ZETA-FUNCTION

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ABSTRACT. We consider the real part $\operatorname{Re} \zeta(s)$ of the Riemann zetafunction $\zeta(s)$ in the half-plane $\operatorname{Re}(s) \geq 1$. We show how to compute accurately the constant $\sigma_0 \approx 1.19$ which is defined to be the supremum of σ such that $\operatorname{Re} \zeta(\sigma + it)$ can be negative (or zero) for some real t. We also consider intervals where $\operatorname{Re} \zeta(1 + it) \leq 0$ and show that they are rare. The first occurs for $t \approx 682112.9$, and has length ≈ 0.05 . We list the first 50 such intervals.

1. INTRODUCTION

In this note we consider the real part of the Riemann zeta-function $\zeta(s)$ in the half-plane $H = \{s \in \mathbb{C} \mid \operatorname{Re}(s) \geq 1\}$. As usual, we write $s = \sigma + it$, so $\operatorname{Re}(s) = \sigma \geq 1$. We are mainly interested in the regions where $\operatorname{Re}\zeta(s) \leq 0$. Since $\lim_{\sigma\uparrow\infty}\zeta(\sigma+it) = 1$ (uniformly in t), $\operatorname{Re}\zeta(\sigma+it)$ cannot be zero for arbitrarily large $\sigma > 1$. We define

$$\sigma_0 := \sup\{\sigma \in \mathbb{R} \mid (\exists t \in \mathbb{R}) \operatorname{Re} \zeta(\sigma + it) = 0\}.$$

Thus, $\operatorname{Re} \zeta(s) > 0$ if $\sigma > \sigma_0$. In van de Lune [9] it was shown that σ_0 is the (unique) positive real root of the equation

$$\sum_{p} \arcsin\left(\frac{1}{p^{\sigma}}\right) = \frac{\pi}{2} \,,$$

where p runs through the primes (we adopt this convention throughout). In [9] it was also shown that $\sigma_0 > 1.192$ and that $\operatorname{Re} \zeta(\sigma_0 + it)$ never vanishes.

The main aim of this note is to show how σ_0 can be computed to arbitrarily high precision by an efficient algorithm. We also mention some results on the behaviour of $\operatorname{Re} \zeta(\sigma + it)$ for $1 \leq \sigma < \sigma_0$, and in particular on the line $\sigma = 1$.

2. Accurate computation of the constant σ_0

In this section we assume that $\sigma \geq \sigma_1 > 1$, where σ_1 is a suitable constant (e.g. 1.1). We show how the constant σ_0 can be computed within a given error bound. There are three main steps.

(1) Give an algorithm to evaluate the prime zeta-function [5]

$$P(\sigma) = \sum_{p} p^{-\sigma},$$

for real $\sigma > 1$.

(2) Using step 1, give an algorithm to evaluate the function $f(\sigma)$ defined by

$$f(\sigma) = \sum_{p} \arcsin\left(\frac{1}{p^{\sigma}}\right) - \frac{\pi}{2}.$$

(3) Use a suitable zero-finding algorithm to locate a zero of $f(\sigma)$ in a (sufficiently small) interval where $f(\sigma)$ changes sign, for example [1.1, 1.2].

Step 1 is easy. From the Euler product for $\zeta(\sigma)$ and Möbius inversion, we have a formula essentially known to Euler [4, 1748]:

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

which is valid for $\sigma > 1$ (see Titchmarsh [13, eqn. (1.6.1)]). The series converges rapidly in view of the following Lemma.

Lemma 2.1. For $\sigma \ge 2$, $0 < \log \zeta(\sigma) < 3/2^{\sigma}$ and $0 < P(\sigma) < 3/2^{\sigma}$.

Proof. For $\sigma \geq 2$, we have

$$0 < \zeta(\sigma) - 1 < 2^{-\sigma} + 3^{-\sigma} + \int_3^\infty x^{-\sigma} dx = 2^{-\sigma} + 3^{-\sigma} + \frac{3^{1-\sigma}}{\sigma - 1} < 3/2^\sigma,$$

so

$$0 < \log \zeta(\sigma) < \zeta(\sigma) - 1 < 3/2^{\sigma}$$

The upper bound on $P(\sigma)$ follows similarly, using $P(\sigma) < \zeta(\sigma) - 1$. \Box

Using (1) and Lemma 2.1, we have

$$P(\sigma) = \log \zeta(\sigma) + \sum_{r=2}^{\infty} \frac{\mu(r)}{r} \log \zeta(r\sigma),$$

where the r-th term in the sum is bounded in absolute value by $3/2^{r\sigma+1}$. Thus, we can evaluate $P(\sigma)$ accurately, for given $\sigma > 1$, using any good algorithm for the evaluation of $\zeta(\sigma)$, for example Euler-Maclaurin summation. If (1) is used to compute $P(\sigma)$, $P(3\sigma)$, $P(5\sigma)$,..., then we should take care to compute the relevant terms $\log \zeta(r\sigma)$ only once.

For step 2, we observe that the arcsin series defining $f(\sigma)$ converges slowly and irregularly, since it is a sum over primes which to first order behaves like $\sum_{n} p^{-\sigma}$. The well-known "trick" is to express $f(\sigma)$

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as a double series and reverse the order of summation, obtaining an expression which is mathematically equivalent but computationally far superior. For some similar examples, see Wrench [15, 1961].

For |x| < 1 we have

$$\arcsin(x) = \sum_{k=0}^{\infty} c_k x^{2k+1},$$

where

$$c_k = \frac{1 \cdot 3 \cdot 5 \cdots (2k-1)}{2 \cdot 4 \cdot 6 \cdots (2k)} \frac{1}{2k+1} = \frac{(2k)!}{(2^k k!)^2 (2k+1)} \quad \text{for } k \ge 0.$$

Note that all c_k are positive so that $f(\sigma)$ is strictly convex. It is also clear that $f(\sigma)$ is strictly decreasing for $\sigma > 1$. From the expression for c_k , we see that, for $k \ge 1$,

$$(2) c_k \le \frac{1}{2(2k+1)}$$

For $\sigma>1$ it is easy to justify interchanging the order of summation in

$$f(\sigma) = \sum_{p} \sum_{k=0}^{\infty} c_k \left(\frac{1}{p^{\sigma}}\right)^{2k+1} - \frac{\pi}{2},$$

obtaining

(3)
$$f(\sigma) = \sum_{k=0}^{\infty} c_k \sum_p \frac{1}{p^{(2k+1)\sigma}} - \frac{\pi}{2} = \sum_{k=0}^{\infty} c_k P((2k+1)\sigma) - \frac{\pi}{2}$$

From Lemma 2.1 and the inequality (2), we see that

$$0 < \sum_{k=K+1}^{\infty} c_k P((2k+1)\sigma) < 2^{-(2K+3)\sigma},$$

so it is easy to determine K such that we can truncate the series in (3) to a finite sum over $k \leq K$ with a rigorous error bound.

If desired, we can substitute (1) into (3) and interchange the order of summation, obtaining

(4)
$$f(\sigma) = \sum_{j \ge 0} d_j \log \zeta((2j+1)\sigma) - \frac{\pi}{2}$$

where

$$d_j = \sum_{k \ge 0, r \ge 1, (2k+1)r = 2j+1} \frac{c_k \mu(r)}{r}$$

From the inequality $c_k \leq 1/(2k+1)$ (valid for $k \geq 0$), it follows that $|d_j| \leq 1$. Using Lemma 2.1, we can determine where to safely truncate the series (4).

For step 3, we can use a zero-finding algorithm which needs only function (not derivative) evaluations, and gives a guaranteed bound on the final result. For example, the method of bisection could be used, but would be slow, taking about $\log_2(1/\varepsilon)$ function evaluations to obtain a solution with error bounded by ε . In the secant method, a sequence (x_n) , converging to a zero of f under suitable conditions, is obtained by computing the approximation x_n by linear interpolation using the two points $(x_{n-1}, f(x_{n-1}))$ and $(x_{n-2}, f(x_{n-2}))$. It converges with order $(1 + \sqrt{5})/2 \approx 1.618$, but does not always give a guaranteed bound on the error. A combination of bisection and linear interpolation, as in the algorithms of Dekker [3] or Brent [2], can give convergence about as fast as the secant method, but with the final result bracketed in a short interval where the function f changes sign.

3. Computational results

The second and third authors independently wrote programs implementing the ideas of §2, using Magma in one case and Mathematica 4 and 8 in the other case. The programs used different strategies to obtain a final interval where f changes sign (in one case taking advantage of the strict convexity of f). The output of the programs agrees to at least 500D. We give here the correctly rounded result to 100D:

$$\begin{split} \sigma_0 &\approx 1.19234\,73371\,86193\,20289\,75044\,27425\,59788\,34011\,19230\,83799\\ &94301\,37194\,92990\,52458\,64848\,30139\,24084\,99863\,83788\,36244\,. \end{split}$$

Programs and higher precision values are available from the authors.

4. The distribution of $\operatorname{Re}\zeta(\sigma+it)$ for $\sigma \geq 1$

Assuming that the limit exists, we define

$$d(\sigma) = \lim_{T \to +\infty} \frac{1}{T} m\{t \in [0, T] \mid \operatorname{Re} \zeta(\sigma + it) < 0\},\$$

where *m* denotes Lebesgue measure. Informally, $d(\sigma)$ is the probability that $\zeta(s)$ has negative real part on a given vertical line Re $(s) = \sigma$.

The results of Section 2 show that $d(\sigma) = 0$ for $\sigma \ge \sigma_0 \approx 1.19$. Here we briefly discuss the region $1 \le \sigma < \sigma_0$.

At least for those values of t that are accessible to computation, Re $\zeta(\sigma + it)$ is "usually" positive for $\sigma \geq 1$. The function $d(\sigma)$ is conjectured to be continuous and monotonic decreasing from a positive value at $\sigma = 1$ to zero at $\sigma = \sigma_0$. Even on the line $\sigma = 1$, Re $\zeta(\sigma + it)$ is usually positive [11]. We can prove that d(1) < 1/4, but a Monte Carlo computation suggests that the true value is much smaller. Based on 5×10^{11} pseudo-random trials, we estimate $d(1) = (3.80 \pm 0.01) \times 10^{-7}$. Similarly, we estimate $d(1.01) = (1.10 \pm 0.01) \times 10^{-7}$ and $d(1.02) \approx$ $(2.66 \pm 0.04) \times 10^{-8}$, so it can be seen that $d(\sigma)$ decreases rapidly as we move to the right of $\sigma = 1$.

Although $\zeta(s)$ has a simple pole at s = 1, the Laurent series

$$\zeta(s) = \frac{1}{s-1} + \gamma + O(|s-1|)$$

shows that $\operatorname{Re} \zeta(1+it)$ has a positive limit $\gamma = 0.577\cdots$ (Euler's constant) as $t \to 0$.

On any fixed vertical line $\sigma > 1$, both $\zeta(\sigma + it)$ and $1/\zeta(\sigma + it)$ are bounded, in fact $\zeta(2\sigma)/\zeta(\sigma) < |\zeta(\sigma + it)| \leq \zeta(\sigma)$. However, the situation is different on the line $\sigma = 1$, as both $\zeta(1+it)$ and $1/\zeta(1+it)$ are unbounded. Their true order of growth is unknown. It follows from Titchmarsh [13, Theorem 11.9] and the continuity of Re $\zeta(1+it)$ that Re $\zeta(1+it)$ attains all real values. Nevertheless, the "usual" values are quite small. As a special case of [13, Theorem 7.2] we have the mean value theorem

$$\lim_{T \to \infty} \frac{1}{T} \int_{1}^{T} |\zeta(1+it)|^2 \, \mathrm{d}t = \zeta(2) = \frac{\pi^2}{6}$$

Using ideas as in the proof of [13, Theorem 7.2], we can prove that

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T \operatorname{Re} \zeta(1+it) \, \mathrm{d}t = 1 \, .$$

Thus, informally, we can say that the typical value of $\operatorname{Re} \zeta(1+it)$ is close to 1. The values have a distribution with mean 1 and variance $\pi^2/6 - 1 \approx 0.645$.

In [9, Table 1], van de Lune gave a list of values of t > 0 such that $\operatorname{Re} \zeta(1+it) < 0$ and is (approximately) a local minimum. The list was not claimed to be exhaustive. The smallest t listed was t = 682112.92 with $\operatorname{Re} \zeta(1+it) \approx -0.003$. We have shown, using the "maximum slope principle" [10], that this is very close to the smallest t for which $\operatorname{Re} \zeta(1+it) \leq 0$. More precisely, $\operatorname{Re} \zeta(1+it) > 0$ for 0 < t < 682112.8913, and there is a local minimum of -.0027652 at $t \approx 682112.9169$. In applying the maximum slope principle we used the bound

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}\arg\zeta(1+it)\right| = \left|\operatorname{Re}\frac{\zeta'(1+it)}{\zeta(1+it)}\right| \le \frac{3}{4}\log(t^2+4) + 7 \text{ for } t\ge 10.$$

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t	$\operatorname{Re}\zeta$	length	t	$\operatorname{Re}\zeta$	length
682112.9169	-0.0028	0.0529	8350473.4853	-0.0019	0.0451
1267065.1710	-0.0040	0.0655	8366684.0439	-0.0197	0.1322
1466782.0667	-0.0013	0.0391	8452317.9526	-0.0090	0.0900
1858650.0915	-0.0282	0.1686	8967566.5926	-0.0148	0.1336
2023654.7671	-0.0221	0.1389	9960968.8748	-0.0184	0.1373
2064996.2141	-0.0117	0.1076	11231380.7309	-0.0099	0.1042
2195056.7909	-0.0755	0.2718	11236680.3350	-0.0262	0.1595
2202620.3296	-0.0111	0.1159	11781932.0257	-0.0170	0.1288
2530662.6360	-0.0072	0.0865	11884021.9776	-0.0035	0.0564
3259774.5293	-0.0471	0.2098	12045289.3337	-0.0644	0.2498
3548283.4160	-0.0189	0.1459	12276788.1573	-0.0182	0.1476
4052438.9330	-0.0023	0.0474	12546625.7916	-0.0455	0.2031
4197235.0783	-0.0331	0.1977	12781127.5748	-0.0102	0.0964
5410820.7150	-0.0008	0.0307	13598773.5889	-0.0543	0.2317
6027913.8513	-0.0181	0.1325	13786262.5457	-0.0826	0.2635
6164063.0008	-0.0263	0.1603	13922411.7750	-0.0222	0.1418
6238849.4877	-0.0071	0.0827	14190358.4974	-0.0632	0.2214
6265907.4688	-0.0030	0.0522	14391623.0217	-0.0016	0.0437
6421627.2235	-0.0241	0.1651	14788310.5330	-0.0149	0.1132
7338152.4379	-0.0043	0.0656	14856540.3430	-0.0220	0.1442
7469838.9709	-0.0009	0.0305	15173904.7533	-0.0041	0.0800
7766995.0303	-0.0742	0.2840	15321273.7219	-0.0131	0.1181
7774558.3985	-0.0672	0.2705	16083163.0244	-0.0098	0.1038
7985493.9836	-0.0324	0.1728	16503899.3235	-0.0060	0.0680
8299958.2327	-0.0022	0.0432	16656258.8346	-0.0155	0.1329

TABLE 1. First 50 negative local minima of $\operatorname{Re} \zeta(1+it)$

Table 1 lists the first 50 local minima of $\operatorname{Re} \zeta(1 + it)$ for which t > 0 and $\operatorname{Re} \zeta(1 + it) \leq 0$ (no minima are exactly zero). The values in the table are rounded to 4 decimal places. The columns headed "length" give the lengths of the intervals containing t in which $\operatorname{Re} \zeta$ is negative. To 8 decimal places, the first interval, of length 0.05291225, is (682112.89133824, 682112.94425049). The sum of the lengths of the first 50 intervals is 6.48390168, giving an estimate $d(1) \approx 3.85 \times 10^{-7}$. This is close to our Monte Carlo estimate $d(1) \approx 3.80 \times 10^{-7}$.

In this brief note we refrain from commenting on the region $\sigma \in [1/2, 1)$, but refer the interested reader to the literature, such as Bohr and Jessen [1], Titchmarsh [13, §11.13], Tsang [14], Joyner [6], Laurinčikas [8], Steuding [12] and Kühn [7].

References

- H. BOHR AND B. JESSEN, Über die Werteverteilung der Riemannschen Zetafunktion, Acta Mathematica 54 (1930), 1–35; ibid 58 (1931), 1–55.
- [2] R. P. BRENT, Algorithms for Minimization without Derivatives, Prentice-Hall, New Jersey, 1973. Reprinted by Dover, New York, 2002.
- [3] T. J. DEKKER, Finding a zero by means of successive linear interpolation, in Constructive Aspects of the Fundamental Theorem of Algebra (B. Dejon and P. Henrici, eds.), Interscience, New York, 1969.
- [4] L. EULER, Introduction à l'Analyse Infinitésimale, Vol. 1, (original 1748, French translation 1796).
- [5] C-E. FRÖBERG, On the prime zeta function. Nordisk Tidskrift für Informationsbehandling (BIT) 8, 3 (1968), 187–202.
- [6] D. JOYNER, Distribution Theorems of L-functions, Pitman Research Notes in Mathematics 142, John Wiley and Sons, New York, 1986.
- [7] P. KÜHN, On Selberg's central limit theorem, Master Thesis, Department of Mathematics, ETH Zürich, Switzerland, March 2011.
- [8] A. LAURINČIKAS, Limit theorems for the Riemann zeta-function, Mathematics and its Applications 352, Kluwer Academic Publishers, Dordrecht, 1996.
- [9] J. VAN DE LUNE, Some observations concerning the zero-curves of the real and imaginary parts of Riemann's zeta function. Afdeling Zuivere Wiskunde [Department of Pure Mathematics], Report ZW 201/83. Mathematisch Centrum, Amsterdam, 1983. i+25 pp.
- [10] J. VAN DE LUNE AND H. J. J. TE RIELE, Numerical computation of special zeros of partial sums of Riemann's zeta function, Computational Methods in Number Theory, Part II, Math. Centrum Tracts, Vol. 155, Math. Centrum, Amsterdam, 1982, 371–387.
- [11] D. C. MILIOTO, A method for zeroing-in on $\operatorname{Re} \zeta(\sigma + it) < 0$ in the half-plane $\sigma > 1$, arXiv:1001.2962v3, 20 Jan. 2010.
- [12] J. STEUDING, Value-distribution of L-functions, Lecture Notes in Mathematics 1877, Springer, 2007.
- [13] E. C. TITCHMARSH, *The Theory of the Riemann Zeta-function*, 2nd edition, edited by D. R. Heath-Brown. The Clarendon Press, Oxford, 1986.
- [14] K. TSANG, The Distribution of the Values of the Riemann Zeta-function, PhD Thesis, Department of Mathematics, Princeton University, Oct. 1984.
- [15] J. W. WRENCH, Evaluation of Artin's constant and the twin prime constant, Math. Comp. 15 (1961), 396–398.

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