let $\sigma_0 = 1.1923473371\cdots$ be the real root in $(1, +\infty)$ of

$$\sum_p \arcsin(p^{-\sigma}) = \frac{\pi}{2}.$$

It was shown by Jan van de Lune (1983) that

$$(\forall \sigma \geq \sigma_0) \;\; \Re\zeta(\sigma + it) > 0\,.$$

Also, for any $\sigma \in (1, \sigma_0)$, there exist arbitrarily large t such that $\Re\zeta(\sigma + it) < 0$. The proof uses Kronecker's theorem.[2]

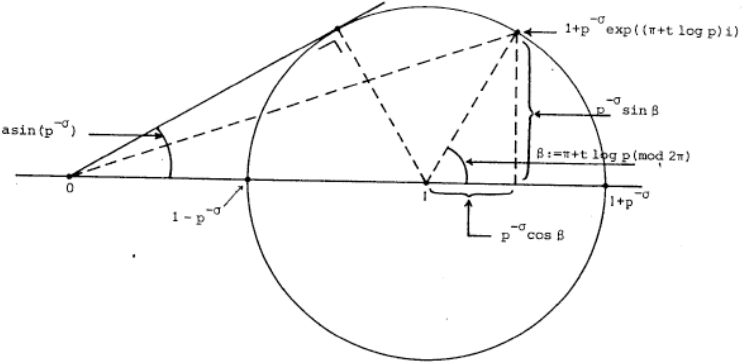
The result is also true for $\sigma \in [1/2, 1]$. In fact, Voronin's "universality" theorem is a vast generalisation of this, but not our topic today.

For future reference, let $\sigma_1 \approx 1.0068232917\cdots$ be the (unique) real root in $(1, +\infty)$ of

$$\sum_p \arcsin(p^{-\sigma}) = \frac{3\pi}{2}.$$

[2] Titchmarsh, §8.3.

Figure from Van de Lune (1983)



From the Figure, we see that the prime p contributes at most $\arcsin(p^{-\sigma})$ to $\arg\zeta(\sigma+it)$. If $\zeta(\sigma+it)<0$ then we must have $|\arg\zeta(\sigma+it)|>\pi/2$.

Some numerical results

If we compute $\zeta(s)$ for "randomly" chosen s with $\sigma = \Re(s) \geq 0.6$ (say), we are unlikely to find any negative values of $\Re\zeta(s)$.

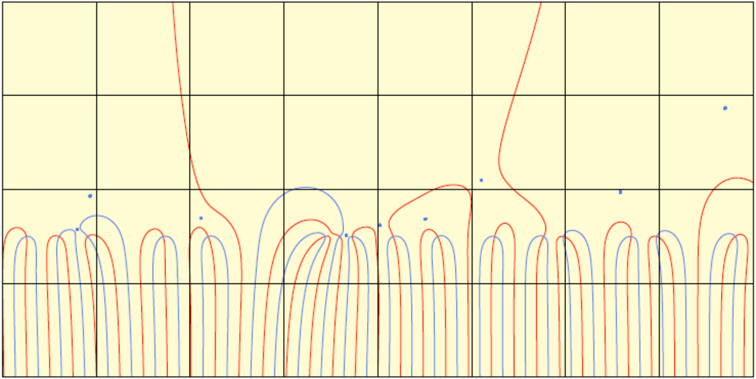
For example, taking $\sigma = 1$, it can be shown that $\Re\zeta(1 + it) > 0$ for all $t \in (0, 682112]$. Near $t = 682112.9169$ there is an interval of length 0.0529 on which $\Re\zeta(1 + it) < 0$.

For $t \in (0, 16656259]$ there are 50 intervals on which $\Re\zeta(1 + it) < 0$; the total length of these intervals is < 6.484.

Note that $16656259/6.484 \approx 2.57 \times 10^6$. Thus, the chance of finding a value of t such that $\Re\zeta(1 + it) < 0$ by random sampling is very small.

The seventh interval where $\Re\zeta(1+it) < 0$

Here is an "x-ray" of $\zeta(\sigma + it)$ for $\sigma \in [-1, 3]$, $t \in [2195052, 2195060]$, enclosing the seventh interval where $\Re\zeta(1+it)$ is negative. $\Re\zeta$ vanishes on the blue lines, and $\Im\zeta$ vanishes on the red lines. The blue dots are zeros of ζ'. The picture is rotated so that the critical strip is horizontal.



Asymptotic densities

Fix $\sigma > 1/2$, and define

$$d_+(\sigma) := \lim_{T\to+\infty} \frac{1}{2T} |\{t \in [-T, +T] : \Re\zeta(\sigma + it) > 0\}| ,$$

$$d_-(\sigma) := \lim_{T\to+\infty} \frac{1}{2T} |\{t \in [-T, +T] : \Re\zeta(\sigma + it) < 0\}| .$$

It can be shown that the limits exist.

$d_+(\sigma)$ can be regarded as the probability that a randomly chosen point $\sigma + it$ gives a positive value of $\Re\zeta(\sigma + it)$; similarly for $d_-(\sigma)$ and negative values.

Since $\Re\zeta(s)$ vanishes on a set of Lebesgue measure zero, we have $d_+(\sigma) + d_-(\sigma) = 1$.

Approximation of $d_\pm(\sigma)$ via $\arg\zeta(s)$

It is easier to work with

$$d(\sigma) = \lim_{T\to+\infty} \frac{1}{2T} |\{t \in [-T, +T] : |\arg\zeta(\sigma + it)| > \pi/2\}| .$$

Observe that $\Re\zeta(s) < 0$ iff

$$|\arg\zeta(s)| \in (\pi/2, 3\pi/2) \cup (5\pi/2, 7\pi/2) \cup \cdots$$

Thus

$$d_-(\sigma) \le d(\sigma),$$

$$d_+(\sigma) \ge 1 - d(\sigma),$$

and $d_-(\sigma) \approx d(\sigma)$ if $\arg\zeta(s)$ is "usually" small, i.e. unless σ is close to $1/2$ (more on this later).

A mean-value result

Using Chebyshev's inequality and a mean-value result[3] for $|\Re\zeta(1+it)|^2$, we can show that

$$d_-(1) \le \frac{\zeta(2)-1}{\zeta(2)+1} = 0.243837\ldots < 1/4\,.$$

However, this result is far from the truth. We shall see later that

$$d_-(1) \approx 3.8 \times 10^{-7}\,.$$

The mean-value approach is simple and elegant, but it throws away too much information to give sharp results.

[3] The proof is similar to that of Theorem 7.2 of Titchmarsh, which gives a mean-value result for $|\zeta(1+it)|^2$.

Intuition

Informally, the idea is that, for a prime p and large t,

$$p^{it} = \exp(it \log(p))$$

behaves like a random variable distributed uniformly on the unit circle.

Moreover, for different primes, the random variables are independent (because the $\log p$ are independent over $\mathbb{Q}$).

A theorem of Bohr and Jessen (to be stated soon) justifies this intuition.

The probability space Ω

Let $\mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$ denote the unit circle with the usual probability measure μ (that is $\frac{d\theta}{2\pi}$ if we identify $\mathbb{T}$ with the interval $[0, 2\pi)$ via $z = \exp(i\theta)$).

Define $\Omega := \mathbb{T}^P$ with the product measure $\mathbb{P} = \mu^P$.

Each point of Ω is a sequence $\omega = (x_p)_{p\in P}$, with each $x_p \in \mathbb{T}$.

This formalises the idea that the x_p may be considered as a random variables, uid[4] on the unit circle.

[4] Uniformly and independently distributed.

The measure $\mathbb{P}_\sigma$ of Bohr and Jessen

Before stating the theorem of Bohr and Jessen we need to define a measure $\mathbb{P}_\sigma$.

Fix $\sigma > 1/2$. The sum of random variables

$$S = -\sum_{p\in P} \log(1 - p^{-\sigma} x_p) := \sum_{p\in P} \sum_{k=1}^{\infty} \frac{1}{k} p^{-k\sigma} x_p^k$$

converges almost everywhere, so S is a well-defined random variable.

The measure $\mathbb{P}_\sigma$ of Bohr and Jessen is defined to be the distribution of S, i.e. for each Borel set $\mathcal{B} \subseteq \mathbb{C}$ we have

$$\mathbb{P}_\sigma(\mathcal{B}) := \mathbb{P}\{\omega = (x_p) \in \Omega : S(\omega) \in \mathcal{B}\}.$$

A theorem of Bohr and Jessen

In modern language, Bohr and Jessen (1930/31) showed that, for each rectangle $\mathcal{B}$ with sides parallel to the axes,

$$\mathbb{P}_\sigma(\mathcal{B}) = \lim_{T\to\infty} \frac{1}{2T} |\{t \in [-T, +T], \log\zeta(\sigma + it) \in \mathcal{B}\}|$$

(and the limit exists).

It is easy to deduce that the same result holds for Jordan-measurable sets $\mathcal{B} \subseteq \mathbb{C}$.

Bohr and Jessen also showed that $\mathbb{P}_\sigma$ is absolutely continuous with respect to the Lebesgue measure on $\mathbb{C}$.

The measure μ_σ on $\mathbb{R}$

We can specialise[5] to sets $\mathcal{B}$ of the form $\mathbb{R} \times B$. For Jordan subsets $B \subseteq \mathbb{R}$, define

$$\mu_\sigma(B) := \mathbb{P}_\sigma(\mathbb{R} \times B).$$

Then

$$d(\sigma) = \mu_\sigma(\mathbb{R} \backslash [-\pi/2, \pi/2]),$$

$$d_+(\sigma) = \mu_\sigma\left(\bigcup_{k\in\mathbb{Z}} (2k\pi - \pi/2,\, 2k\pi + \pi/2)\right).$$

The measure μ_σ is the distribution function of the random variable $\Im S$:

$$\begin{aligned} \mu_\sigma(B) = \mathbb{P}_\sigma(\mathbb{R} \times B) &= \mathbb{P}\{\omega \in \Omega : S(\omega) \in \mathbb{R} \times B\} \\ &= \mathbb{P}\{\omega \in \Omega : \Im S(\omega) \in B\}. \end{aligned}$$

[5] Since $\mathbb{R}$ is not bounded, we need a limiting argument to justify this.

The characteristic function ψ_σ

Recall that the *characteristic function* $\psi(y)$ of a random variable X is defined by

$$\psi(y) := \mathrm{E}[\exp(iXy)]\,.$$

This is just a Fourier transform; we omit a factor 2π in the exponent to agree with the statistical literature.

The characteristic function associated with μ_σ is the characteristic function ψ_σ of the random variable $\Im S$:

$$\psi_\sigma(x) := \int_\Omega e^{ix\Im S(\omega)}\,d\omega\,.$$

ψ_σ as an infinite product over the primes

We have

$$\psi_\sigma(x) = \prod_p I(p^\sigma, x)\,,$$

where (as usual) the product is over all primes p, and

$$I(b, x) := \frac{1}{2\pi} \int_0^{2\pi} e^{-ix \arg(1 - b^{-1} e^{it})}\, dt\,.$$

Sketch of the proof

By definition

$$\psi_\sigma(x) = \int_\Omega e^{ix\Im S(\omega)}\,d\omega = \int_\Omega \prod_p e^{-ix\arg(1-p^{-\sigma}x_p)}\,d\omega.$$

By independence the integral of the product is the product of the integrals:

$$\psi_\sigma(x) = \prod_p \int_\Omega e^{-ix\arg(1-p^{-\sigma}x_p)}\,d\omega.$$

Each random variable x_p is distributed as $e^{i\theta}$ on the unit circle. □

$I(b,x)$ as an integral

Assume $b > 1$. Recall the definition

$$I(b,x) := \frac{1}{2\pi}\int_0^{2\pi} e^{-ix\arg(1-b^{-1}e^{it})}\,dt\,.$$

Then we have two equivalent expressions for $I(b,x)$ as a definite integral:

$$\begin{aligned} I(b,x) &= \frac{1}{\pi}\int_0^{\pi}\cos\left(x\arctan\left(\frac{\sin\theta}{b-\cos\theta}\right)\right)\,d\theta \\ &= \frac{2}{\pi}\int_0^{1}\cos\left(x\arcsin\frac{u}{b}\right)\frac{du}{\sqrt{1-u^2}}\,. \end{aligned}$$

Connection with Bessel functions

Suppose b is large in the first representation

$$I(b,x) = \frac{1}{\pi}\int_0^\pi \cos\left(x \arctan\left(\frac{\sin\theta}{b-\cos\theta}\right)\right)\,d\theta\,.$$

Approximating $\arctan(\sin\theta/(b-\cos\theta))$ by $\sin(\theta)/b$, we get

$$I(b,x) \approx \frac{1}{\pi}\int_0^\pi \cos\left(\frac{x}{b}\sin\theta\right)\,d\theta = J_0(x/b)$$

from an integral representation of the Bessel function J_0.

A more detailed asymptotic analysis shows that $I(b,x)$ has infinitely many real zeros near the points

$$\{\pm(3\pi/4 + k\pi)/\arcsin(1/b) : k \in \mathbb{Z}_{\geq 0}\}.$$

What does ψ_σ look like?

$\psi_\sigma(x)$ is a product:

$$\psi_\sigma(x) = \prod_p I(p^\sigma, x)\,.$$

Each factor in the product has infinitely many real zeros, and the same is true for $\psi_\sigma(x)$.

We have the bound

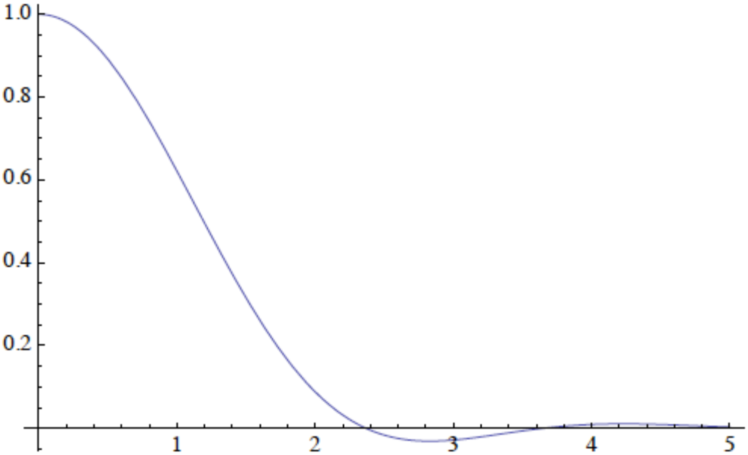
$$|\psi_\sigma(x)| \le C \exp\left(-c\frac{x^{1/\sigma}}{\log x}\right)$$

for some positive constants $C = C(\sigma)$, $c = c(\sigma)$ and $x \ge 2$.

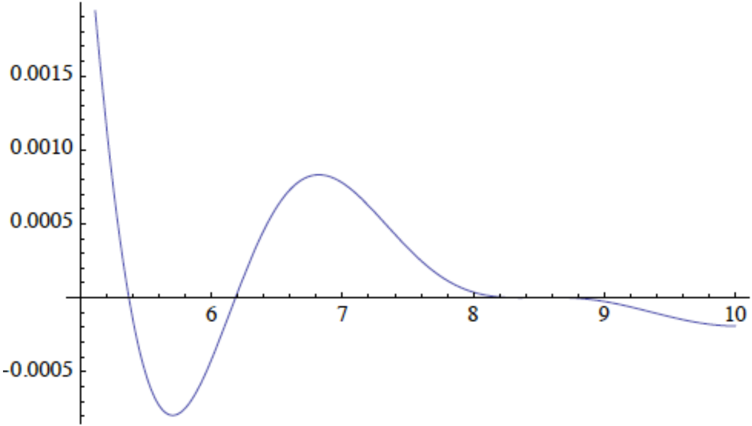
The best possible constants are not known, but empirically we can take $C = c = 1$ for all $x \ge 7$ and $\sigma > 1/2$.

Pictures of $\psi_{1.02}(x)$

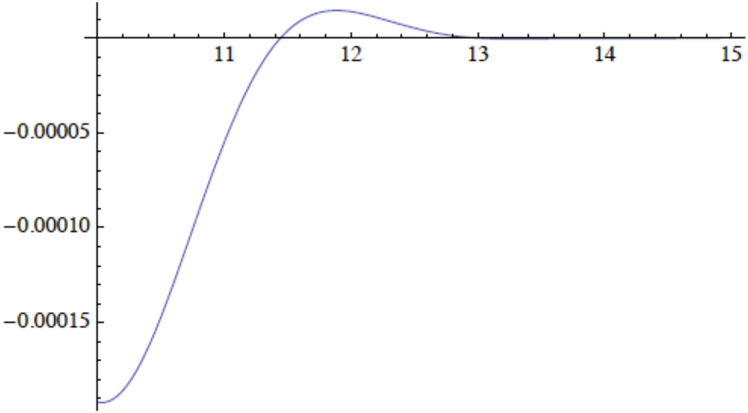
Due to the exponential decay of $|\psi_\sigma(x)|$ it is difficult to give a single plot that shows its behaviour. Following are plots for $\sigma = 1.02$ and x in the intervals $[0,5]$, $[5,10]$, ..., $[25,30]$.



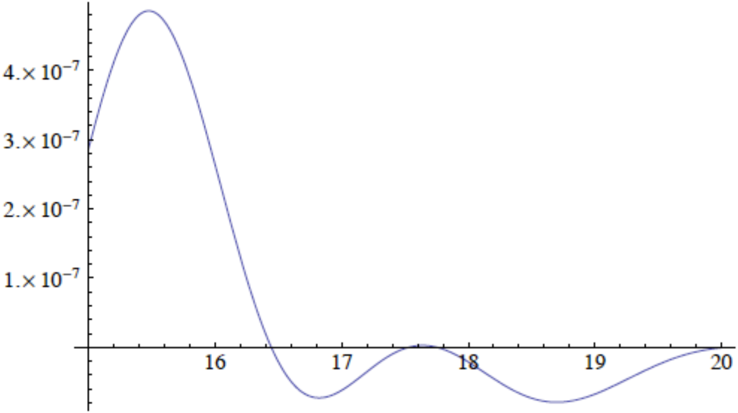
$x \in [5, 10]$



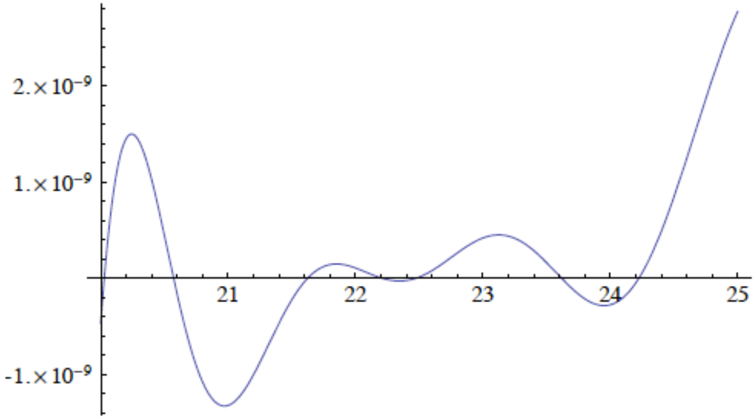
$x \in [10, 15]$



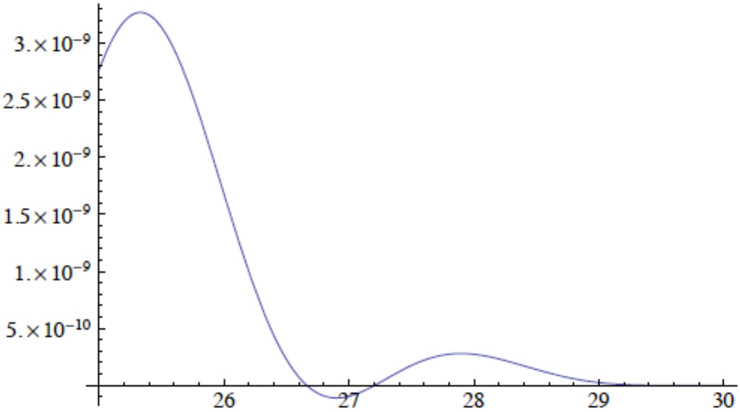
$x \in [15, 20]$



$x \in [20, 25]$



$x \in [25, 30]$



Digression – the hypergeometric differential equation

The *hypergeometric differential equation* is the second-order linear equation

$$z(1-z)w'' + (c-(a+b+1)z)w' - abw = 0,$$

where primes denote differentiation with respect to z. Here a, b, c are constants. In a neighbourhood of the origin, the *hypergeometric function*

$${}_2F_1(a,b;c;z) = \sum_{n=0}^{\infty} \frac{(a)_n(b)_n}{(c)_n} \frac{z^n}{n!}$$

is a solution; a second solution is

$$z^{1-c}{}_2F_1(1+a-c, 1+b-c; 2-c; z).$$

$\cos(2x \arcsin u)$ as a hypergeometric function

For $|u| < 1$ and all $x \in \mathbb{C}$,

$$\cos(2x \arcsin u) = 1 + \sum_{n=1}^{\infty} \frac{(2u)^{2n}}{(2n)!} \prod_{j=0}^{n-1} (j^2 - x^2).$$

To prove this, let $f(u) :=$ LHS, $g(u) :=$ RHS above. Then

$$(1 - u^2)f''(u) - uf'(u) + 4x^2 f(u) = 0.$$

Also, $g(u)$ satisfies the same differential equation. Since $g(0) = f(0) = 1$ and $g'(0) = f'(0) = 0$, the two solutions coincide. □

Notes. When $x \in \mathbb{Z}$ the series reduces to a polynomial. The differential equation can be put in standard hypergeometric form by a linear change of variables.

Corollary

For $|b| > 1$ we have

$$I(b, 2x) = 1 + \sum_{n=1}^{\infty} \frac{1}{b^{2n} n!^2} \prod_{j=0}^{n-1} (j^2 - x^2).$$

Combining this result with the product formula for ψ_σ, we obtain an explicit expression for ψ_σ, valid for $\sigma > 1/2$ (next slide).

An explicit expresson for ψ_σ

The characteristic function ψ_σ is given by the following product

$$\psi_\sigma(2x) = \prod_p \left(1 + \sum_{n=1}^{\infty} \frac{1}{n!^2} \prod_{j=0}^{n-1} (j^2 - x^2) \cdot \frac{1}{p^{2n\sigma}} \right).$$

Marc Kac[6] gave the probability of $\log(\varphi(n)/n)$ being in a given interval (ω_1, ω_2) as

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{i\omega_2\xi} - e^{i\omega_1\xi}}{i\xi} \prod_p \left(1 - \frac{1}{p} + \frac{1}{p} \exp\left[i\xi \log\left(1 - \frac{1}{p}\right)\right]\right) d\xi\,,$$

and referred to this as "an explicit but nearly useless formula". Is our formula for $\psi_\sigma(2x)$ in the same category ?

[6] Mark Kac, *Statistical Independence in Probability, Analysis and Number Theory*, 1959, page 64.

Remarks

- Formally, the problem is solved. We can use a Fourier transform to compute the distribution function μ_σ from ψ_σ, and hence compute $d(\sigma)$, $d_\pm(\sigma)$ etc.
- In practice there are still severe difficulties (recall the quote from Kac). The product over prime p converges slowly, and we need to compute ψ_σ accurately to compensate for cancellation in computing the Fourier transform.
  Also, some of the results of interest, such as $d_-(\sigma)$ for $\sigma \in [1, \sigma_0)$, are tiny, so we need to compute the Fourier transform accurately.
- In the following slides we show how these difficulties can be overcome.

Computing sums/products over primes

There is a well-known technique, going back at least to Wrench (1961), for accurately computing certain sums/products over primes.

The idea is to express what we want to compute in terms of the *prime zeta function*

$$P(s) := \sum_p p^{-s} \quad (\Re(s) > 1).$$

The prime zeta function can be computed from $\log\zeta(s)$ using Möbius inversion:

$$P(s) = \sum_{r=1}^{\infty} \frac{\mu(r)}{r} \log\zeta(rs)\,.$$

This formula was essentially known to Euler (1748).

Application to computation of ψ_σ

Recall that

$$\psi_\sigma(x) = \prod_p I(p^\sigma, x),$$

so the obvious approach is to take logarithms of each side:

$$\log \psi_\sigma(x) = \sum_p \log I(p^\sigma, x)\,,$$

and try to express the RHS as a sum $\sum_{k\geq 1} a_k(x,\sigma)P(k\sigma)$.

Problem – $I(p^\sigma, x)$, considered as a function of x, has zeros. Thus, the series for $\log \psi_\sigma(x)$ fails to converge.

Solution – If we consider x fixed, then $I(p^\sigma, x) > 0$ for $p > p_0(x,\sigma)$. Thus, we can apply a variant of the "prime zeta function" technique after all, provided we sum over $p > p_0$ rather than over all primes. The finite number of cases $p \leq p_0$ can be handled in a different manner.

The function $\log I(b, x)$

Suppose $x > 0$. There exist even polynomials $Q_n(x)$ of degree $2n$ such that

$$\log I(b, 2x) = -\sum_{n=1}^{\infty} \frac{Q_n(x)}{n!^2} \frac{1}{b^{2n}},$$

and the series converges for $b > \max(1, |x|)$.

The polynomials $Q_n(x)$ are determined by the following recurrence:

$$Q_{n+1}(x) = (n!)^2 x^2 + \sum_{j=0}^{n-1} \binom{n}{j} \binom{n}{j+1} Q_{j+1}(x) Q_{n-j}(x), \ \ n \geq 0.$$

Sketch of proof

The existence of the $Q_n(x)$ follows easily from the fact that

$$I(b, 2x) = 1 + \sum_{n=1}^{\infty} \frac{P_n(x)}{n!^2} \frac{1}{b^{2n}}$$

for certain even polynomials $P_n(x)$.

To prove the recurrence for $Q_n(x)$, consider x as fixed and define $f(y) := I(y^{-1/2}, 2x)$. Then $f(y) = {}_2F_1(x, -x; 1; y)$ satisfies the hypergeometric differential equation

$$y(1-y)f'' + (1-y)f' + x^2 f = 0.$$

Sketch of proof continued

Define $g(y) := f'(y)/f(y)$. Then g satisfies the Riccati equation

$$y(g' + g^2) + g + \frac{x^2}{1-y} = 0.$$

Now $g(y) = \sum_{n\geq 0} g_n y^n$, where the g_n are polynomials in x, in fact

$$g_n = -\frac{Q_{n+1}}{n!(n+1)!} .$$

Equating coefficients gives the recurrence

$$g_n = -\left(\frac{1}{n+1}\right)\left(x^2 + \sum_{j=0}^{n-1} g_j g_{n-1-j}\right) \quad \text{for} \quad n \geq 0,$$

from which the recurrence for the Q_n follows. □

The coefficients of the polynomials $Q_n(x)$

From the recurrence it is clear that $Q_n(x)$ is an even polynomial of degree $2n$ such that $Q_n(0) = 0$. Define coefficients $q_{n,k}$ by

$$Q_n(x) = \sum_{k=1}^{n} q_{n,k} x^{2k}.$$

The numbers $q_{n,k}$ are determined by $q_{n,1} = (n-1)!^2$ for $n \geq 1$, and, for $2 \leq k \leq n+1$, by the recurrence

$$q_{n+1,k} = \sum_{j=0}^{n-1} \binom{n}{j} \binom{n}{j+1} \sum_{r=\max(1,k-n+j)}^{\min(j+1,k-1)} q_{j+1,r} q_{n-j,k-r} \,.$$

It follows that $q_{n,k}$ is a positive integer for $1 \leq k \leq n$.

The integers $q_{n,k}$

Table: The integers $q_{n,k}$, $1 \le k \le n \le 6$.

$n \setminus k$	1	2	3	4	5	6
1	1					
2	1	1				
3	4	4	4			
4	36	33	42	33		
5	576	480	648	720	456	
6	14400	10960	14900	18780	17900	9460

Question. Do the $q_{n,k}$ have a natural combinatorial interpretation?

The first column is Sloane's A001044, and the diagonal is Sloane's A002190.

Further remarks on the integers $q_{n,k}$

1. It is easy to show that $\sum_{k=1}^{n} q_{n,k} = n!\,(n-1)!$.
2. We also have

$$q_{n,n} = n!(n-1)! \sum_{k=1}^{\infty} \left(\frac{2}{j_{0,k}}\right)^{2n},$$

   where $(j_{0,k})_{k\geq 1}$ is the sequence of positive zeros of the Bessel function $J_0(z)$ [Carlitz, 1963].
3. The numbers $q_{n,n}$ enjoy interesting congruence properties. They are analogous to Bernoulli numbers. Compare Euler's identity

$$|B_{2n}| = 2(2n)! \sum_{k=1}^{\infty} \left(\frac{1}{2\pi k}\right)^{2n}.$$

4. There are other recurrences giving the polynomials Q_n and the integers $q_{n,k}$.

An algorithm for the computation of ψ_σ

We want to compute

$$\psi_\sigma(2x) = \prod_p I(p^\sigma, 2x).$$

Choose $p_0^\sigma > |x|$ (a good choice is $p_0^\sigma \approx 8|x|$).
Split the product at p_0, so $\psi_\sigma(2x) = AB$ say.
Then $A = \prod_{p \le p_0} \cdots$ is computed using

$$A = \prod_{p \le p_0} \left(1 + \sum_{n=1}^{\infty} \frac{1}{p^{2n\sigma} n!^2} \prod_{j=0}^{n-1} (j^2 - x^2) \right) ,$$

and $B = \prod_{p > p_0} \cdots$ is computed using

$$B = \exp\left(- \sum_{n=1}^{\infty} \frac{Q_n(x)}{n!^2} \left[P(2n\sigma) - \sum_{p \le p_0} p^{-2n\sigma} \right] \right) .$$

Remarks

1. The summations required for A involve some cancellation, so the working precision has to be increased (by $O(x)$ bits) to compensate.
2. There is inevitably cancellation in computing
$$\left[P(2n\sigma) - \sum_{p \le p_0} p^{-2n\sigma} \right] ,$$
so here too the working precision has to be increased (by about $2n\sigma \log_2 p_0$ bits) to compensate.
3. The $Q_k(x)$ can be computed directly from the recurrence for Q_k, or by using a precomputed table of the coefficients $q_{n,k}$.
4. The whole computation is polynomial-time in the sense that, for fixed x, the time required to compute $\psi_\sigma(2x)$ with absolute error $O(2^{-d})$ is bounded by a polynomial in d (the number of digits).

The density ρ_σ

Suppose for the moment that $\sigma > 1$. Then the support of the measure μ_σ is the interval $[-L(\sigma), L(\sigma)]$, where

$$L(\sigma) := \sum_p \arcsin(p^{-\sigma}).$$

Recall that

$$\psi_\sigma(x) = \int_{\mathbb{R}} e^{ixt}\, d\mu_\sigma(t).$$

μ_σ is the Fourier transform of a function in $L^2(\mathbb{R})$, so it is a measure with density

$$\rho_\sigma(t) = \frac{1}{2\pi}\int_{\mathbb{R}} \psi_\sigma(x) e^{-itx}\, dx.$$

The function ρ_σ is a Fourier transform of a function in $L^1(\mathbb{R})$, hence is continuous.

Computation of the density $d(\sigma)$

Theorem

Let $\sigma > 1$ *and* $\ell > \max(\pi/2, L(\sigma))$*. Then we have*

$$d(\sigma) = 1 - \frac{\pi}{2\ell} - \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\psi\Big(\frac{\pi n}{\ell}\Big)\sin\Big(\frac{n\pi^2}{2\ell}\Big).$$

Sketch of proof. Consider the function $\widetilde{\rho}(x)$ equal to $\rho_\sigma(x)$ in the interval $[-\ell, \ell]$. Extend $\widetilde{\rho}(x)$ to the entire real line $\mathbb{R}$, making it periodic with period 2ℓ. We have

$$\widetilde{\rho}(x) = \sum_{n\in\mathbb{Z}} f_n e^{\frac{2\pi i n x}{2\ell}}, \quad \text{with} \quad f_n = \frac{1}{2\ell}\int_{-\ell}^{\ell}\widetilde{\rho}(x)e^{-\frac{2\pi i n x}{2\ell}}\,dx\,.$$

Now $\widetilde{\rho}(x) = \rho_\sigma(x)$ for $|x| \le \ell$, and $\rho_\sigma(x) = 0$ for $|x| > \ell$. Therefore

$$f_n = \frac{1}{2\ell}\int_{-\ell}^{\ell}\rho_\sigma(x)e^{-\frac{2\pi i n x}{2\ell}}\,dx = \frac{1}{2\ell}\int_{\mathbb{R}}\rho_\sigma(x)e^{-\frac{2\pi i n x}{2\ell}}\,dx = \frac{1}{2\ell}\psi\Big(\frac{\pi n}{\ell}\Big)\,.$$

Sketch of proof continued

Since $\psi(x)$ is an even function,

$$\widetilde{\rho}(x) = \frac{1}{2\ell}\sum_{n\in\mathbb{Z}}\psi\Big(\frac{\pi n}{\ell}\Big)e^{\frac{2\pi inx}{2\ell}} = \frac{1}{2\ell} + \frac{1}{\ell}\sum_{n=1}^{\infty}\psi\Big(\frac{\pi n}{\ell}\Big)\cos\frac{\pi nx}{\ell}.$$

Now

$$d(\sigma) = 1 - \mu_\sigma([-\pi/2, \pi/2]) = 1 - \int_{-\pi/2}^{\pi/2}\rho_\sigma(t)\,dt\,.$$

Since we assume $\pi/2 \leq \ell$, we may replace $\rho_\sigma(t)$ by $\widetilde{\rho}$. Hence, multiplying the above equality by the characteristic function of $[-\pi/2, \pi/2]$ and integrating, we get the result. □

Remarks

1. The formula for $d(\sigma)$ is exact, on the assumption that $\sigma > 1$ and $\ell > \max(\pi/2, L(\sigma))$. If $\sigma \in (1/2, 1]$ the formula is approximate, but converges rapidly to $d(\sigma)$ as $\ell \to \infty$, because ψ_σ is exponentially small outside a small compact interval $[-L, L]$.
2. If we take $m := 4\ell/\pi$ in the theorem, we get the slightly simpler form

$$d(\sigma) = 1 - \frac{2}{m} - \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \psi_\sigma \left(\frac{4n}{m} \right) \sin \left(\frac{2\pi n}{m} \right)$$

   for $m > \max(2, M(\sigma))$, where $M(\sigma) = 4L(\sigma)/\pi$.
3. A good choice is $m = 4$; then only the odd terms in the sum contribute, since $\sin(2\pi n/4) = 0$ when n is even.

Computation of $d_-(\sigma)$

Recall that $d_-(\sigma)$ is the probability that $\Re(\zeta(\sigma+it)<0$.
Let a_k be the probability that $|\arg\zeta(\sigma+it)|>(2k+1)\pi/2$.
Then

$$d_-(\sigma)=\sum_{k=0}^{\infty}(a_{2k}-a_{2k+1}).$$

We have seen that

$$a_0=d(\sigma)=1-\frac{2}{m}-\frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\psi_\sigma\left(\frac{4n}{m}\right)\sin\left(\frac{2\pi n}{m}\right).$$

Similarly, we have

$$a_k=1-\frac{4k+2}{m}-\frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\psi_\sigma\left(\frac{4n}{m}\right)\sin\left(\frac{(4k+2)\pi n}{m}\right).$$

Some numerical results

We have three varieties of numerical results:

1. *Monte Carlo results.* Here we replace p^{it} in the (truncated) Euler product by a pseudo-random variable uniformly distributed on the unit circle. In this way we can estimate $d(\sigma)$ or $d_{-}(\sigma)$ from the outcome of a number of trials. To give one example, we estimated

$$d(1) = (3.806 \pm 0.020) \times 10^{-7}$$

   from 10^{11} trials taking about 22 hours of computer time.

   The method is time-consuming and inaccurate when $d(\sigma)$ is small. It is also inaccurate when σ is close to $1/2$.

   On the positive side, the Monte Carlo method was easy to program and provided a "sanity check". It was very helpful for debugging the "exact" method.

Numerical results continued

2. *Exhaustive search in an interval* $(0, T]$. For example, we already mentioned that for $t \in (0, 16656259]$ there are 50 intervals on which $\Re\zeta(1 + it) < 0$, and the total length of these intervals is < 6.484.

   The problems with this approach are:

   - It requires a bound on $|\zeta'(s)|$ to ensure that we do not miss any intervals where $\Re(s)$ changes sign.
   - It is slow, requiring computation of $\zeta(s)$ at many points.
   - The results may not be "typical", because T is limited by our computational power.

     For example, on the critical line $\sigma = 1/2$, for $T \leq 1.1 \times 10^{10}$, we find that $\Re(1/2 + it)$ is predominantly ($> 66\%$) positive, but analytic results due to Selberg (see e.g. Kühn/Tsang) suggest that $\Re(1/2 + it)$ is positive with probability $1/2 + o(1)$ as $T \to \infty$. The "$o(1)$" term tends to zero, but too slowly for this to be observable!

Numerical results continued

3. *"Exact" computation.* Using our algorithm for the computation of $d(\sigma)$ via ψ_σ, as described above, we have computed the following results (next slide), believed to be correct to the number of decimals given.

   We used two independent programs, one written in Mathematica and the other in Magma.

   The results are consistent with those obtained by the Monte Carlo method, at least in the range $0.7 \le \sigma \le 1.05$ where Monte Carlo is feasible.

Values of $d(\sigma)$

Table: $d(\sigma)$ for various $\sigma \in [1/2, \sigma_0]$, $\sigma_0 = 1.192347\cdots$

σ	$d(\sigma)$
$0.5+$	$1-$
$0.5 + 10^{-11}$	0.65335922491489174970
$0.5 + 10^{-5}$	0.49627342044466974340
0.6	$7.92029192674327531250 \times 10^{-2}$
0.7	$2.52287827960689629690 \times 10^{-2}$
0.8	$5.14018886001872476410 \times 10^{-3}$
0.9	$3.14017436106421124270 \times 10^{-4}$
1.0	$3.78866236066887186710 \times 10^{-7}$
1.1	$6.30887499525050140380 \times 10^{-22}$
1.15	$1.38153280809070342470 \times 10^{-103}$
1.16	$1.11720748157793681250 \times 10^{-194}$
1.165	$1.27982077523185346030 \times 10^{-283}$
1.19234	positive
σ_0	zero

$d(\sigma)$ and $d_{-}(\sigma)$

For $\sigma > 0.8$, there is no appreciable difference between $d(\sigma)$ and $d_{-}(\sigma)$. This is because the probability that $|\arg\zeta(\sigma+it)| > 3\pi/2$ is very small in this region.

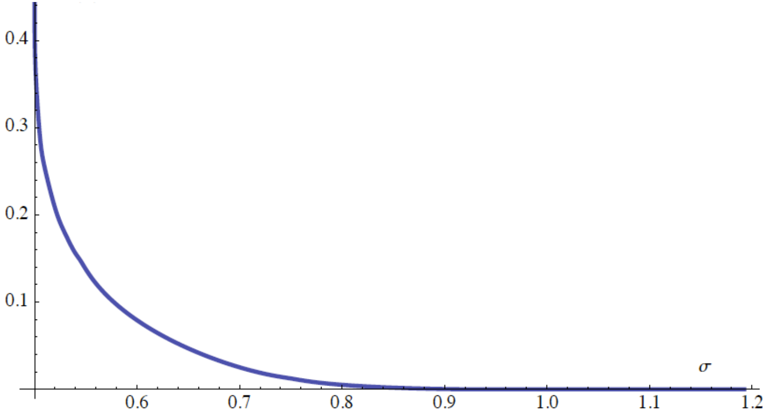
There is an appreciable difference very close to the critical line. For example,

$$d_{-}(0.5+10^{-11}) = 0.4986058426,$$
$$d(0.5+10^{-11}) = 0.6533592249.$$

Table: The difference $d(\sigma) - d_{-}(\sigma)$

σ	$d(\sigma) - d_{-}(\sigma)$
$0.5+$	$0.5-$
$0.5+10^{-11}$	0.1547533823
0.6	$8.073328981 \times 10^{-11}$
0.7	$2.676004881 \times 10^{-32}$
0.8	$7.655052120 \times 10^{-210}$
$\sigma_1 \approx 1.006823$	0

Plot of $d_{-}(\sigma)$



This is a plot of $d_{-}(\sigma)$ for $0.5 < \sigma \leq \sigma_0$.

A plot of $d(\sigma)$ is indistinguishable to the naked eye, but

$$\lim_{\sigma \downarrow 0.5} d(\sigma) = 1 \neq \lim_{\sigma \downarrow 0.5} d_{-}(\sigma) = 0.5\,.$$

Asymptotics of $d(\sigma)$ near σ_0

Recall that $d(\sigma) = 0$ if $\sigma \geq \sigma_0 \approx 1.19235$, so we might expect $\lim_{\sigma \uparrow \sigma_0} d^{(k)}(\sigma) = 0$ for all $k \geq 0$.

The table of values presented earlier confirms that $d(\sigma)$ decreases extremely fast as $\sigma \uparrow \sigma_0$, e.g. $d(1.165) < 10^{-282}$.

Let $\delta := \sigma_0 - \sigma > 0$. A reasonable fit to the computed data for $\sigma > 1$ is given by a function of the form

$$a\,\delta^{b/\delta^2}$$

for constants $a \approx 7.14 \times 10^{-6}$, $b \approx 0.1326$.

It is plausible to conjecture that

$$d(\sigma) \ll \exp(-1/\delta^2) \;\text{ as }\; \delta \to 0+\,,$$

but we have no idea how to prove this. Obtaining analytic results as $\delta \to 0$ appears to be difficult.

Asymptotics of ψ_σ near the critical line

What is the behaviour of ψ_σ as $\sigma \downarrow 1/2$?

It is clear that $\psi_\sigma(x)$ does not tend (pointwise) to a limit as $\sigma \downarrow 1/2$. However, a suitably normalised version of ψ_σ does tend to a limit. More precisely, let

$$\overline{\psi}_\sigma(x) = \exp\left(\frac{x^2}{4}P(2\sigma)\right)\psi_\sigma(x).$$

Then there exists

$$\overline{\psi}_{1/2}(x) := \lim_{\sigma\downarrow 1/2} \overline{\psi}_\sigma(x).$$

Thus, for σ close to $1/2$ and x small, we have

$$\psi_\sigma(x) = \exp(-z^2/2)(1 + O(z^2/P(2\sigma))),$$

where $z = x\sqrt{P(2\sigma)/2}$ is the "natural" variable.

Remarks

We can replace $P(2\sigma)$ by $\log\zeta(2\sigma)$ or by $\log(1/(2\sigma-1))$ since the difference between these is bounded as $\sigma \downarrow 1/2$.

We can write

$$\overline{\psi}_\sigma(x) = \prod_p \left(\exp\left(\frac{x^2}{4p^{2\sigma}}\right) \sum_{n=0}^{\infty} \frac{1}{p^{2n\sigma} 2^{2n} n!^2} \prod_{j=0}^{n-1} (4j^2 - x^2) \right) .$$

The product converges for $\sigma > 1/4$. In particular,

$$\overline{\psi}_{1/2}(x) = \prod_p \left(\exp\left(\frac{x^2}{4p}\right) \sum_{n=0}^{\infty} \frac{1}{p^n 2^{2n} n!^2} \prod_{j=0}^{n-1} (4j^2 - x^2) \right) .$$

Asymptotics of $d(\sigma)$ near the critical line

Using the asymptotic behaviour of $\psi_\sigma(x)$ for σ close to $1/2$, we expect (though have not proved) that

$$1 - d(\sigma) \sim c/\sqrt{-\log(2\sigma - 1)} \text{ as } \sigma \downarrow 1/2.$$

A good fit to the numerical data is

$$d(\sigma) \approx 1 - \frac{A}{\sqrt{B - \log(2\sigma - 1)}}$$

with $A = 1.7786$, $B = 1.6479$.

This explains why the convergence of $d(\sigma)$ to 1 as $\sigma \downarrow 1/2$ is so slow.

What happens on the critical line?

We have seen that $\Re\zeta(\sigma + it)$ has a limiting distribution on any line to the right of the critical line. This is not true on the critical line. Selberg showed that, for $t \sim \mathrm{unif}(T, 2T)$,

$$\frac{\log \zeta(1/2 + it)}{\sqrt{\frac{1}{2} \log \log T}} \xrightarrow{d} X + iY$$

as $T \to \infty$, with $X, Y \sim N(0, 1)$. This implies that $d(1/2) = 1$. We also expect that

$$d_{-}(1/2) = d_{+}(1/2) = 1/2,$$

but proving this seems more difficult.

Computational verification is impossible, because the function $\sqrt{\log \log T}$ grows far too slowly.

Why the difference?

There are several reasons why the critical line $\sigma = 1/2$ is special – for example, it is the line of symmetry for the functional equation of $\zeta(s)$, and a positive proportion (maybe all) of the nontrivial zeros of $\zeta(s)$ lie on it.

If we look at Selberg's proof to see how the $\sqrt{\log\log T}$ scaling factor arises, we see that it comes from

$$\sum_{p<T} \frac{1}{p} \sim \log\log T \quad \text{as} \quad T \to \infty\,.$$

Thus, so far as the distribution of $\arg\zeta(\sigma + it)$ is concerned, the essential difference is that

$$\sum_{p<T} p^{-2\sigma}$$

is bounded as $T \to \infty$ if $\sigma > 1/2$, but unbounded if $\sigma = 1/2$.

Other L-functions

We have only discussed the Riemann zeta function, but similar results hold for all Dirichlet L-functions because the character $\chi(p)$ in the Euler product

$$L(s,\chi) = \prod_p (1 - \chi(p)p^{-s})^{-1}$$

can usually be absorbed into the random variable x_p.

In more detail – we replaced p^{-s} by $p^{-\sigma}x_p$. In the case of an L-function we get $p^{-\sigma}\chi(p)x_p$, but $\chi(p)x_p$ is a random variable distributed uniformly on the unit circle whenever $|\chi(p)| = 1$. Thus, we merely have to omit (from sums/products over primes) all primes p for which $\chi(p) = 0$, i.e. all primes that divide the modulus of the L-function.

References

J. Arias de Reyna, X-ray of Riemann's zeta-function, arXiv:math/0309433v1, 26 Sept. 2003.

J. Arias de Reyna, R. P. Brent and J. van de Lune, A note on the real part of the Riemann zeta-function, *Herman te Riele Liber Amicorum*, CWI, Amsterdam, 2011. arXiv:1112:4910v1

H. Bohr and B. Jessen, *Über die Werteverteilung der Riemannschen Zetafunktion*, Acta Mathematica **54** (1930) 1–35; *ibid* **58** (1931), 1–55.

L. Carlitz, *A sequence of integers related to the Bessel function*, Proc. Amer. Math. Soc., **14** (1963), 1–9.

P. R. Halmos, *Measure Theory*, Springer Verlag, NY, 1974.

P. Kühn, *On Selberg's central limit theorem*, Master's Thesis, Department of Mathematics, ETH Zürich, March 2011.

References continued

J. van de Lune, *Some observations concerning the zero-curves of the real and imaginary parts of Riemann's zeta function*. Afdeling Zuivere Wiskunde, Report ZW 201/83. Mathematisch Centrum, Amsterdam, 1983. i+25 pp.

A. van der Poorten, *A proof that Euler missed . . . Apéry's proof of the irrationality of* $\zeta(3)$, Math. Intel. **1** (1979), 196–203.

J. Steuding, *Value-distribution of L-functions*, Lecture Notes in Mathematics **1877**, Springer, 2007.

E. C. Titchmarsh, *The Theory of the Riemann Zeta-function*, 2nd edition, revised by D. R. Heath-Brown. The Clarendon Press, Oxford, 1986.

K. Tsang, *The Distribution of the Values of the Riemann Zeta-function*, PhD Thesis, Department of Mathematics, Princeton University, Oct. 1984.

J. W. Wrench, *Evaluation of Artin's constant and the twin prime constant*, Math. Comp. **15** (1961), 396–398.