A sum over non-trivial zeros of the Riemann zeta-function

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Abstract

Sums over non-trivial zeros of the Riemann zeta-function often arise in analytic number theory. We consider a special case that is analogous to the harmonic series. Although the sum diverges, we can estimate its "finite part" H by a process of normalisation, analogous to how we can estimate Euler's constant $C \approx 0.5772$ using the harmonic series.

We describe three algorithms for the numerical approximation of H. The first is straightforward, with error $\ll (\log T)/T$ if we use the zeros ρ satisfying $0 < \Im \rho \leqslant T$.

The second algorithm is more accurate, with error $\ll (\log T)/T^2$. It obtains about twice as many correct digits in the same time as the first algorithm.

The first two algorithms and their error bounds are unconditional. The third algorithm, due to Juan Arias de Reyna, is faster for the same accuracy, but assumes the Riemann Hypothesis.



Motivation

- In analytic number theory we often encounter sums of the form $\sum \phi(\rho)$ or $\sum \phi(\gamma)$, where ϕ is some specified function, and the sum is taken over the non-trivial zeros $\rho = \beta + i\gamma$ of $\zeta(s)$, perhaps restricted to some finite interval $\gamma \in [T_1, T_2]$, or the semi-infinite case $\gamma \in [T_1, \infty)$.
- For example, consider $\sum_{0<\gamma\leqslant T}1/\gamma^2$. In some applications it is sufficient to know that the sum converges as $T\to\infty$. In other applications, especially when obtaining "explicit" bounds, we may need numerical upper and lower bounds on the sum (for specific values of T, or as $T\to\infty$).
- ▶ Similarly for $\sum_{0<\gamma\leqslant T}1/\gamma$, except that here the sum diverges as $T\to\infty$, and we may want bounds valid for large T.

Identities and a comment on RH

Occasionally a sum over zeros can be obtained analytically. For example, with *C* denoting Euler's constant,

$$\frac{1}{2} \sum_{\rho} \left(\frac{1}{1-\rho} + \frac{1}{\rho} \right) = \sum_{\rho} \Re \frac{1}{\rho} = \frac{C}{2} + 1 - \frac{1}{2} \log 4\pi \approx 0.0230957$$

This identity follows from the functional equation and Hadamard product for $\xi(s)$, see [MV, 1 (10.24)–(10.30)].

Note that a generic non-trivial zero is $\rho = \beta + i\gamma$, which gives $\gamma = (\rho - \beta)/i$, so if β is constant (i.e. if RH is true) there is no essential difference between sums over ρ and sums over γ .

¹MV = Montgomery and Vaughan, *Multiplicative Number*, Theory, I. = > = = -

A special case

To illustrate the main ideas we'll consider a special case

$$G(T) := \sum_{0 < \gamma \leqslant T} \frac{1}{\gamma}.$$

More general results are covered in the references (last slide).

For simplicity, in this talk we'll assume that T is not the ordinate of a non-trivial zero.

Multiple zeros (if any) are weighted by their multiplicities.

Analogy – the harmonic series

G(T) is analogous to the harmonic sum

$$H(N) := \sum_{n \leq N} \frac{1}{n} = \log N + C + O(1/N).$$

Here $\log N = \int_1^N t^{-1} dt$ is an integral approximation to H(N), and may be regarded as a "normalisation" to convert a divergent series into an expression with a finite limit.

We'll show that something similar works for

$$G(T) = \sum_{0 < \gamma \leqslant T} \frac{1}{\gamma}.$$

In this case a suitable integral approximation is

$$\int_{2\pi}^{T} \frac{\log(t/2\pi)}{2\pi} \frac{dt}{t} = \frac{\log^2(T/2\pi)}{4\pi}.$$

A further analogy between C and H

The Dirichlet series $\zeta(s) = \sum_{n \ge 1} n^{-s}$ formally gives the harmonic

series $\sum_{n\geqslant 1} n^{-1}$ at s=1. Of course, this series diverges,

because $\zeta(s)$ has a pole at s=1.

In fact $\zeta(s)$ has a Laurent expansion that may be written as

$$\zeta(1+z) = \frac{1}{z} + C_0 + C_1 z + \cdots,$$

where $C_0 = C$ is Euler's constant.

We'll see later that, assuming RH, the Laurent expansion of a meromorphic function known as the *secondary zeta function* can be used to find H.

Some notation

 $\rho = \beta + i\gamma$ is a non-trivial zero of $\zeta(s)$, with $\beta, \gamma \in \mathbb{R}$.

N(T) is the number of zeros with $0 < \gamma \leqslant T$.

 $S(T) = \pi^{-1} \arg \zeta(\frac{1}{2} + iT)$ defined in the usual way. (Remember, we are assuming that $T \neq \gamma$.)

We can write

$$N(T) = L(T) + Q(T),$$

where L(T) is a smooth approximation to N(T), and

$$Q(T) = S(T) + O(1/T)$$

is an error term which has jumps at the ordinates of non-trivial zeros.

Approximation of N(T)

In Titchmarsh, Ch. 9, we find N(T) = L(T) + Q(T), where

$$L(T) = \frac{T}{2\pi} \left(\log \left(\frac{T}{2\pi} \right) - 1 \right) + \frac{7}{8}$$

and the "remainder term" Q(T) = S(T) + O(1/T). More precisely [BPT 2021b], for all $T \geqslant 2\pi$,

$$Q(T) = S(T) + \frac{\vartheta}{150T}$$
, where $|\vartheta| \leq 1$.

It is known that $S(T) \ll \log T$, so $Q(T) \ll \log T$.

Also, if $S_1(T) := \int_0^T S(t) dt$, then

$$S_1(T) \ll \log T$$
.

Explicit bounds on Q(T), S(T) and $S_1(T)$ are known, e.g. $|Q(T)| \le 0.28 \log T$ for all $T \ge 2\pi$ [BPT 2020].

Existence of the limit, and an integral expression

Theorem (BPT 2021a, Thm. 2.1) If

$$G(T) := \sum_{0 < \gamma \leqslant T} \frac{1}{\gamma},$$

then the limit

$$H := \lim_{T o \infty} \left(G(T) - \frac{\log^2(T/2\pi)}{4\pi} \right)$$

exists, and

$$H=\int_{2\pi}^{\infty}\frac{Q(t)}{t^2}\,dt-\frac{1}{16\pi}\,.$$

Sketch of proof.

$$G(T) = \int_{2\pi}^{T} \frac{dN(t)}{t} = \int_{2\pi}^{T} \frac{dL(t)}{t} + \int_{2\pi}^{T} \frac{dQ(t)}{t}.$$

Using integration by parts and the fact that $Q(2\pi) = 1/8$, we find that

$$G(T) - \frac{\log^2(T/2\pi)}{4\pi} = \int_{2\pi}^T \frac{Q(t)}{t^2} dt - \frac{1}{16\pi} + \frac{Q(T)}{T}.$$
 (*)

Now let
$$T \to \infty$$
 and use $Q(T) \ll \log T = o(T)$.



Algorithm 1

In the most obvious algorithm, we use

$$H = G(T) - \frac{\log^2(T/2\pi)}{4\pi} + E(T).$$

Here $G(T) = \sum_{0 < \gamma \leqslant T} 1/\gamma$ can easily be evaluated after computing the non-trivial zeros up to height T.

The error term E(T) can be bounded using a lemma due to Lehman (see the next two slides). The result is

$$|\boldsymbol{E}(T)| \leqslant 0.28 \left(\frac{1+2\log T}{T}\right) \ll \frac{\log T}{T}$$
.

Remark

Since $\lim_{T\to\infty} E(T) = 0$, this gives another proof of the existence of the limit defining H, but it does not give the integral expression for H.



Motivation for Lehman's Lemma

Suppose that we want to estimate a sum of the form

$$\sum_{T_1\leqslant\gamma\leqslant T_2}'\phi(\gamma).$$

We can think of this as a sum approximating

$$\int_{T_1}^{T_2} \phi(t) w(t) dt,$$

where w(t) is a weight function that takes into account the non-uniform spacing of the γ s. The natural weight function is

$$w(t) := L'(t) = \frac{1}{2\pi} \log(t/2\pi).$$

Lehman's lemma bounds the difference between the sum and integral with this choice of w(t).



Lehman's Lemma

Lemma (Lehman, 1966)

If $2\pi e \leqslant T_1 \leqslant T_2$ and $\phi : [T_1, T_2] \mapsto [0, \infty)$ is monotone decreasing on $[T_1, T_2]$, then

$$\sum_{T_1 \leqslant \gamma \leqslant T_2}' \phi(\gamma) = \frac{1}{2\pi} \int_{T_1}^{T_2} \phi(t) \log(t/2\pi) \, dt + E(T_1, T_2),$$

where

$$|E(T_1,T_2)|\leqslant A\left(2\phi(T_1)\log T_1+\int_{T_1}^{T_2}\frac{\phi(t)}{t}\,dt\right),$$

and A is an absolute constant.

Lehman gave A = 2, but this can be reduced to A = 0.28. [BPT 2020, Corollary 1].



A closer look at the error term in Algorithm 1

From the identity (*) four slides back, we can write

$$E(T) = -\frac{Q(T)}{T} + \int_{T}^{\infty} \frac{Q(t)}{t^2} dt \ll \frac{\log T}{T}.$$

Now Q(t) = S(t) + O(1/t), so

$$\int_{T}^{\infty} \frac{Q(t)}{t^2} dt = \int_{T}^{\infty} \frac{S(t)}{t^2} dt + O(1/T^2).$$

Recall that $S_1(T) = \int_0^T S(t) dt \ll \log T$, so we expect cancellation in $\int_T^\infty (S(t)/t^2) dt$. Integration by parts gives

$$\int_{T}^{\infty} \frac{S(t)}{t^2} \, dt = -\frac{S_1(T)}{T^2} + 2 \int_{T}^{\infty} \frac{S_1(t)}{t^3} \, dt \ll \frac{\log T}{T^2} \, .$$

By evaluating Q(T)/T, the error bound can be reduced by a factor of order T.



Algorithm 2A

Use

$$H = G(T) - \frac{\log^2(T/2\pi)}{4\pi} - \frac{Q(T)}{T} + E_2(T),$$

where

$$E_2(T) = \int_T^\infty \frac{Q(t)}{t^2} dt \ll \frac{\log T}{T^2}.$$

G(T) can be computed as in Algorithm 1, using the ordinates of nontrivial zeros up to height T. While doing this, we can compute N(T), so Q(T) = N(T) - L(T) is easily obtained.

Thus, the "correction term" -Q(T)/T is cheap to compute, and the overall work is about the same as for Algorithm 1. The error bound improves from

$$\frac{0.28 + 0.56 \log T}{T}$$
 to $\frac{4.27 + 0.12 \log T}{T^2}$,

where the numerical constants are as in [BPT 2021a, §4].



Algorithm 2B

By absorbing the computation of the correction term into the computation of the sum, we obtain Algorithm 2B, which uses the following theorem.

Theorem (BPT 2021a, Theorem 4.1) For all $T \ge 2\pi$,

$$H = \sum_{0 < \gamma \leqslant T} \left(\frac{1}{\gamma} - \frac{1}{T}\right) - \frac{\log^2(T/2\pi e) + 1}{4\pi} + \frac{7}{8T} + E_2(T),$$

where $E_2(T)$ is as above.

This shows that the error term $E_2(T)$ is a continuous function of T, unlike E(T), which has jumps. The continuity of $E_2(T)$ also follows from its expression as an integral.



Algorithm 2C

Recall that
$$H=\int_{2\pi}^{\infty} \frac{Q(t)}{t^2} dt - \frac{1}{16\pi}$$
, $Q(t)=N(t)-L(t)$.

Suppose we use the first n ordinates γ_j (j = 1, ..., n) of non-trivial zeros of $\zeta(s)$ in the upper half-plane, and define $\gamma_0 := 2\pi$, $T := \gamma_n$. Then

$$H = \sum_{j=0}^{n-1} \int_{\gamma_j}^{\gamma_{j+1}} \frac{j - L(t)}{t^2} dt - \frac{1}{16\pi} + \int_T^{\infty} \frac{Q(t)}{t^2} dt.$$

The n integrals in the sum can each be evaluated in closed form, and the infinite integral is just $E_2(T)$. Thus, this gives an algorithm that is equivalent to Algorithms 2A and 2B, modulo the effect of rounding errors.

Numerical approximation of *H*

Corollary (BPT 2021a, Corollary 4.2)

$$H = -0.0171594043070981495 + \vartheta(10^{-18}),$$

where $|\vartheta| \leqslant 1$.

Proof.

This follows from Algorithm 2B, via an interval-arithmetic computation using the first $n = 10^{10}$ zeros, with $T = \gamma_n \approx 3293531632.4$.

Remarks

Ignoring rounding errors, the error bound is 6.4×10^{-19} . Algorithms 2A and 2C should give the same result. With Algorithm 1, the error bound is 3.9×10^{-9} . Previous algorithms gave about 5*D*, and no error bound.

Generalisation

Nearly everything can be generalised to cover sums of the form

$$\sum_{T \leqslant \gamma < U} \phi(\gamma),$$

where $\phi:[T,U)\subseteq[1,\infty)\mapsto[0,\infty)$ is in C^2 and satisfies:

$$\phi'(t) \leqslant 0, \ \phi''(t) \geqslant 0 \text{ for all } t \in [T, U),$$

and (if $U = \infty$)

$$\int_{T}^{U} \frac{\phi(t)}{t} dt < \infty.$$

For example, $\phi(t) = t^{-c}$ satisfies these conditions for any c > 0 and $1 = T \le U \le \infty$.

For details of the generalisation, see [BPT 2021b].



The secondary zeta function

The secondary zeta function Z(s) is defined by

$$Z(s) := \sum_{n=1}^{\infty} \alpha_n^{-s}, \Re s > 1,$$

where $\rho_n=\frac{1}{2}+i\alpha_n$ runs through the zeros ρ of $\zeta(s)$ with $\Im \rho>0$. The α_n are zeros of the Riemann-Landau Ξ function. Note that α_n is real (and $\alpha_n=\gamma_n$) for all $n\geqslant 1$ iff RH is true. Without assuming RH, we have $\Re \alpha_n=\gamma_n$ and $|\Im \alpha_n|<\frac{1}{2}$. Z(s) extends to a meromorphic function on $\mathbb C$, with a double pole at s=1, and simple poles at $s=-1,-3,-5,\ldots$ Its properties have been studied by many authors, starting with Mellin (1917) and Cramér (1919). See [AdR 2020] for details.

The Laurent expansion of Z(s) at s = 1

Z(s) is a meromorphic function with a double pole at s=1, and we have the Laurent expansion

$$Z(1+z) = \frac{1}{2\pi z^2} - \frac{\log(2\pi)}{2\pi z} + A_0 + A_1 z + A_2 z^2 + \cdots$$

Arias de Reyna (2021) has shown that

$$A_0 = H' + \frac{\log^2(2\pi)}{4\pi}$$

where

$$H' = \lim_{T \to \infty} \left(\sum_{\Re lpha_n < T} \frac{1}{lpha_n} - \frac{\log^2(T/2\pi)}{4\pi} \right).$$

We have $H' \leq H$, and H' = H iff RH is true. In this respect, H - H' is analogous to the *de Bruijn-Newman* constant Λ .



Computing A₀

If $C_{1/4}$ is the circle with centre 1 and radius $r = \frac{1}{4}$, then

$$A_0 = rac{1}{2\pi i} \int_{C_{1/4}} rac{Z(s)}{s-1} \, ds = rac{1}{2\pi} \int_0^{2\pi} Z(1+re^{i heta}) \, d heta.$$

Thus A_0 can be computed by numerical integration if we have a way of evaluating Z(s) on $C_{1/4}$. This can be done using the method that Delsarte (1966) used to establish the analytic continuation of Z(s) into the region $\Re s \leqslant 1$, and implemented by Arias de Reyna in mpmath.

Once A_0 has been computed, we easily get

$$H'=A_0-\frac{\log^2(2\pi)}{4\pi}\,.$$

Algorithm 3

This leads to a conditional algorithm for computing H: evaluate A_0 (and hence H') to the desired accuracy using numerical integration around the circle $C_{1/4}$, as on the previous slide. Assuming RH, we have H = H'.

Using this algorithm, Arias de Reyna computed H' to 100 decimal places. His result

H' = 0.017159404307098149454...

confirms our unconditional 18-decimal place result (for H).

The advantage of Algorithm 3 over the other algorithms that we have mentioned is its speed.

The disadvantage is that it assumes RH. Also, it is difficult to give a completely rigorous error bound, due to the numerical integration and the difficulty of evaluating Z(s), which involves much cancellation if $\Re s < 1$.



An obvious question and answer

Question:

Should we attempt to disprove RH by showing that $H \neq H'$?

Answer: NO.

In order to find H sufficiently accurately, we would have to compute so many zeros of $\zeta(s)$ that an exception to RH (if it exists) would already have shown up.

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