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LI’S CRITERION FOR THE RIEMANN HYPOTHESIS —
NUMERICAL APPROACH

Abstract. There has been some interest in a criterion for the Riemann hypothesis proved recently by Xian-Jin Li [9]. The present paper reports on a numerical computation of the first 3300 of Li’s coefficients which appear in this criterion. The main empirical observation is that these coefficients can be separated in two parts. One of these grows smoothly while the other is very small and oscillatory. This apparent smallness is quite unexpected. If it persisted till infinity then the Riemann hypothesis would be true.

Keywords: Riemann zeta function, Riemann hypothesis, Li’s criterion, numerical methods in analytic number theory.

Mathematics Subject Classification: 11M26, 11Y60.

1. INTRODUCTION

The distribution of prime numbers is an old problem in number theory. It is very easy to state but extremely hard to resolve, see Figure 1. In his famous paper written in 1859 Bernhard Riemann connected this problem with a function investigated earlier by Leonhard Euler. He also formulated certain hypothesis concerning the distribution of complex zeros of this function. At first this hypothesis appeared as a relatively simple analytical conjecture to be proved sooner rather than later. However, future development of the theory proved otherwise: since then the Riemann hypothesis (hereafter called RH) is commonly regarded as both the most challenging and the most difficult task in number theory [12]. It states that all complex zeros of the zeta function, defined by the following series if Re\(s\) > 1

\[
\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}
\]

(1)
and by analytic continuation to the whole plane, are located right on the critical line \( \text{Re} \ s = \frac{1}{2} \). RH, if true, would shed more light on our knowledge of the distribution of prime numbers. More precisely, the absence of zeroes of \( \zeta(s) \) in the half-plane \( \text{Re} \ s > \theta \) implies that (see [5], theorem 30)

\[
\pi(x) = \text{li}(x) + O(x^\theta \log x)
\]

where \( \pi(x) \) is the number of primes not exceeding \( x \) and \( \text{li}(x) \) denotes logarithmic integral. Therefore, the value \( \theta = \frac{1}{2} \) (as Riemann conjectured) makes the theorem useful since the error term in (2) is the smallest possible.

**Fig. 1.** The distribution of prime numbers can be most naturally described using function \( \pi(x) \) which gives the number of primes less than or equal to \( x \). The argument \( x \) can be any positive real number and \( \pi(1) \) gives 0. On small scales \( \pi(x) \) has apparently random-like behavior. On the basis of extensive empirical material two asymptotes of \( \pi(x) \) were independently and almost simultaneously discovered: \( \frac{x}{\log x} \) (A.-M. Legendre, lower smooth curve) and logarithmic integral: \( \text{li}(x) := \int_0^x \frac{dt}{\log t} \), \( x > 1 \) (C. F. Gauss, upper smooth curve)

2. **LI’S CRITERION**

In 1997 Xian-Jin Li [9] presented an interesting criterion equivalent to the Riemann hypothesis (see Fig. 2).
**Theorem 1.** RH is true if and only if all coefficients

$$\lambda_n := \frac{1}{\Gamma(n)} \frac{d^n}{ds^n} \left[ s^{n-1} \ln \xi(s) \right]_{s=1}$$

are non-negative, where

$$\xi(s) = 2(s-1)\pi^{-s/2}\Gamma\left(1 + \frac{s}{2}\right)\zeta(s).$$

![Graph](image-url)  

**Fig. 2.** Real and imaginary parts of the zeta-function of Riemann. Vertical lines denote 10 first complex zeros on the critical line \( \text{Re} \ z = \frac{1}{2} \).

An equivalent definition of \( \lambda_n \) is (see [9], formula 1.4):

$$\lambda_n = \sum_{\rho} \left( 1 - \left( 1 - \frac{1}{\rho} \right)^n \right)$$

where the sum runs over all (paired) complex zeros of the Riemann zeta-function. However, the above definitions of \( \lambda_n \) are not suitable for numerical calculations. It should be mentioned that we know only one exact value, namely \( \lambda_1 \) which may be expressed in closed form using mathematical constants:

$$\lambda_1 = \sum_{\rho} \frac{1}{\rho} = 1 + \frac{1}{2} \gamma - \frac{1}{2} \log 4\pi = 0.0234967 \ldots$$

The idea of relating Riemann Hypothesis to the rate of growth of certain sequences of real numbers is an old one. For example, in 1916 Marcel Riesz proved that RH is equivalent to the assertion that

$$\sum_{k=1}^{\infty} \frac{(-1)^{k+1}k^k}{(k-1)!\zeta(2k)} \ll x^{1/2+\epsilon}, \quad \epsilon > 0$$
The same idea, in its formulation very similar to Li’s approach, appeared also in 1992 in a little-known paper by Jerry Keiper in which he presented certain new and efficient method of calculating Stieltjes constants [6]. This method has been later implemented in Wolfram’s package Mathematica. Xian-Jin Li was clearly unaware of Keiper’s result. (Keiper tragically died in a bicycle accident in 1995.)

In the present paper I shall put forward an effective method for calculating coefficients introduced by Li. The gathered data investigated numerically up to $n = 3300$ reveals unexpected properties: it contains a strictly growing trend plus extremely small oscillations superimposed on this trend.

The following decomposition of $\lambda_n$ is already implicitly given in a recent paper by Bombieri and Lagarias ([2], Theorem 2):

\[
\lambda_n = 1 - \left( \log(4\pi) + \gamma \right) \frac{n}{2} + \sum_{j=2}^{n} (-1)^j \binom{n}{j} (1 - 2^{-j}) \zeta(j) \tag{6}
\]

\[
= - \sum_{j=1}^{n} \binom{n}{j} \eta_j - 1
\]

\[
\equiv \tilde{\lambda}_n + \lambda_n
\]

Using the language of signal theory (perhaps not very common but sometimes appropriate in number theory) one can say that the decomposition (6) uniquely “splits” the behavior of the sequence of $\{\lambda_n\}$ into a strictly growing trend $\tilde{\lambda}_n$ and certain tiny oscillations $\lambda_n$ superimposed on it. It may be proved that the trend can be expressed as

\[
\tilde{\lambda}_n = \frac{1}{\Gamma(n)} \frac{d^n}{ds^n} \left[ s^{n-1} \ln \left( \pi^{-s/2} \Gamma \left( 1 + \frac{s}{2} \right) \right) \right]_{s=1} \tag{7}
\]

It may also be proved that the trend is indeed strictly growing as $n$ tends to infinity. It is evident that (7) differs from the main definition (3) simply by replacing $\xi(s)$ by much simpler function: $\pi^{-s/2} \Gamma(1 + s/2)$. On the other hand, the oscillatory behavior of $\lambda_n$ is not so evident, nevertheless it may be investigated numerically. I shall return to this decomposition later.

The starting point of Li’s approach to RH is certain transformation of the complex plane into itself using the map $s \mapsto z = 1 - 1/s$ (which is a special case of Möbius transformation). Under this transformation the half-plane $\Re s > 1/2$ is mapped into the unit disk (with the critical line $\Re s = 1/2$ becoming the unit circle, see Figs. 3 and 4). This was Li’s original idea. However, he was inspired by studying A. Weil’s proof of RH for function fields over finite fields where the critical line is also transformed into a unit circle [10].
Fig. 3. Möbius transformation of the complex plane used by Li. The lower part is an image of the upper part under $s \mapsto z = 1 - 1/s$ in which the critical line is mapped into unit circle centered at the origin. (See text for details)

Fig. 4. Plot of $1/|\zeta(1/z)|$ on a small part of the transformed complex plane containing all nontrivial zeroes. Nontrivial zeroes are visible as sharp “pins”. The apparent lack of peaks in the center is an artifact. All complex zeroes are very crowded near $z = 1$ and the corresponding peaks are increasingly thinner.
3. THE MAIN DERIVATION

It has been known since medieval times that the harmonic series $\sum_{k=1}^{\infty} \frac{1}{k}$ diverges. This was proved long ago with the use of elementary methods by Nicole d'Oresme in the 14th century (in his work *Questiones super Geometriam Euclidis*), and, much later, independently, by Pietro Mengoli (in his book on arithmetic series *Novae quadraturae arithmeticae*, 1650) as well as, using yet another method, by the Bernoulli brothers.

A natural question emerges: how fast does this series diverge? It turns out that its divergence is “weak”, more precisely: logarithmic. The quantitative answer to this question implies the definition of the following famous number called the Euler–Mascheroni constant:

$$\gamma := \lim_{x \to \infty} \left( \sum_{k \leq x} \frac{1}{k} - \log x \right) = 0,5772156649 \ldots$$

(8)

Its natural generalization is the sequence $\gamma_n$ defined by

$$\gamma_n = \frac{(-1)^n}{n!} \lim_{x \to \infty} \left( \sum_{k \leq x} \frac{1}{k} (\log k)^n - \frac{(\log x)^{n+1}}{n+1} \right)$$

(9)

where $\gamma_0 = \gamma$. These are the so-called Stieltjes constants$^1)$. Another “similar” very useful sequence denoted by $\eta_n$ is defined by

$$\eta_n := \frac{(-1)^n}{n!} \lim_{x \to \infty} \left( \sum_{k \leq x} \frac{\Lambda(k)}{k} (\log k)^n - \frac{(\log x)^{n+1}}{n+1} \right),$$

(10)

where $\Lambda(k)$ is the so-called von Mangoldt function defined for any positive integer $k$ as:

$$\Lambda(k) = \begin{cases} \log p & \text{if } k \text{ is a prime } p \text{ or any power of a prime } p^n \\ 0 & \text{otherwise} \end{cases}$$

(11)

The von Mangoldt function is related to the Riemann zeta function $\zeta(s)$ by

$$\frac{\zeta'(s)}{\zeta(s)} = \sum_{n=1}^{\infty} \frac{\Lambda(n)}{n^s}$$

The above sequences (9) and (10) are important on their own right since they appear in the Laurent expansions for $\zeta(s)$ and its logarithmic derivative around

$^1)$ It should be noted that the function *StieltjesGamma*[n] implemented in Wolfram’s Mathematica, which employs Keiper’s algorithm [6], uses a different convention. It is related to our $\gamma_n$ via

$$\gamma_n = \frac{(-1)^n}{n!} \text{StieltjesGamma}[n]$$
There are different conventions in the literature when defining these numbers, here I have adopted those of Bombieri and Lagarias [2]:

\[ \zeta(s + 1) = \frac{1}{s} + \sum_{n=0}^{\infty} \gamma_n s^n \]  
(12) 

\[ -\frac{\zeta'}{\zeta}(s + 1) = \frac{1}{s} + \sum_{n=0}^{\infty} \eta_n s^n \]  
(13)

Integrating the second equation (13) with respect to \( s \), inserting the result into the first one and equating coefficients in the appropriate powers of the variable \( s \), one can find explicit relations between the \( \gamma_n \) and the \( \eta_n \):

\[ \sum_{n=0}^{\infty} \eta_n s^{n+1} = -\log \left( 1 + \sum_{n=0}^{\infty} \gamma_n s^{n+1} \right) \]  
(14)

\[ \sum_{n=0}^{\infty} \eta_n s^{n+1} = \sum_{k=1}^{\infty} \frac{(-1)^k}{k} s^k \left( \sum_{n=0}^{\infty} \gamma_n s^n \right)^k \]

Now introduce the coefficients \( c_n^{(k)} \) defined by

\[ \sum_{n=0}^{\infty} c_n^{(k)} s^n = \left( \sum_{n=0}^{\infty} \gamma_n s^n \right)^k \]

Employing a certain formula from [4] (formula 0.314, i.e., raising a power series to an arbitrary integral exponent) one can express the \( c \) coefficients by the following recurrence relations:

\[ c_0^{(k)} = \gamma^k \]  
(15)

\[ c_m^{(k)} = \frac{1}{m! \gamma} \sum_{i=0}^{m-1} [km - (k + 1)i] \gamma_m - c_i^{(k)} \]

The matrix of coefficients \( c \) depends on \( \{\gamma_n\} \):

\[
\begin{array}{cccccc}
  & m = 0 & m = 1 & m = 2 & m = 3 & m = 4 \\
  k = 1 & \gamma_0 & \gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 \\
  k = 2 & \gamma_0^2 & 2\gamma_0\gamma_1 & \gamma_1^2 + 2\gamma_0\gamma_2 & 2\gamma_1\gamma_2 + 2\gamma_0\gamma_3 & \ldots \\
  k = 3 & \gamma_0^3 & 3\gamma_0^2\gamma_1 & 3\gamma_0\gamma_1^2 + 3\gamma_0^2\gamma_2 & \ldots & \ldots \\
  k = 4 & \gamma_0^4 & 4\gamma_0^3\gamma_1 & \ldots & \ldots & \ldots \\
  k = 5 & \gamma_0^5 & \ldots & \ldots & \ldots & \ldots \\
\end{array}
\]  
(16)

(In what follows only the upper triangular part of this infinite matrix will be needed, see Fig. 5)
With the help of (14) the coefficients $\eta_n$ may further be expressed using the elements of the matrix $c$ as

$$\eta_n = (n+1) \sum_{k=0}^{n} \frac{(-1)^{k+1}}{k+1} c_{n-k}^{(k+1)}$$  \hspace{1cm} (17)

From this we have:

$$\eta_0 = -\gamma_0$$
$$\eta_1 = +\gamma_0^2 - 2\gamma_1$$
$$\eta_2 = -\gamma_0^3 + 3\gamma_0\gamma_1 - 3\gamma_2$$
$$\eta_3 = +\gamma_0^4 - 4\gamma_0^2\gamma_1 + 2\gamma_1^2 + 4\gamma_0\gamma_2 - 4\gamma_3$$
$$\eta_4 = -\gamma_0^5 + 5\gamma_0^3\gamma_1 - 5\gamma_0^2\gamma_1^2 - 5\gamma_0^2\gamma_2 + 5\gamma_1\gamma_2 + 5\gamma_0\gamma_3 - 5\gamma_4,$$

$$\ldots$$

Finally, the oscillating parts of $\lambda_n$ are expressible as polynomials in the Stieltjes constants:

$$\tilde{\lambda}_n = -\sum_{j=1}^{n} \binom{n}{j} \eta_{j-1}.$$  \hspace{1cm} (19)
Using now (18) and (19) we finally obtain:

\[ \tilde{\lambda}_1 = \gamma_0 \]
\[ \tilde{\lambda}_2 = 2\gamma_0 - \frac{\gamma_0^2}{2} + 2\gamma_1 \]
\[ \tilde{\lambda}_3 = 3\gamma_0 - 3\frac{\gamma_0^2}{2} + \gamma_0^3 + 6\gamma_1 - 3\gamma_0\gamma_1 + 3\gamma_2 \]
\[ \tilde{\lambda}_4 = 4\gamma_0 - 6\frac{\gamma_0^2}{2} + 4\gamma_0^3 - \gamma_0^4 - 12\gamma_1 + 12\gamma_0\gamma_1 + 4\gamma_0^2\gamma_1 - 2\gamma_1^2 + 12\gamma_2 - 4\gamma_0\gamma_2 + 4\gamma_3 \]

\[ \ldots \]

4. APPLICATIONS AND CONCLUSIONS

The recurrence formulae (15) together with (17) and (19) allow in principle to compute both \( \eta_n \) and \( \tilde{\lambda}_n \) with arbitrary accuracy for any value of \( n \), but it is clear that with increasing \( n \) the number of terms increases very rapidly\(^2\). It would be desirable to simplify the polynomials in (18) and (20), or at least to reveal some hidden regularities in them, but I doubt whether this is possible. The Table 1 demonstrates that it would be even impractical to write down explicit expressions for, say, \( \tilde{\lambda}_n \) for \( n \) greater than 15 or 20.

<table>
<thead>
<tr>
<th>( n )</th>
<th># of terms in ( \eta_n ) (eq. 18)</th>
<th># of terms in ( \tilde{\lambda}_n ) (eq. 20)</th>
</tr>
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<tr>
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<td>1</td>
<td>–</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>1</td>
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<td>2</td>
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</tr>
<tr>
<td>50</td>
<td>239943</td>
<td>1295970</td>
</tr>
</tbody>
</table>

\(^2\) Using the On-Line Encyclopedia of Integer Sequences (http://www.research.att.com/~njas/sequences/) one can see that number of terms in \( \eta_n \) is related to the number of partitions of \( n \) (partition number, \texttt{PartitionsP}[n] in \texttt{Mathematica} notation), which grows like \( \exp(\text{const}\sqrt{n}) \), whereas the number of terms in \( \tilde{\lambda}_n \) is equal to the number of sums \( S \) of positive integers satisfying \( S \leq n \) (\texttt{Sum[PartitionsP}[k], \{k,1,n\}] in \texttt{Mathematica} notation). Using conventions of the above mentioned \textit{Encyclopedia} the first is denoted by A000041 and the second by A026905.
Using the above formulae (15), (17) and (20) I have computed quite a lot of initial values of $\eta_n$ and $\lambda_n$. First it was necessary to tabulate Stieltjes constants $\gamma_n$ with sufficient number of significant digits. In order to obtain these I used Mathematica 5 which can handle arbitrary precision numbers and performs automatically full control of accuracy in numerical calculations. This part of computations took over 60 hours on a computer with AMD 1667 MHz processor.

The main calculations ($\eta_n$ and $\lambda_n$) were also time consuming (about 20 hours) and required considerable amount of computer memory (3×256 Mb). In particular, having 2000 pre-computed Stieltjes constants, with 800 significant digits each, I calculated 2000 $\eta_n$ and over 3300 $\lambda_n$.

The main conclusion which stems from the above calculations is contained in the following plots showing the trend of $\lambda$ (Fig. 6a) and the oscillating part of $\lambda$ (Fig. 6b). Their sum gives the coefficients which appear in Li’s criterion for RH. Note that the scales on both plots differ by nearly two orders of magnitude. As mentioned before, it is easy to show that the trend (7) is strictly growing. Therefore, if the oscillations were bounded or, at least, if their amplitude would grow with $n$ slower than the trend, then RH would be true. In other words, we have a new RH criterion, which is simply a reformulation the original Li’s result, but from the viewpoint of the present paper it has an obvious interpretation. It states that if for all positive integer $n$

$$-\tilde{\lambda}_n \leq \tilde{\lambda}_n$$

then RH is true.

The numerical data gathered so far and presented in Figures 6a and 6b is in its favor. Of course, one should bear in mind that in number theory the numerical evidence, no matter how “convincing”, may be just illusory. In fact, Oesterlé observed recently (in an unpublished note, [15]) that if the first $n$ complex zeros of zeta are located on the critical line, then the Li positivity criterion should hold for about the first $n^2$ Li coefficients (see [1], p. 441). Therefore, direct numerical search for a possible counterexample to RH using Li’s criterion is rather a hopeless task.

Finally I would like to stress out that so far there are no published extensive tables of Li’s coefficients. Several numerical values of $\lambda_n$ with small accuracy are given in [1]. All the numerical data obtained during preparation of this paper as well as appropriate Mathematica notebook are available from the author.

**Note added in proof.** The present paper, initially posted as preprint at e-Print archive http://arxiv.org [11], has since then motivated some further work, cf. [7] and [14]. In particular, Voros, using classic technique of saddle-point method, proved that the trend behaves asymptotically as

$$\tilde{\lambda}_n \sim \frac{1}{2} (1 + n \ln n) + cn$$

where

$$c = \frac{1}{2} (\gamma - 1 - \ln 2\pi).$$
Fig. 6. The trend of $\lambda_n$ (a) in comparison with the oscillating part of $\lambda_n$ (b). Note different vertical scales. In fact, the sum of the trend and the oscillating part, i.e. full $\lambda_n \equiv \lambda_n + \bar{\lambda}_n$, would look exactly like the upper plot since the amplitude of the oscillations is smaller than the thickness of the graph line.

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