THE ERROR FOR THE SECOND MOMENT OF COTANGENT SUMS RELATED TO THE RIEMANN HYPOTHESIS

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Abstract. In various papers the authors have derived asymptotics for moments of certain cotangent sums related to the Riemann Hypothesis. S. Bettin [4] has given an upper bound for the error term in these asymptotic results. In the present paper the authors establish a lower bound for the error term for the second moment.

Key words: Riemann Hypothesis, Riemann zeta function, Nyman-Beurling-Báez-Duarte criterion.

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1. Introduction

The authors in joint work (cf. [8, 9, 10, 11]) and the second author in his thesis ([12]) investigated the distribution of cotangent sums

$$c_0 \left( \frac{r}{b} \right) := \sum_{m=1}^{b-1} \frac{m}{b} \cot \left( \frac{\pi mr}{b} \right),$$

as \( r \) ranges over the set

$$\{r : (r, b) = 1, A_0 b \leq r \leq A_1 b\}, \text{ where } 1/2 < A_0 < A_1 < 1.$$

These cotangent sums are related to the Estermann zeta function

$$E \left( s, \frac{r}{b}, \alpha \right) := \sum_{n \geq 1} \frac{\sigma_\alpha(n) \exp(2\pi inr/b)}{n^s},$$

where \( \Re s > \Re \alpha + 1 \), \( b \geq 1 \), \( (r, b) = 1 \) and

$$\sigma_\alpha(n) := \sum_{d|n} d^\alpha.$$

The cotangent sum \( c_0(r/b) \) can be associated to the study of the Riemann Hypothesis through its relation with the Vasyunin sum \( V \), which is defined by

$$V \left( \frac{r}{b} \right) := \sum_{m=1}^{b-1} \left\{ \frac{mr}{b} \right\} \cot \left( \frac{\pi mr}{b} \right),$$

where \( \{u\} := u - \lfloor u \rfloor \), \( u \in \mathbb{R} \).

It can be shown that

$$V \left( \frac{\bar{r}}{b} \right) = -c_0 \left( \frac{\bar{r}}{b} \right),$$

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where \( r\bar{r} \equiv 1 \pmod{b} \). We have
\[
\frac{1}{2\pi \sqrt{rb}} \int_{-\infty}^{\infty} \left| \zeta \left( \frac{1}{2} + it \right) \right|^2 \left( \frac{r}{b} \right)^it \frac{dt}{\frac{4}{t} + t^2} = \log 2 \pi - \frac{\gamma}{2} \left( \frac{1}{r} + \frac{1}{b} \right) + \frac{b - r}{2rb} \log \frac{r}{b} - \pi \left( \frac{V(\frac{r}{b}) + V(\frac{b}{r})}{2} \right).
\]
The above formula is related to the Nymann-Beurling-Báez-Duarte-Vasyunin approach to the Riemann Hypothesis (see [14]). Let
\[
d_N^2 := \inf_{D_N} \frac{1}{2\pi} \int_{-\infty}^{\infty} \left| 1 - \zeta D_N \left( \frac{1}{2} + it \right) \right|^2 \frac{dt}{\frac{4}{t} + t^2}
\]
and the infimum is over all Dirichlet polynomials
\[
D_N(s) := \sum_{n=1}^{N} \frac{a_n}{n^s}, \quad a_n \in \mathbb{C},
\]
of length \( N \) (see [3]).
The Riemann Hypothesis is true if and only if
\[
\lim_{N \to +\infty} d_N = 0.
\]
The authors of the present paper in joint work (cf. [9]), considered the moments defined by
\[
H_k := \lim_{b \to +\infty} \phi(b)^{-1} b^{-2k} (A_1 - A_0)^{-1} \sum_{a_0b \leq r \leq A_1b \atop (r,b)=1} c_0 \left( \frac{r}{b} \right)^{2k}, \quad k \in \mathbb{N},
\]
where \( \phi(\cdot) \) denotes the Euler phi-function. They could show that
\[
H_k = \int_0^1 \left( \frac{g(x)}{\pi} \right)^{2k} dx,
\]
where
\[
g(x) := \sum_{l \geq 1} \frac{1 - 2\{lx\}}{l}
\]
a function that has been investigated by de la Bretèche and Tenenbaum ([9]), as well as Balazard and Martin ([2, 3]).
Bettin [4] could replace the interval \((1/2, 1]\) for \( A_0, A_1 \) by the interval \((0, 1)\). In a series of papers the authors investigated the moments \( H_k \). In [10] they showed:
Let \( K \in \mathbb{N} \). There is an absolute constant \( C > 0 \), such that
\[
\int_0^1 |g(x)|^K dx = \frac{e^\gamma}{\pi} \Gamma(K + 1)(1 + O(\exp(-CK)))
\]
for \( K \to +\infty \).
In [11] the authors could generalise this result for arbitrary positive exponents.
The size of the error term in (1.1) has been investigated by Bettin ([4]). Using the Mellin transform and complex integration he could show the following result:
\[
\frac{1}{\phi(q)} \sum_{(a,q)=1} c_0 \left( \frac{a}{q} \right)^k = H_{k/2} q^k + O(q^{k-1+\epsilon}(Ak \log q)^{2k}).
\]
In this paper we show that for the special case \( k = 2 \) and \( q \) a prime number Bettin’s upper bound for the error term is close to best possible. Our main result is the following:

**Theorem 1.1.** Let \( q \) be a prime number, \( H_1 \) resp. \( g \) be given by (1.2) resp. (1.3) and let

\[
\frac{1}{q-1} \sum_{a=1}^{q-1} c_0 \left( \frac{a}{q} \right)^2 = H_1 q^2 + E(q) .
\]

Then there is an absolute constant \( C > 0 \), such that

\[
E(q) \geq C q (\log q)^2 , \quad q \geq q_0 .
\]

2. **Continued Fractions**

We recall some fundamental definitions and results from [3].

**Definition 2.1.** Let \( X := [0, 1] \setminus \mathbb{Q} \) and \( \alpha(x) := \{1/x\} \) for all \( x \in X \), where \( \{ \cdot \} \) denotes the fractional part. We define the iterates of \( \alpha \) by:

\[
\alpha_0(x) := x , \quad \alpha_k(x) := \alpha(\alpha_{k-1}(x)) , \quad \text{for all } k \in \mathbb{N} .
\]

We write

\[
a_0(x) := 0 \quad \text{and} \quad a_k(x) := \left\lfloor \frac{1}{\alpha_{k-1}(x)} \right\rfloor , \quad k \geq 1 .
\]

If \( x \) is irrational, then the sequence of partial fractions of \( x \) is defined by the recursion:

\[
\begin{align*}
p_0(x) &:= 0 , \quad q_0(x) := 1 ; \quad p_1(x) := 1 , \quad q_1(x) := a_1(x) , \\
p_k(x) &:= a_k(x)p_{k-1}(x) + p_{k-2}(x) , \\
q_k(x) &:= a_k(x)q_{k-1}(x) + q_{k-2}(x) , \quad k \geq 2 .
\end{align*}
\]

One writes

\[
\frac{p_k(x)}{q_k(x)} := [0; a_1(x), \ldots, a_k(x)] .
\]

The sequence

\[
\left( \frac{p_k(x)}{q_k(x)} \right)_{k=0}^{+\infty}
\]

is called the continued fraction expansion of \( x \) and is denoted by

\[
[0; a_1(x), \ldots, a_k(x), \ldots] .
\]

If \( x \) is a rational number, then \( a_K(x) = 0 \) for some \( K \in \mathbb{N} \) and we have:

\[
x = [0; a_1(x), \ldots, a_K(x)] .
\]

\( K \) is called the depth of \( x \).

We shall also apply the Definitions 2.1, 2.2 for the case that the last term \( a_k(x) \) is not an integer.

We define the functions \( \beta_k \) and \( \gamma_k \) by

\[
\beta_k(x) := \alpha_0(x)\alpha_1(x)\ldots\alpha_k(x) , \quad (\beta_{-1} = 1)
\]

and

\[
\gamma_k(x) := \beta_{k-1}(x) \log \frac{1}{\alpha_k(x)} ,
\]
with
\[(2.5)\]
\[\gamma_0(x) := \log(1/x).\]

**Definition 2.2. (cells)**

Let \(k \in \mathbb{N}, b_0 := 0\) and \(b_1, \ldots, b_k \in \mathbb{N}^* = \mathbb{N} \setminus \{0\}\). The **cell of depth** \(k\), \(C(b_1, \ldots, b_k)\) is the open interval with the endpoints \([0; b_1, \ldots, b_k]\) and \([0; b_1, \ldots, b_{k-1}, b_k + 1]\).

In the cell \(C(b_1, \ldots, b_k)\) the functions \(a_j, p_j, q_j\) are constant for \(j \leq k\).

For \(x \in C(b_1, \ldots, b_k)\) we have:
\[a_j(x) = b_j, \quad \frac{p_j(x)}{q_j(x)} = [0; b_1, \ldots, b_j], \quad j \leq k.\]

**Lemma 2.3.** Within the cell \(C(b_1, \ldots, b_k)\), \(\alpha_k\) and \(\gamma_k\) are differentiable functions of \(x\). We have:
\[\alpha_k' = (-1)^k (q_k + \alpha_k q_{k-1})^2, \quad \gamma_k' = (-1)^{k-1} q_{k+1} \log \left(\frac{1}{\alpha_k}\right) + \frac{(-1)^{k-1}}{\beta_k}.\]

*Proof.* (2), Formula (34), p. 207 and (36), p. 208. \(\square\)

**Lemma 2.4.**
\[\beta_k(x) = (-1)^{k-1} (p_k(x) - x q_k(x)) = |p_k(x) - x q_k(x)| = \frac{1}{q_{k+1}(x) + \alpha_{k+1}(x) q_k(x)}.\]

*Proof.* This is formula (14) of [3]. \(\square\)

**3. A representation of \(g(x)\) related to Wilton’s function**

We now recall the following definition from [3]. The number \(x\) is called a Wilton number if the series
\[(3.1)\]
\[\sum_{k \geq 0} (-1)^k \gamma_k(x)\]
converges. Wilton’s function \(W(x)\) is defined by
\[(3.2)\]
\[W(x) := \sum_{k \geq 0} (-1)^k \gamma_k(x)\]
for each Wilton number \(x \in (0, 1)\).

The operator \(T : L^p \rightarrow L^p\) (\(p > 1\)) is defined by
\[(3.3)\]
\[Tf(x) := xf(\alpha(x))\]

For \(n \in \mathbb{N}, x \in X\), we define
\[(3.4)\]
\[\mathcal{L}(x, n) := \sum_{v=0}^{n} (-1)^v (T^v l)(x).\]

For \(\lambda \geq 0\) we set
\[(3.5)\]
\[A(\lambda) := \int_0^{+\infty} \left\{t\right\} \lambda t \ dt \frac{dt}{t^2}\]
\[(3.6)\]
\[F(x) := \frac{x + 1}{2} A(1) - \frac{x}{2} A(x) - \frac{x}{2} \log x\]
\[(3.7)\]
\[H(x) := -2 \sum_{j \geq 0} (-1)^j \beta_{j-1}(x) F(\alpha_j(x)).\]
Lemma 3.1. We have

\begin{equation}
L(x, n) = \sum_{k=0}^{n} (-1)^k \gamma_k(x) .
\end{equation}

\begin{equation}
g(x) = L(x, n) + H(x) + (-1)^{n+1} T^{n+1} W(x).
\end{equation}

Proof. Equality (3.8) follows from (2.3)-(2.5) and (3.4). Equality (3.9) follows from Lemma 2.7 of [2]. □

4. An expression for the error-term

We recall the following definition from [2].

Definition 4.1.

\[ D_{\sin}(s, x) := \sum_{n=1}^{+\infty} \frac{d(n) \sin(2\pi nx)}{n^s}. \]

Lemma 4.2.

\[ c_0 \left( \frac{a}{q} \right) = 2q\pi^{-2} D_{\sin}(1, \bar{a}/q), \]

where

\[ D_{\sin}(1, x) = \pi g(x). \]

Proof. The first fact is due to Ishibashi [7], the second to de la Bretêche and Tenenbaum [6] (see also [4]). □

Lemma 4.3. Let

\[ \frac{1}{q-1} \sum_{a=1}^{q-1} g \left( \frac{a}{q} \right)^2 = H_1 + \tilde{E}(q). \]

Then Theorem 4.1 is equivalent to

\[ \tilde{E}(q) \geq Cq^{-1} (\log q)^2, \quad q \geq q_0, \]

for an absolute constant \( C > 0 \).

Proof. This follows from Lemma 4.2. To estimate \( \tilde{E}(q) \) we thus have to investigate the sums in the following. □

Definition 4.4.

\[ \Sigma_1 := \sum_{k \leq K} \sum_{a=1}^{q-1} \int_{\frac{a}{q} - \frac{1}{2q}}^{\frac{a}{q} + \frac{1}{2q}} \gamma_k(x)^2 - \gamma_k \left( \frac{a}{q} \right)^2 \, dx \]

\[ \Sigma_2 := \sum_{k_1 < k_2 \leq K} (-1)^{k_1 + k_2} \sum_{a=1}^{q-1} \int_{\frac{a}{q} - \frac{1}{2q}}^{\frac{a}{q} + \frac{1}{2q}} \left( \gamma_{k_1}(x) - \gamma_k \left( \frac{a}{q} \right) \right) \left( \gamma_{k_2}(x) - \gamma_k \left( \frac{a}{q} \right) \right) \, dx \]

\[ \Sigma_3 := \sum_{k \leq K} \sum_{a=1}^{q-1} \int_{\frac{a}{q} - \frac{1}{2q}}^{\frac{a}{q} + \frac{1}{2q}} \left( H(x) - H \left( \frac{a}{q} \right) \right) \left( \gamma_k(x) - \gamma_k \left( \frac{a}{q} \right) \right) \, dx \]

\[ \Sigma_4 := \sum_{k \leq K} \sum_{a=1}^{q-1} \int_{\frac{a}{q} - \frac{1}{2q}}^{\frac{a}{q} + \frac{1}{2q}} \left( H(x) - H \left( \frac{a}{q} \right) \right)^2 \, dx \]
5. A LOWER BOUND FOR \( \Sigma_1 \)

We first give some facts and definitions which are also of importance in the estimate of the other terms.

**Lemma 5.1.** Let \( r \) be a rational number of depth \( k \),

\[
r = [0; b_1, \ldots, b_k] , \ k \geq 2 .
\]

Then there is exactly one pair \( P_k = (C_1, C_2) \), \( C_1 \) a cell of depth \( k \) and \( C_2 \) a cell of depth \( k + 1 \), such that \( r \) is a common endpoint of both of the cells, namely

\[
C_1 = C(b_1, \ldots, b_k) \text{ and } C_2 = C(b_1, \ldots, b_k - 1, 2) .
\]

**Proof.** By definition a cell \( \tilde{C} \) of depth \( k + 1 \) that has an endpoint of depth \( k \) must be of the form

\[
\tilde{C} = C(a_1, \ldots, a_k - 1, 2) , \ a_k \geq 2 .
\]

Thus we must have

\[
C_2 = C(b_1, \ldots, b_k - 1, 2) .
\]

By Definition 2.2 the cells of order \( k \) bordering on \( r \) are

\[
\tilde{C} = C(b_1, \ldots, b_k - 1) \text{ and } \tilde{C} = C(b_1, \ldots, b_k) .
\]

Since \( C(b_1, \ldots, b_k - 1, 2) \) is a proper subset of \( \tilde{C} \), we must have \( C_1 = C(b_1, \ldots, b_k) \). \( \square \)

**Definition 5.2.** We call the pair \( P_k = (C_1, C_2) \) of Lemma 5.1 the pair of order \( k \) of \( r \). For each \( k \) we partition the set of intervals

\[
I_a := \left[ \frac{a}{q}, \frac{a+1}{q} \right]
\]

into two classes:

\[
C_{k,1} := \{ I_a : I_a \text{ and } I_{a+1} \text{ do not contain a rational number of depth } k \}
\]

\[
C_{k,2} := \{ I_a : I_a \text{ or } I_{a+1} \text{ contains a rational number of depth } k \} .
\]

We first give a lower bound for the contribution of the intervals of class \( C_{k,1} \). Each \( I_a^* \in C_{k,1} \) is entirely contained in a cell \( c(I_a^*) = C(b_1, \ldots, b_k) \) of order \( k \). Let

\[
[b_1, \ldots, b_k] := \frac{p_k}{q_k} .
\]

We write \( a = a_0 + b \), where

\[
a_0 = \min \{ a : I_a \subset c(I_a^*) \} .
\]

We now evaluate

\[
C_a = \int \frac{\alpha_{k+1}}{\alpha_k} - \gamma_k(x)^2 - \gamma_k \left( \frac{a}{q} \right)^2 \ dx
\]

From Lemmas 2.3 and 2.4 we obtain:

\[
\gamma_k(x) = -q_k - 1 \log \left( \frac{1}{\alpha_k(x)} \right) + q_k^{-1} \left( \frac{p_k}{q_k} - x \right)^{-1}
\]

and thus

\[
\gamma_k''(x) = 2q_k^{-1} \left( \frac{p_k}{q_k} - x \right)^{-2} + O \left( \left( \frac{p_k}{q_k} - x \right)^{-1} \right) .
\]
We also have that
\[ \left| \frac{p_k}{q_k} \right| - a_k \geq \frac{1}{qq_k}. \]

This leads to
\[ \frac{d^2}{dx^2}(\gamma_k(x)^2) = 2\gamma_k'(x)^2 + 2\gamma_k(x)\gamma_k''(x) \geq 4q_k^{-2} \frac{q^2 \log(q)}{(h + \theta(x))^2}, \quad 0 \leq \theta(x) \leq 1, \]
if \( q_k \leq q^{1/3} \).

By Taylor’s theorem we obtain with \( \theta_1(u), \theta_2(u) \in (0, 1) \),
\[ C_a = \int_0^{a/q} \gamma_k \left( \frac{a}{q} + u \right)^2 + \gamma_k \left( \frac{a}{q} - u \right)^2 - 2\gamma_k \left( \frac{a}{q} \right)^2 \, du 
\]
\[ = \int_0^{a/q} \frac{1}{2} \left( \frac{d^2}{dx^2} \left( \gamma_k \left( \frac{a}{q} + \theta_1(u) \right)^2 \right) + \frac{d^2}{dx^2} \left( \gamma_k \left( \frac{a}{q} - \theta_2(u) \right)^2 \right) \right) \, du 
\]
\[ \geq c_1 q_k^{-2} q^{-1} h^{-2} \log \left( \frac{q}{h} \right) \]
for \( q_k \leq q^{1/3} \) (where \( c_1 > 0 \) is an absolute constant).

We now investigate the contribution of the intervals \( I_a \subset c_{k,2} \). We assume that \( k \) is odd. The case \( k \) even is treated similarly.

Let \( r \) be a rational number of depth \( k \) in
\[ I_a = \left( \frac{a}{q}, \frac{a + 1}{q} \right). \]

We write
\[ r = \frac{a}{q} + \frac{1}{2q} + w_0, \quad w_0 \in \left( -\frac{1}{2q}, \frac{1}{2q} \right). \]

By Lemma \textbf{2.1} there is exactly one pair \( P_k \) of cells \( (C_1, C_2) \), \( C_1 \) of depth \( k \), \( C_2 \) of depth \( k + 1 \), such that \( r \) is a common endpoint of both, namely
\[ C_1 = C(b_1, \ldots, b_k) \quad \text{and} \quad C_2 = C(b_1, \ldots, b_k - 1, 2). \]

We combine the contributions of order \( k \) to \( I_a \) and of order \( k + 1 \) to \( I_{a+1} \), i.e. we consider
\[ C(a, k) := \int_{\frac{a}{q} + \frac{1}{2q} + w_0}^{\frac{a}{q} + \frac{1}{2q} + w_0 + v} \gamma_k(x)^2 - \gamma_k \left( \frac{a}{q} \right)^2 \, dx + \int_{\frac{a}{q} + \frac{1}{2q} + w_0}^{\frac{a}{q} + \frac{1}{2q} + w_0 + v} \gamma_{k+1}(x)^2 - \gamma_{k+1} \left( \frac{u + 1}{q} \right)^2 \, dx 
\]
\[ =: I(a, k, w_0). \]

and study \( I(a, k, w_0) \) as a function of \( w_0 \). We first treat the case \( w_0 = 0 \).

For \( u > 0 \) we write
\[ r - u = [b_1, \ldots, b_k + v] = [b_1, \ldots, b_k - 1, (1 + v)^{-1}] . \]

By Lemma \textbf{2.2} we obtain:
\[ \gamma_k(r - u) - \gamma_k \left( \frac{a}{q} \right) = \left( \gamma_{k+1}(r + u) - \gamma_{k+1} \left( \frac{a + 1}{q} \right) \right) (1 + O(q^{-1})). \]

We obtain
\[ I(a, k, 0) \geq c_2 q_k^{-2} q^{-1} \log q \]
A simple computation shows that
\[ \frac{d^2 I(a, k, w_0)}{dw_0^2} > 0. \]
Thus we also have:

\[(5.3) \quad C(a, k) \geq c_3q_k^{-2}q^{-1}\log q, \quad \text{for } q_k \leq q^{1/3}. \]

We still need a bound for the contribution of a cell, which is uniform in \( q_k \). The width of the cell of depth \( k \) with partial denominators \( q_k \) is \( O(1/q_k^2) \). From the bound

\[ \beta_k(x) \leq \frac{1}{q_k}, \]

we obtain

\[(5.4) \quad \int C \gamma_k(x)^2 dx = O(q_k^{-4}). \]

We now collect the estimates (5.2), (5.3), (5.4). Summing over \( h, p_k \) and \( q_k \) we obtain

\[(5.5) \quad \Sigma_1 \geq c_4q^{-1}(\log q)^2, \quad \text{for } K \text{ sufficiently large.} \]

6. Upper bound for the other sums

The estimate of the other sums is carried out with very similar methods. To estimate the sum \( \Sigma_2 \) - the most difficult case - we again collect pairs \( P_k \) of order \( k \) and estimate integrals

\[ \int_{-w_0}^{w_0} \gamma_k(r + v)(\gamma_k(r + v) - \gamma_{k+1}(r + v)) dv, \]

which arise from the alternating signs in (3.8). We obtain

\[(6.1) \quad \Sigma_i = o(q^{-1}(\log q)^2) \quad (i = 2, 3, 4). \]

Theorem 1.1 now follows from (5.4) and (6.1).

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