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ACCURATE ESTIMATION OF SUMS OVER ZEROS OF THE RIEMANN ZETA-FUNCTION

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Abstract. We consider sums of the form $\sum \phi(\gamma)$, where ϕ is a given function, and γ ranges over the ordinates of nontrivial zeros of the Riemann zeta-function in a given interval. We show how the numerical estimation of such sums can be accelerated by a simple device, and give examples involving both convergent and divergent infinite sums.

1. Introduction

Let the nontrivial zeros of the Riemann zeta-function $\zeta(s)$ be denoted by $\rho = \beta + i\gamma$. In order of increasing height, the ordinates of the zeros in the upper half-plane are $\gamma_1 \approx 14.13 < \gamma_2 < \gamma_3 < \cdots$.

We are interested in sums of the form $\sum'_{T_1 \leqslant \gamma \leqslant T_2} \phi(\gamma)$ and $\sum'_{T_1 \leqslant \gamma} \phi(\gamma)$, where $T_1 \leqslant T_2$, and where $\phi(t)$ is a function with certain properties, which we specify later. Here the prime symbol $(')$ indicates that if $\gamma = T_1$ or $\gamma = T_2$ then the term $\phi(\gamma)$ is given weight $\frac{1}{2}$. If multiple zeros exist, then terms involving such zeros are weighted by their multiplicities. Sums of this form can be bounded using a lemma of Lehman [10, Lem. 1] that we state for reference. We have changed Lehman's wording slightly, but the proof is the same. In the lemma and elsewhere, ϑ denotes a real number in $[-1, 1]$, possibly different at each occurrence.

Lemma 1 (Lehman). *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*

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

where A is an absolute constant.[1]

To avoid repetition, it is convenient to make the following definition.

Condition A. We say that $\phi : [T_0, \infty) \mapsto \mathbb{R}$ satisfies *Condition A* if $\phi(t)$ is twice continuously differentiable and satisfies $\phi(t) \geqslant 0$, $\phi'(t) \leqslant 0$, and $\phi''(t) \geqslant 0$ for all $t \in [T_0, \infty)$.

Our Lemma 3 may be seen as a refinement of Lehman's lemma, with the additional assumption that ϕ satisfies Condition A. This assumption allows us to

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[1] In Lemma 1, A is a constant such that $|Q(T)| \leqslant A \log T$ for all $T \geqslant 2\pi e$, where $Q(T)$ is as in (5). From [3, Cor. 1], we may take $A = 0.28$.

obtain a smaller error term in most cases of interest (two numerical examples are given below). Lemma 3 is stated and proved in §3. For simplicity we outline here the case $T_2 \to \infty$, since this case has one fewer parameter and is of interest in many applications.

If the infinite sum $\sum'_{T\leqslant\gamma} \phi(\gamma)$ converges, then the error term in Lemma 1 is $\gg \phi(T)\log T$. In Theorem 1 we express the error as $-\phi(T)Q(T) + E_2(T)$, where the discontinuous term $Q(T) \ll \log T$ can be computed from (5)–(6), and the continuous term $E_2(T)$ is generally of lower order than $\phi(T)\log T$ (see also Remark 2). We state Theorem 1 here; the proof depends on Lemma 3 and is given in §4.

Theorem 1. *Suppose that $2\pi \leqslant T_0 \leqslant T$ and that ϕ satisfies Condition* A. *Suppose further that $\int_T^\infty \phi(t)\log(t/2\pi)\,dt < \infty$. Let*

$$E(T) := \sum_{T\leqslant\gamma}{}' \phi(\gamma) - \frac{1}{2\pi}\int_T^\infty \phi(t)\log(t/2\pi)\,dt. \tag{1}$$

Then $E(T) = -\phi(T)Q(T) + E_2(T)$, where

$$E_2(T) = -\int_T^\infty \phi'(t)Q(t)\,dt, \tag{2}$$

and $Q(T) = N(T) - L(T)$ is defined by (5)*–*(6)*. Also,*

$$|E_2(T)| \leqslant 2(A_0 + A_1\log T)\,|\phi'(T)| + (A_1 + A_2)\phi(T)/T, \tag{3}$$

where we may take $A_0 = 2.067$, $A_1 = 0.059$, and $A_2 = 1/150$.

In Theorem 1, A_0 and A_1 are constants satisfying condition (12), and A_2 is as in Lemma 2. We note that $E_2(T)$ is a continuous function of T, as can be seen from (2), whereas $E(T)$ has jumps at the ordinates of nontrivial zeros of $\zeta(s)$.

Disregarding the constant factors, Theorem 1 shows that

$$E_2(T) \ll |\phi'(T)|\log T + \phi(T)/T.$$

For example, if $\phi(t) = t^{-c}$ for some $c > 1$, then $E(T) \ll T^{-c}\log T$, and $E_2(T) \ll T^{-(c+1)}\log T$ is smaller by a factor of order T.

Theorem 1 deals with (convergent) infinite sums. Lemma 3 gives a similar result for finite sums. We deduce Theorem 1 from Lemma 3 instead of giving an independent proof (which would be similar to but slightly easier than the proof of Lemma 3).

Example 1. We consider computation of the constant

$$c_1 := \sum_{\gamma>0} \frac{1}{\gamma^2} = 0.02310499\ldots.$$

The approximation 0.023105 was given in [14, Lemma 2.9], where it was computed using a finite sum with (essentially) Lemma 1 to bound the tail.

Taking $\phi(t) = 1/t^2$ in Lemma 1, with T_1 replaced by T and $T_2 \to \infty$, gives an error term

$$|E(T)| \leqslant A\left(\frac{\frac{1}{2} + 2\log T}{T^2}\right) = \frac{0.14 + 0.56\log T}{T^2}\,,$$

using the value $A = 0.28$ mentioned above.[1] The corresponding error term given by Theorem 1 is

$$|E_2(T)| \leqslant \frac{(4A_0 + A_1 + A_2) + 4A_1\log T}{T^3} \leqslant \frac{8.334 + 0.236\log T}{T^3}\,,$$

using the values of A_0, A_1, A_2 above. For example, taking $T = 1000$ (corresponding to the first 649 nontrivial zeros), we get $|E(T)| \leqslant 4.009 \times 10^{-6}$ and $|E_2(T)| \leqslant 9.965 \times 10^{-9}$, an improvement by a factor of 400. If we use 10^{10} zeros, as in Corollary 1, the improvement is by a factor of 3×10^9.

Corollary 1. *We have*

$$c_1 = \sum_{\gamma>0} \frac{1}{\gamma^2} = 0.023104993115418970788933810 4 + \vartheta(5 \times 10^{-28}).$$

Proof. This follows from Theorem 1 by an interval-arithmetic computation using the first $n = 10^{10}$ zeros, with $T = 3293531632.542\cdots \in (\gamma_n, \gamma_{n+1})$, and $Q(T)$ computed from $Q(T) = N(T) - L(T)$; see (5). We used the database of 10^{11} zeros of $\zeta(s)$ whose computation is described in Platt [13]. These are correct to $\pm 2^{-102}$ and this limits the accuracy we can ultimately obtain. To control rounding errors, we used the Arb package [9]. □

Remark 1. Assuming the Riemann Hypothesis (RH), there is an equivalent expression[2]

$$c_1 = \tfrac{1}{2} d^2 \log\zeta(s)/ds^2|_{s=1/2} + G + \pi^2/8 - 4, \tag{4}$$

where $G = \beta(2)$ is Catalan's constant $0.915965\cdots$. This enables us to confirm Corollary 1 without summing over any zeros of $\zeta(s)$, but assuming RH. It is only rarely that such a closed form is known.[3]

As well as convergent sums, we also consider certain divergent sums. Theorem 2 shows that, if $\int_{T_0}^{\infty} t^{-1}\phi(t)\,dt < \infty$, then there exists

$$F(T_0) := \lim_{T\to\infty} \left(\sum_{T_0 \leqslant \gamma \leqslant T}{}^{'} \phi(\gamma) - \frac{1}{2\pi} \int_{T_0}^{T} \phi(t) \log(t/2\pi)\,dt \right).$$

In Theorem 3 we consider approximating $F(T_0)$ by computing a finite sum (over $\gamma \leqslant T$), with error term $E_2(T)$ the same as in Theorem 1.

For example, if $\phi(t) = 1/t$ and $T_0 = 2\pi$, we have $E(T) \ll T^{-1}\log T$ and $E_2(T) \ll T^{-2}\log T$. The latter bound allows us to obtain an accurate approximation to the constant $H = F(2\pi)$ that can equally well be defined, in analogy to Euler's constant, by

$$H := \lim_{T\to\infty} \left(\sum_{0<\gamma\leqslant T} \frac{1}{\gamma} - \frac{1}{4\pi} \log^2(T/2\pi) \right).$$

This example is considered in detail in [4], where it is shown that

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

The motivation for this paper was an attempt to generalise the results of [4].

In §2 we define some notation and mention some relevant results in the literature. We also state Lemma 2, which sharpens a result of Trudgian [18] and gives an almost best-possible explicit bound on $Q(t) - S(t)$. Lemma 3 in §3 covers finite sums. In

[2]The formula (4) is stated in [8, (21)] and is proved in [1, p. 13]. An almost indecipherable sketch of this result may be found in Riemann's Nachlass. We are indebted to Juan Arias de Reyna for information on the identity (4), and for his translation of the relevant page from Riemann's Nachlass.

[3]Some examples may be found in [5, Ch. 12] and [12, pp. 349, 443].

§4–§5 we deduce Theorems 1–3 from Lemma 3. Thus, in a sense, Lemma 3 is the key result, but we have called it a lemma in deference to Lehman's lemma.

We remark that the lower bound on T in Theorem 1 (and in other results below) is chosen to be 2π, not $2\pi e$ as in Lehman's lemma. This is convenient in applications because $2\pi < \gamma_1 < 2\pi e$. In fact, any positive lower bound could be chosen, provided the constants A_0, A_1 and A_2 were adjusted accordingly.

Our results are independent of the RH. However, it should be noted that we consider summands of the form $\phi(\gamma)$ which depend only on the imaginary parts of nontrivial zeros $\beta + i\gamma$. As to whether sharper bounds could be obtained on the assumption of RH, see the remarks at the end of §2.

Finally, we remark that Condition A can be weakened. It is sufficient for $\phi''(t)$ to exist and be non-negative for *almost all* $t \in [T_0, \infty)$ because the assumption $\phi''(t) \geqslant 0$ is only used in the proof of Lemma 3, and there $\phi''(t)$ only appears inside integrals.

2. Preliminaries

The *Riemann-Siegel theta function* $\theta(t)$ is defined for real t by

$$\theta(t) := \arg \Gamma\left(\frac{1}{4} + \frac{it}{2}\right) - \frac{t}{2}\log \pi,$$

see for example [6, §6.5]. The argument is defined so that $\theta(t)$ is continuous on $\mathbb{R}$, and $\theta(0) = 0$.

Let $\mathcal{F}$ denote the set of positive ordinates of zeros of $\zeta(s)$. Following Titchmarsh [16, §9.2–§9.3], if $0 < T \notin \mathcal{F}$, then we let $N(T)$ denote the number of zeros $\beta + i\gamma$ of $\zeta(s)$ with $0 < \gamma \leqslant T$, and $S(T)$ denote the value of $\pi^{-1}\arg\zeta(\frac{1}{2} + iT)$ obtained by continuous variation along the straight lines joining 2, $2 + iT$, and $\frac{1}{2} + iT$, starting with the value 0. If $0 < T \in \mathcal{F}$, we take $S(T) = \lim_{\delta\to 0}[S(T - \delta) + S(T + \delta)]/2$, and similarly for $N(T)$. This convention is the reason why we consider sums of the form $\sum'_{T_1 \leqslant \gamma \leqslant T_2} \phi(t)$ instead of $\sum_{T_1 \leqslant \gamma \leqslant T_2} \phi(t)$.

By [16, Thm. 9.3], we have

$$N(T) = L(T) + Q(T), \tag{5}$$

$$L(T) = \frac{T}{2\pi}\left(\log\left(\frac{T}{2\pi}\right) - 1\right) + \frac{7}{8}, \text{ and} \tag{6}$$

$$S(T) = Q(T) + O(1/T). \tag{7}$$

From [16, Thm. 9.4]), $S(T) \ll \log T$. Thus, from (7), $Q(T) \ll \log T$.

Trudgian [18, Cor. 1] gives the explicit bound $|Q(T) - S(T)| \leqslant 0.2/T$ for all $T \geqslant e$. In Lemma 2 we obtain a sharper constant, assuming that $T \geqslant 2\pi$. Our result is close to optimal, since the proof shows that the constant 150 could at best be replaced by $48\pi \approx 150.8$. We note that $Q(t) - S(t)$ is continuous for $t > 0$. This follows from the continuity of $\theta(t)$ and (8); see also [16, §9.3].

Lemma 2. *If $Q(t)$ and $S(t)$ are as above then, for all $t \geqslant 2\pi$, $|Q(t) - S(t)| \leqslant A_2/t$, where we may take $A_2 = 1/150 < 0.007$.*

Proof. We shall assume that $t \notin \mathcal{F}$, since otherwise the result follows by continuity of $Q(t) - S(t)$. The Riemann-von Mangoldt formula states, in its most precise form,

$$N(t) = \theta(t)/\pi + 1 + S(t).$$

From (5), this implies that

$$Q(t) - S(t) = \theta(t)/\pi + 1 - L(t). \tag{8}$$

Now $\theta(t)$ has a well-known asymptotic expansion as $t \to \infty$. Fix a positive integer k. Then, from [7, Satz 4.2.3(c)],

$$\theta(t) = \frac{t}{2}\left(\log\left(\frac{t}{2\pi}\right) - 1\right) - \frac{\pi}{8} + \sum_{j=1}^{k} \widetilde{T}_j(t) + O_k(t^{-(2k+1)}), \tag{9}$$

where, using the notation of [2],

$$\widetilde{T}_j(t) = \frac{(1-2^{1-2j})|B_{2j}|}{4j(2j-1)t^{2j-1}},$$

where $B_2 = \frac{1}{6}, B_4 = -\frac{1}{30}, \ldots$ are the Bernoulli numbers. Thus, using (6), $Q(t) - S(t)$ has an asymptotic expansion

$$Q(t) - S(t) = \frac{1}{\pi}\sum_{j=1}^{k} \widetilde{T}_j(t) + O_k(t^{-(2k+1)}). \tag{10}$$

In order to give an explicit bound on $Q(t) - S(t)$, we use an explicit bound from [2, (47)] on the error term in (9). The bound, valid for all $t > 0$, is

$$|\widetilde{R}_{k+1}(t)| < (1-2^{1-2k})^{-1}\,(\pi k)^{1/2}\,\widetilde{T}_k(t) + \tfrac{1}{2}e^{-\pi t}. \tag{11}$$

Substituting the expression for $\widetilde{T}_k(t)$ into (11) gives a bound

$$\frac{|\widetilde{R}_{k+1}(t)|}{\pi} < \frac{|B_{2k}|}{4(\pi k)^{1/2}(2k-1)\,t^{2k-1}} + \frac{e^{-\pi t}}{2\pi}$$

for the error term in (10). Thus, for all $k \geqslant 1$ and $t > 0$,

$$Q(t) - S(t) = \frac{1}{\pi}\sum_{j=1}^{k} \widehat{T}_j(t) + \vartheta\left(\frac{|B_{2k}|}{4(\pi k)^{1/2}(2k-1)\,t^{2k-1}} + \frac{e^{-\pi t}}{2\pi}\right).$$

Taking $k = 3$ and using the assumption $t \geqslant 2\pi$, we obtain the result. □

Define $S_1(T) := \int_0^T S(t)\,dt$. From Littlewood [11], $S_1(T) \ll \log T$. Explicit bounds on $S_1(T)$ are known [6, 17, 19]. From [17, Thm 2.2],

$$|S_1(T) - c_0| \leqslant A_0 + A_1 \log T \text{ for all } T \geqslant 168\pi, \tag{12}$$

where $c_0 = S_1(168\pi)$, $A_0 = 2.067$, and $A_1 = 0.059$. However, a small computation shows that (12) also holds for $T \in [2\pi, 168\pi]$. Hence, from now on we assume that $T_0 \geqslant 2\pi$ and that (12) holds for $T \geqslant T_0$.

We know that $S_1(T) = o(\log T)$ if and only if the Lindelöf Hypothesis (LH) is true — see Titchmarsh [16, Thm. 9.9(A), Thm. 13.6(B), and Note 13.8]. Since RH implies LH, one might expect better constants under the assumption of RH (or LH). However, it is likely that any improvement would be significant only for T very large. See, for example, Simonič [15].

3. Finite sums

In this section we prove Lemma 3, which may be seen as a refinement of Lemma 1 if the conditions $\phi'(t) \leqslant 0$, $\phi''(t) \geqslant 0$ are satisfied. The proof of Lemma 3 is essentially the same as the proof of Lehman's lemma up to equation (15), but then differs in the way that $\int_{T_1}^{T_2} \phi'(t)Q(t)\,dt$ is bounded. In particular, the proof of Lemma 3 uses the explicit bound (12) on $S_1(T)$, whereas the proof of Lehman's lemma does not use a bound on $S_1(T)$.

Lemma 3. *Suppose that $2\pi \leqslant T_0 \leqslant T_1 \leqslant T_2$ and that ϕ satisfies Condition* A. *If A_0, A_1, and A_2 are as in Theorem* 1, *and*

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

then $E(T_1, T_2) = \phi(T_2)Q(T_2) - \phi(T_1)Q(T_1) + E_2(T_1, T_2)$, where

$$E_2(T_1, T_2) = -\int_{T_1}^{T_2} \phi'(t)Q(t)\,dt \tag{13}$$

and

$$|E_2(T_1, T_2)| \leqslant 2(A_0 + A_1 \log T_1)\,|\phi'(T_1)| + (A_1 + A_2)\phi(T_1)/T_1. \tag{14}$$

Proof. Assume initially that $T_1 \notin \mathcal{F}$, $T_2 \notin \mathcal{F}$. Using Stieltjes integrals, we see that

$$\begin{aligned}\sideset{}{'}\sum_{T_1 \leqslant \gamma \leqslant T_2} \phi(\gamma) &= \int_{T_1}^{T_2} \phi(t)\,dN(t) = \int_{T_1}^{T_2} \phi(t)\,dL(t) + \int_{T_1}^{T_2} \phi(t)\,dQ(t)\\ &= \frac{1}{2\pi}\int_{T_1}^{T_2} \phi(t)\log(t/2\pi)\,dt + \int_{T_1}^{T_2} \phi(t)\,dQ(t),\end{aligned}$$

so

$$\begin{aligned}E(T_1, T_2) &= \int_{T_1}^{T_2} \phi(t)\,dQ(t) = \left[\phi(t)Q(t) - \int \phi'(t)Q(t)\,dt\right]_{T_1}^{T_2}\\ &= \phi(T_2)Q(T_2) - \phi(T_1)Q(T_1) - \int_{T_1}^{T_2} \phi'(t)Q(t)\,dt. \qquad (15)\end{aligned}$$

This proves (13). To prove (14), note that, from Lemma 2,

$$\int_{T_1}^{T_2} \phi'(t)Q(t)\,dt = \int_{T_1}^{T_2} \phi'(t)S(t)\,dt + \vartheta A_2 \int_{T_1}^{T_2} \frac{\phi'(t)}{t}\,dt, \tag{16}$$

and the last integral can be bounded using

$$\left|\int_{T_1}^{T_2} \frac{\phi'(t)}{t}\,dt\right| \leqslant \frac{1}{T_1}\int_{T_1}^{T_2} |\phi'(t)|\,dt = \frac{\phi(T_1) - \phi(T_2)}{T_1} \leqslant \frac{\phi(T_1)}{T_1}, \tag{17}$$

where we used $\phi(t) \geqslant 0$, $\phi'(t) \leqslant 0$ (from Condition A).

Also,

$$\begin{aligned}\int_{T_1}^{T_2} \phi'(t)S(t)\,dt &= \left[\phi'(t)(S_1(t) - c_0) - \int \phi''(t)(S_1(t) - c_0)\,dt\right]_{T_1}^{T_2}\\ &= \phi'(T_2)(S_1(T_2) - c_0) - \phi'(T_1)(S_1(T_1) - c_0) - \int_{T_1}^{T_2} \phi''(t)(S_1(t) - c_0)\,dt.\end{aligned}$$

Now, using $\phi'(t) \leqslant 0$ and $|S_1(t) - c_0| \leqslant A_0 + A_1 \log t$, we have

$$|\phi'(t)(S_1(t) - c_0)| \leqslant -(A_0 + A_1 \log t)\phi'(t)$$

for $t = T_1, T_2$. Thus

$$\begin{aligned}
&\left|\int_{T_1}^{T_2} \phi'(t)S(t)\,dt\right| \\
&\leqslant -\sum_{j=1}^{2}(A_0 + A_1 \log T_j)\phi'(T_j) + \left|\int_{T_1}^{T_2} \phi''(t)(S_1(t) - c_0)\,dt\right|. \qquad (18)
\end{aligned}$$

Also, using $\phi''(t) \geqslant 0$, we have

$$\begin{aligned}
&\left|\int_{T_1}^{T_2} \phi''(t)(S_1(t) - c_0)\,dt\right| \leqslant A_0 \int_{T_1}^{T_2} \phi''(t)\,dt + A_1 \int_{T_1}^{T_2} \phi''(t)\log t\,dt \\
&= A_0(\phi'(T_2) - \phi'(T_1)) + A_1\left[\phi'(t)\log t - \int \frac{\phi'(t)}{t}\,dt\right]_{T_1}^{T_2} \\
&= (A_0 + A_1 \log T_2)\phi'(T_2) - (A_0 + A_1 \log T_1)\phi'(T_1) - A_1 \int_{T_1}^{T_2} \frac{\phi'(t)}{t}\,dt. \qquad (19)
\end{aligned}$$

Inserting (19) in (18) and simplifying, terms involving T_2 cancel, giving

$$\left|\int_{T_1}^{T_2} \phi'(t)S(t)\,dt\right| \leqslant -2(A_0 + A_1 \log T_1)\phi'(T_1) - A_1 \int_{T_1}^{T_2} \frac{\phi'(t)}{t}\,dt. \qquad (20)$$

Combining (13) with (16), (17), and (20) gives (14). Finally, we note that (13)–(14) hold even if $T_1 \in \mathcal{F}$ and/or $T_2 \in \mathcal{F}$, because of the way that we defined $N(T)$ (and hence $Q(T) = N(T) - L(T)$) for $T \in \mathcal{F}$. □

Remark 2. With the assumptions and notation of Lemma 3, Lemma 1 gives the bound

$$|E(T_1, T_2)| \leqslant A\left(2\phi(T_1)\log T_1 + \int_{T_1}^{T_2} \frac{\phi(t)}{t}\,dt\right). \qquad (21)$$

Our bound (14) on $E_2(T_1, T_2)$ is often smaller than the bound (21) on $E(T_1, T_2)$. We can take advantage of this if the terms $\phi(T_j)Q(T_j)$ $(j = 1, 2)$ are known. This is often the case, because we can easily compute $Q(T_j) = N(T_j) - L(T_j)$ if the nontrivial zeros up to height T_j have been enumerated.

4. Convergent sums

In this section we assume that $\sum_{T \leqslant \gamma} \phi(\gamma) < \infty$, or equivalently (given our conditions on ϕ) that $\int_T^\infty \phi(t)\log(t/2\pi)\,dt < \infty$. We first state an easy lemma, and then prove Theorem 1.

Lemma 4. *Suppose that $2\pi \leqslant T_0 \leqslant T$, that ϕ satisfies Condition* A, *and that* $\int_T^\infty \phi(t)\log(t/2\pi)\,dt < \infty$. *Then*

$$\phi(t)\log t = o(1) \text{ as } t \to \infty, \tag{22}$$

$$\phi'(t)\log t = o(1) \text{ as } t \to \infty, \text{ and} \tag{23}$$

$$\int_T^\infty |\phi'(t)|\log t\,dt < \infty. \tag{24}$$

Proof. For $u \geqslant T$,

$$\int_u^{u+1} \phi(t)\log(t/2\pi)\,dt \geqslant \phi(u+1)\log(u/2\pi).$$

Thus $\phi(u+1)\log(u/2\pi) = o(1)$ as $u \to \infty$, and $\phi(t)\log((t-1)/2\pi) = o(1)$. Since $\log((t-1)/2\pi) \sim \log t$, (22) follows.

For (23), we have

$$\phi(u) \geqslant \phi(u) - \phi(u+1) = \int_u^{u+1} |\phi'(t)|\,dt \geqslant |\phi'(u+1)|, \tag{25}$$

so (22) implies that $\phi'(u+1)\log u = o(1)$. Taking $t = u+1$, we have $\phi'(t)\log(t-1) = o(1)$. Since $\log(t-1) \sim \log t$, (23) follows.

Finally, from (25), $|\phi'(t)| \leqslant \phi(t-1)$ for $t \geqslant T+1$, so

$$\int_{T+1}^\infty |\phi'(t)|\log t\,dt \leqslant \int_{T+1}^\infty \phi(t-1)\log t\,dt \ll \int_T^\infty \phi(t)\log(t/2\pi)\,dt < \infty,$$

and (24) follows. □

Proof of Theorem 1. We have $\phi(t)\log t = o(1)$ by Lemma 4 and convergence of the integral in (1). Also, from Lemma 4 we have $\int_T^\infty |\phi'(t)|\log t\,dt < \infty$, but $Q(t) \ll \log t$, so $\int_T^\infty \phi'(t)Q(t)\,dt$ converges absolutely. Now, Lemma 3 gives

$$\begin{aligned}\sideset{}{'}\sum_{T\leqslant\gamma\leqslant T_2} \phi(\gamma) - \frac{1}{2\pi}\int_T^{T_2} \phi(t)\log(t/2\pi)\,dt \\ = \phi(T_2)Q(T_2) - \phi(T)Q(T) - \int_T^{T_2} \phi'(t)Q(t)\,dt.\end{aligned} \tag{26}$$

If we let $T_2 \to \infty$ in (26), $\phi(T_2)Q(T_2) \to 0$ and $\int_T^{T_2} \phi'(t)Q(t)\,dt$ tends to a finite limit. Thus, the right side of (26) tends to a finite limit, and the left side must tend to the same limit. This gives

$$\sideset{}{'}\sum_{T\leqslant\gamma} \phi(\gamma) - \frac{1}{2\pi}\int_T^\infty \phi(t)\log(t/2\pi)\,dt = -\phi(T)Q(T) - \int_T^\infty \phi'(t)Q(t)\,dt.$$

We have proved (1)–(2) of Theorem 1. The bound (3) follows by observing that the bound (14) of Lemma 3 is independent of T_2, so

$$\left|\int_T^\infty \phi'(t)Q(t)\,dt\right| \leqslant 2(A_0 + A_1\log T)\,|\phi'(T)| + (A_1 + A_2)\phi(T)/T.$$

This completes the proof of Theorem 1. □

5. Divergent sums

In this section we give two theorems that apply, subject to a mild condition (31) on $\phi(t)$, even if $\sum_{T\leqslant\gamma}\phi(\gamma)$ diverges. Theorem 2 shows the existence of a limit for the difference between a sum and the corresponding integral. Theorem 3 shows how we can accurately approximate the limit.

First we prove two lemmas that strengthen the first and third parts of Lemma 4. In Lemma 5, f is non-increasing but need not be differentiable.

Lemma 5. *Suppose that, for some $T\geqslant 1$, $f:[T,\infty]\mapsto[0,\infty)$ is non-negative and non-increasing on $[T,\infty)$. If*

$$\int_T^\infty \frac{f(t)}{t}\,dt<\infty, \tag{27}$$

then $f(t)\log t=o(1)$.

Proof. Assume, by way of contradiction, that $f(t)\log t\neq o(1)$. Thus, there exists a constant $c>0$ and an unbounded increasing sequence $(t_n)_{n\geqslant 1}$ such that $t_1>T$ and

$$f_n:=f(t_n)\geqslant\frac{c}{\log t_n}\,. \tag{28}$$

Moreover, by taking a subsequence of $(t_n)_{n\geqslant1}$ if necessary, we can assume that $t_{n+1}\geqslant t_n^2$ for all $n\geqslant1$. Thus

$$\log\left(\frac{t_{n+1}}{t_n}\right)\geqslant\frac{\log t_{n+1}}{2}\,. \tag{29}$$

Since $f(t)$ is non-increasing, we have $f(t)\geqslant f_{n+1}$ on $[t_n,t_{n+1}]$, and

$$\int_{t_n}^{t_{n+1}}\frac{f(t)}{t}\,dt\geqslant\int_{t_n}^{t_{n+1}}\frac{f_{n+1}}{t}\,dt=f_{n+1}\log\left(\frac{t_{n+1}}{t_n}\right).$$

Using (28)–(29), this gives

$$\int_{t_1}^{t_{n+1}}\frac{f(t)}{t}\,dt\geqslant\frac12\sum_{k=1}^{n}f_{k+1}\log t_{k+1}\geqslant\frac{c}{2}\sum_{k=1}^{n}1=\frac{cn}{2}\to\infty.$$

This contradicts the condition (27). Thus, our assumption is false, and we must have $f(t)\log t=o(1)$. □

Lemma 6. *If ϕ satisfies Condition* A *with $T_0\geqslant1$, and $\int_{T_0}^\infty\frac{\phi(t)}{t}\,dt<\infty$, then $\int_{T_0}^\infty\phi'(t)\log t\,dt$ is absolutely convergent.*

Proof. For $T\geqslant T_0$ we have

$$\int_{T_0}^{T}\phi'(t)\log t\,dt=\phi(T)\log T-\phi(T_0)\log T_0-\int_{T_0}^{T}\frac{\phi(t)}{t}\,dt. \tag{30}$$

As $T\to\infty$ in (30), the term $\phi(T)\log T\to0$ by Lemma 5, and the integral on the right-hand side tends to a finite limit. Thus, the integral on the left-hand side tends to a finite limit. Since $\phi'(t)\log t\leqslant0$ has constant sign on $[T_0,\infty)$, the integral is absolutely convergent. □

Theorem 2. *Suppose that $T_0 \geqslant 2\pi$, that ϕ satisfies Condition* A, *and that*

$$\int_{T_0}^{\infty} \frac{\phi(t)}{t}\, dt < \infty. \tag{31}$$

Then there exists

$$F(T_0) := \lim_{T\to\infty} \left(\sideset{}{'}\sum_{T_0 \leqslant \gamma \leqslant T} \phi(\gamma) - \frac{1}{2\pi} \int_{T_0}^{T} \phi(t) \log(t/2\pi)\, dt \right),$$

and

$$F(T_0) = -\phi(T_0)Q(T_0) - \int_{T_0}^{\infty} \phi'(t)Q(t)\, dt. \tag{32}$$

Proof. Suppose that $T \geqslant T_0$. Applying Lemma 3, we have

$$\sideset{}{'}\sum_{T_0 \leqslant \gamma \leqslant T} \phi(\gamma) - \frac{1}{2\pi} \int_{T_0}^{T} \phi(t) \log(t/2\pi)\, dt$$
$$= \phi(T)Q(T) - \phi(T_0)Q(T_0) - \int_{T_0}^{T} \phi'(t)Q(t)\, dt. \tag{33}$$

Let $T \to \infty$ in (33). On the right-hand side, $\phi(T)Q(T) \to 0$ by Lemma 5, and the integral tends to a finite limit by Lemma 6, using $Q(t) \ll \log t$. Thus the left-hand side tends to a finite limit $F(T_0)$. This gives (32). □

The identity (32) is not convenient for accurately approximating $F(T_0)$ when T_0 is small, because $\int_{T_0}^{\infty} \phi'(t)Q(t)\, dt$ is not necessarily small. In Theorem 3 we use a finite sum (over $\gamma \leqslant T$) and integral to approximate $F(T_0)$. Theorem 3 has the same expression for the error term E_2 as Theorem 1, essentially because the bounds in both theorems are proved using Lemma 3.

Theorem 3. *Suppose that $2\pi \leqslant T_0 \leqslant T_1$, that ϕ satisfies Condition* A, *and that* (31) *holds. Let*

$$F(T_0) := \lim_{T\to\infty} \left(\sideset{}{'}\sum_{T_0 \leqslant \gamma \leqslant T} \phi(\gamma) - \frac{1}{2\pi} \int_{T_0}^{T} \phi(t) \log(t/2\pi)\, dt \right).$$

If A_0, A_1, A_2 are as in Theorem 1, *then*

$$F(T_0) = \sideset{}{'}\sum_{T_0 \leqslant \gamma \leqslant T_1} \phi(\gamma) - \frac{1}{2\pi} \int_{T_0}^{T_1} \phi(t) \log(t/2\pi)\, dt - \phi(T_1)Q(T_1) + E_2(T_1),$$

where $E_2(T_1) = -\int_{T_1}^{\infty} \phi'(t)Q(t)\, dt$, and

$$|E_2(T_1)| \leqslant 2(A_0 + A_1 \log T_1)\, |\phi'(T_1)| + (A_1 + A_2)\phi(T_1)/T_1.$$

Proof. We note that, from Theorem 2, the limit defining $F(T_0)$ exists. Also, from Lemmas 5–6, $\phi(T)Q(T) = o(1)$ and $\int_{T_0}^{\infty} \phi'(t)Q(t)\, dt < \infty$. Thus, using Lemma 3 as in the proof of Theorem 1, we see that

$$\lim_{T_2\to\infty} \left(\sideset{}{'}\sum_{T_1 \leqslant \gamma \leqslant T_2} \phi(\gamma) - \frac{1}{2\pi} \int_{T_1}^{T_2} \phi(t) \log(t/2\pi)\, dt \right)$$
$$= -\phi(T_1)Q(T_1) - \int_{T_1}^{\infty} \phi'(t)Q(t)\, dt$$

and $\left|\int_{T_1}^{\infty} \phi'(t)Q(t)\,dt\right| \leqslant 2(A_0 + A_1 \log T_1)\,|\phi'(T_1)| + (A_1 + A_2)\phi(T_1)/T_1$. Since

$$F(T_0) = \lim_{T_2\to\infty} \left(\sum_{T_1 \leqslant \gamma \leqslant T_2}{}' \phi(\gamma) - \frac{1}{2\pi}\int_{T_1}^{T_2} \phi(t)\log(t/2\pi)\,dt \right) + \sum_{T_0 \leqslant \gamma \leqslant T_1}{}' \phi(\gamma) - \frac{1}{2\pi}\int_{T_0}^{T_1} \phi(t)\log(t/2\pi)\,dt,$$

the result follows. □

Example 2. To illustrate the divergent case, we consider the example $\phi(t) = 1/(\log(t/2\pi))^2$. The constant 2π here is unimportant, but this choice simplifies some of the expressions below.

From Lemma 1, the asymptotic behaviour of $\sum_{0<\gamma\leqslant T} \phi(\gamma)$ is given by

$$\frac{1}{2\pi}\int_c^T \phi(t)\log(t/2\pi)\ dt = \mathrm{li}(T/2\pi) - \mathrm{li}(c/2\pi) \sim \frac{T}{2\pi\log T},$$

where $c \geqslant 2\pi e$ is an arbitrary constant, and $\mathrm{li}(x)$ is the logarithmic integral, defined in the usual way by a principal value integral. This motivates the definition of a constant c_2 by

$$c_2 := \lim_{T\to\infty}\left(\sum_{0<\gamma\leqslant T}{}' \phi(\gamma) - \mathrm{li}(T/2\pi) \right), \tag{34}$$

where the limit exists by Theorem 2.

If we use (34) to estimate c_2 then, by Theorem 3, the error is

$$E(T) = -\phi(T)Q(T) + O(|\phi'(T)|\log T) + O(\phi(T)/T) \ll \frac{1}{\log T}.$$

Convergence is so slow that it is difficult to obtain more than two correct decimal digits. On the other hand, if we estimate c_2 using the approximation

$$\sum_{0<\gamma\leqslant T}{}' \phi(\gamma) - \mathrm{li}(T/2\pi) - \phi(T)Q(T) \tag{35}$$

suggested by Theorem 3, then the error is $E_2(T) \ll (T\log^2 T)^{-1}$, smaller by a factor of order $T\log T$. More precisely, from Theorem 3 we have

$$\begin{aligned} |E_2(T)| &\leqslant \frac{4(A_0 + A_1\log T)}{T\log^3(T/2\pi)} + \frac{A_1 + A_2}{T\log^2(T/2\pi)} \\ &\leqslant \frac{0.302\log(T/2\pi) + 8.702}{T\log^3(T/2\pi)}. \end{aligned} \tag{36}$$

Corollary 2. *If c_2 is defined by* (34)*, then*

$$c_2 = -0.5276697875 + \vartheta(10^{-10}).$$

Proof. Using the first $n = 10^9$ nontrivial zeros with $T = (\gamma_n + \gamma_{n+1})/2$ in (35), and the error bound (36), an interval-arithmetic computation gives the result. The sum over zeros was performed as described in the proof of Corollary 1, again using Arb [9] and computing $Q(T)$ in the obvious way. □

Table 1. Numerical estimation of $c_2 \approx -0.5276697875$

n	estimate via (34)	estimate via (35)	$\lvert E_2\rvert$ bound (36)
10	-0.49986259	-0.52733908	1.96×10^{-2}
10^2	-0.54054724	-0.52767238	8.64×10^{-4}
10^3	-0.52244974	-0.52767173	4.58×10^{-5}
10^4	-0.53117846	-0.52766980	2.78×10^{-6}
10^5	-0.53026260	-0.52766977	1.87×10^{-7}

We used fewer nontrivial zeros in the proof of Corollary 2 than in the proof of Corollary 1 because the computation in the inner loop, involving a logarithm evaluated using interval arithmetic, was more expensive, and 10^9 zeros were sufficient to obtain the desired error bound.

To illustrate the speed of convergence, in Table 1 we give the estimates of c_2 obtained from (34) and (35) by summing over the first n nontrivial zeros, and the error bound (36), with $T = (\gamma_n + \gamma_{n+1})/2$.

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