EFFECTIVE METHOD OF COMPUTING LI’S COEFFICIENTS AND THEIR PROPERTIES

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Abstract. In this paper we present an effective method for computing certain real coefficients $\lambda_n$ which appear in a criterion for the Riemann hypothesis proved by Xian-Jin Li. With the use of this method a sequence of over three-thousand $\lambda_n$’s has been calculated. This sequence reveals a peculiar and unexpected behavior: it can be split into a strictly growing trend and some tiny oscillations superimposed on this trend.

1. Introduction

Since its formulation almost a century and a half ago the Riemann hypothesis (hereafter called RH) is commonly regarded as both the most challenging and the most difficult task in number theory [14]. It states that all complex zeroes of the zeta function, defined by the following series if $\Re s > 1$

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

and by analytic continuation to the whole plane, are located right on the critical line $\Re s = \frac{1}{2}$. 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 $\Re s > \theta$ implies that (see [6], theorem 30)

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

where $\pi(x)$ is the number of primes not exceeding $x$ and li($x$) denotes logarithmic integral. Therefore, the value $\theta = \frac{1}{2}$ (as Riemann conjectured) makes the theorem useful since the error term in (1.2) is the smallest possible. We do know that on the critical line lie infinitely many complex zeroes and that among several billions of initial zeroes there is no counterexample to RH, cf. [13], [17].

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2. Li’s Criterion

In 1997 Xian-Jin Li [10] presented an interesting criterion equivalent to the Riemann hypothesis:

**Theorem 2.1.** RH is true if and only if all coefficients

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

are non-negative, where

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

An equivalent definition of \( \lambda_n \) is (see [10], 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 zeroes of the Riemann zeta-function. However, the above definitions of \( \lambda_n \) are not suitable for numerical calculations. In this paper I shall present an effective method for calculating these coefficients. 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 implicitly given in a recent paper by Bombieri and Lagarias ([2], Theorem 2):

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

Using the language of signal theory (perhaps not very common but sometimes appropriate in number theory) one can say that the decomposition (2.4) uniquely “splits” the behavior of the sequence of \( \{\lambda_n\} \) into a strictly growing trend \( \bar{\lambda}_n \) and certain tiny oscillations \( \tilde{\lambda}_n \) superimposed on it. It may be proved that the trend can be expressed as

\[ \bar{\lambda}_n = \frac{1}{\Gamma(n)} \frac{d^n}{ds^n} \left[ s^{n-1} \ln \left( \pi^{-s/2} \Gamma \left( 1 + \frac{s}{2} \right) \zeta(s) \right) \right] \bigg|_{s=1} \]

while the oscillations are

\[ \tilde{\lambda}_n = \frac{1}{\Gamma(n)} \frac{d^n}{ds^n} \left[ s^{n-1} \ln \left( (s - 1) \zeta(s) \right) \right] \bigg|_{s=1} \]
It may also be proved that the trend is indeed strictly growing as \( n \) tends to infinity. It is evident that (2.5) differs from the main definition (2.1) simply by replacing \( \xi(s) \) by the much simpler function \( \pi^{-s/2}\Gamma(1+s/2) \). On the other hand, the oscillatory behavior of \( \sim \) is not so evident, nevertheless it may be investigated numerically. I shall return to this decomposition later.

The problem of calculating numerically both components of \( \lambda_n \) (i.e. trend and oscillations), using directly (2.5) and (2.6), is rather hopeless, not to say: malicious. One has to take the \( n^{th} \) derivatives of functions which depend of variable \( s \) and are labelled by parameter \( n \). When \( n \) tends to infinity both families of differentiated functions tend to right angle shaped figures and the derivatives are to be taken just at the almost singular point \( s = 1 \). What is interesting, the first derivative in \( s = 1 \) for all functions related to the oscillating part is the same and equal to the Euler constant.

However, it is possible to calculate several tens of initial derivatives using direct numerical approach, for example Mathametica’s ND built-in function. This function has several parameters which enable to control the required accuracy. One must be aware, however, that there is no guarantee that the result will be correct. As with all numerical techniques for evaluating the infinite via finite samplings, it is sometimes possible to "fool" ND into giving an incorrect result.

(Place Figure 2 about here.)

It turns out that the following function fits very well to the numerically tabulated values of (2.5):

\[
(2.7) \quad a(1 + n \ln n) + cn
\]

with

\[
a = \frac{1}{2} \pm 8 \cdot 10^{-9}
\]

\[
c = -1.130330701...
\]

(A choice very similar to (2.7) was suggested to me by J. Lagarias, [9].) Recently I learned that A. Voros [16] using classic technique of saddle-point method calculated the exact value of \( c \)

\[
c = \frac{1}{2} (\gamma - 1 - \ln 2\pi)
\]

where \( \gamma \) is Euler constant. Simple fitting procedure gives also coefficients of consecutive terms which appear to be related to Bernoulli numbers \( B_k \)

\[
(2.8) \quad -\sum_{k=1} B_k \frac{k^{k-1}}{2kn^{k-1}} = \frac{1}{4} - \frac{1}{24n} + \frac{1}{240n^3} - \frac{1}{504n^5} + \frac{1}{480n^7} - \ldots
\]

This series works well for a dozen or so initial terms although it is formally divergent.
The starting point of Li’s approach to RH is a 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 $\Re s > \frac{1}{2}$ is mapped into the unit disk (with the critical line $\Re s = \frac{1}{2}$ 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 transformed into a unit circle [11].

(Place Figures 3 and 4 about here.)

3. THE MAIN DERIVATION

It has been known since medieval times that the harmonic series $\sum_{k=1}^{\infty} 1/k$ diverges. This was proved long ago with the use of elementary methods by Nicole d’Oresme in the 14th century, 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:

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

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

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

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

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

\[\text{It should be noted that the function } \text{StieltjesGamma}[n] \text{ implemented in Wolfram’s Mathematica, which employs Keiper’s algorithm [7], uses a different convention. It is related to our } \gamma_n \text{ via}
\]

\[
\gamma_n = \frac{(-1)^n}{n!} \text{StieltjesGamma}[n]
\]
where $\Lambda(k)$ is the so-called von Mangoldt function defined for any positive integer $k$ as:

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

The above sequences are important on their own right since they appear in the Laurent expansions for $\zeta(s)$ and its logarithmic derivative around $s = 1$. (There are different conventions when defining these numbers, here I have adopted those of Bombieri and Lagarias [2]):

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

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

Integrating the second equation (3.6) 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 $\eta_n$:

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

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

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:

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

\[ c_m^{(k)} = \frac{1}{m^k \gamma} \sum_{i=0}^{m-1} [km - (k + 1) i] \gamma_{m-i} c_i^{(k)} \]
The matrix of coefficients \( c \) depends on \( \{ \gamma_n \} \):

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

(In what follows only the upper triangular part of this infinite matrix will be needed.)

(Place Figure 5 about here.)

With the help of (3.7) the coefficients \( \eta_n \) may further be expressed using the elements of the matrix \( c \) as

\[
(3.10) \quad \eta_n = (n + 1) \sum_{k=0}^{n} \frac{(-1)^{k+1}}{k+1} c_{n-k}^{(k+1)}
\]

From this we have:

\[
(3.11) \quad \eta_0 = -\gamma_0 \\
\eta_1 = +\gamma_0^2 - 2\gamma_1 \\
\eta_2 = -\gamma_0^3 + 3\gamma_0\gamma_1 - 3\gamma_2 \\
\eta_3 = +\gamma_0^4 - 4\gamma_0^2\gamma_1 + 2\gamma_1^2 + 4\gamma_0\gamma_2 - 4\gamma_3 \\
\eta_4 = -\gamma_0^5 + 5\gamma_0^3\gamma_1 - 5\gamma_0\gamma_1^2 - 5\gamma_0^2\gamma_2 + 5\gamma_1\gamma_2 + 5\gamma_0\gamma_3 - 5\gamma_4, \\
\]

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

\[
(3.12) \quad \tilde{\lambda}_n = -\sum_{j=1}^{n} \binom{n}{j} \eta_{j-1}.
\]

Using now (3.11) and (3.12) we finally obtain:

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

......
Here are some numerical values of various numbers used in this paper:

| $n$ | $\gamma_n$ | $\eta_n$ | $\tilde{\lambda}_n$ | $\lambda_n$ |
|-----|-------------|-----------|----------------------|------------|
| 0   | +0.577215664902 | -0.577215664902 | - | - |
| 1   | -0.0728158454837 | +0.187546232840 | 0.577215664902 | 0.0230957089661 |
| 2   | -0.00969036319287 | -0.0516886320332 | 0.96688096963 | 0.0923457352280 |
| 3   | +0.002357096547 | -0.00452447788850 | 1.37558813187 | 0.207638920554 |
| 4   | +0.00793323817301 | +0.0144679520453 | 1.458268956963 | 0.0923457352280 |
| 5   | -0.000238769345430 | -0.000471544078185 | 1.48829832721 | 0.827566012282 |
| 6   | -0.000527869345430 | +0.00144679520453 | 1.48019084024 | 1.1246011757 |
| 7   | -0.000527289567058 | +0.00155180294164 | 1.4829832721 | 1.827566012282 |
| 8   | -0.000352123353803 | +0.00144679520453 | 1.48485574412 | 2.07638920554 |
| 9   | +0.000793323817301 | +0.0144679520453 | 1.48829832721 | 2.57557667715 |
| 10  | +0.000205332814909 | +0.00144679520453 | 1.48829832721 | 2.57557667715 |
| 11  | -0.000205332814909 | +0.00144679520453 | 1.48829832721 | 2.57557667715 |
| 12  | -0.000027463806638 | +0.00144679520453 | 1.48829832721 | 2.57557667715 |
| 13  | -0.000027463806638 | +0.00144679520453 | 1.48829832721 | 2.57557667715 |
| 14  | -0.000205332814909 | +0.00144679520453 | 1.48829832721 | 2.57557667715 |
| 15  | -0.000205332814909 | +0.00144679520453 | 1.48829832721 | 2.57557667715 |
| 16  | -0.000205332814909 | +0.00144679520453 | 1.48829832721 | 2.57557667715 |
| 17  | -0.000205332814909 | +0.00144679520453 | 1.48829832721 | 2.57557667715 |
| 18  | -0.000205332814909 | +0.00144679520453 | 1.48829832721 | 2.57557667715 |
| 19  | -0.000205332814909 | +0.00144679520453 | 1.48829832721 | 2.57557667715 |
| 20  | -0.000205332814909 | +0.00144679520453 | 1.48829832721 | 2.57557667715 |

4. APPLICATIONS AND CONCLUSIONS

The recurrence formulae (3.8) together with (3.10) and (3.12) 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 (3.11) and (3.13), or at least to reveal some hidden regularities in them, but I doubt whether this is possible. The table below demonstrates that it would be even impractical to write down explicit expressions for, say, $\tilde{\lambda}_n$ for $n$ greater than 15 or 20.

\(^2\)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(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 the above formulae (3.8), (3.10) and (3.13) 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. (For details concerning Mathematica interval arithmetic see e.g. [12]). This part of computations took over 60 hours on AMD 1667 MHz processor.

Recently Kreminski [8] published an effective method of computing Stieltjes gamma using Newton-Cotes integration algorithm. His method would be of considerable interest since, due to some "hardcoded" limitations, the current Mathematica version can’t give $\gamma_n$ (with sufficient accuracy) beyond $n \approx 2050$.

The main calculations ($\eta_n$ and $\lambda_n$) were also time consuming (about 20 hours) and required also considerable amount of computer memory ($3 \times 256$ Mb). In particular, having 2000 pre-computed Stieltjes constants, with 800 significant digits each, I calculated 2000 $\eta_n$ and almost 3300 $\lambda_n$. Due to finite accuracy and the obvious phenomenon of error accumulation, the number of significant digits in $\eta_n$ and $\lambda_n$ decreases with increasing $n$ (see Fig. 6).

In order to verify the computations as well as to compare various packages I also tried to repeat the whole procedure using Maple 8. However, it turned out that it is impossible to get Stieltjes constants $\gamma_n$ for relatively small $n = 100$ with the required precision 800 significant digits.

(Place Figure 6 about here.)

The main conclusion which stems from the above calculations is contained in the following plots showing the trend of $\lambda$ (Fig. 7a) and the oscillating part of $\lambda$ (Fig. 7b). 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 \( (2.5) \) 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 \( n \)

\[
-\tilde{\lambda}_n \leq \lambda_n
\]

then RH is true. The numerical data gathered so far and presented in Figures 7a and 7b 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 that if the first \( n \) zeta zeros are on the critical line, then the Li positivity 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 \( \lambda_n \) 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.

\( \text{(Place Figures 7a and 7b about here.)} \)

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Note added in proof. After completing the calculations I become aware of the paper by Keiper [7]. His Figure 1 looks similar to Figure 7b of the present paper. However it is not exactly the same, insofar as he is subtracting off an approximation to the ”main term”. But presumably the error is a constant plus \( O(1/n) \) term, in view of my asymptotic series approximation \( (2.8) \), so it must be pretty close.

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Figure captions

- Figure 1. Distribution of zeroes of $\zeta$ in the complex plane.
- Figure 2. Understanding the Li’s lambda: inevitable difficulties encountered when calculating numerically both parts of $\lambda_n$. The sequence of consecutive derivatives is to be taken near $s = 0$.
- Figure 3. Möbius transformation of the complex plane used by Li. The left fragment of the picture is just Fig. 1 reduced to its essential part: the critical strip. The half-plane $\Re s > \frac{1}{2}$ (left picture) is mapped into the unit disk $|z| < 1$ (right picture).
- Figure 4. Plot of $1/|\zeta(\frac{1}{1-z})|$ on a small part of the transformed complex plane containing all nontrivial zeroes. On the right fragment of Fig. 2 this part of complex plane is a small, very narrow rectangle near $z = 1$. Nontrivial zeroes are visible as sharp “pins”. White dots are added to help visualize that the zeroes indeed lie on a circle (which looks rather like an ellipse here since the scales on $\Re z$ and $\Im z$ are different). 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. Obtaining a better picture would require much higher density of points in which values of zeta are calculated (hence more computer memory) and much higher resolution of the picture.
• Figure 5. Signs of the coefficients of matrix $c$ (3.8) for $k = 100$ with rows and columns labelled as in (3.9). Little white squares denote plus sign, black squares denote minus sign; grey squares mark unused entries of the matrix.

• Figure 6. Accuracies of various numbers used in this paper: $\gamma_n$, $\eta_n$ and $\tilde{\lambda}_n$. Having 2000 precomputed Stieltjes constants $\gamma_n$, with 800 significant digits each, I could (using Mathematica 5) obtain 2000 coefficients $\eta_n$ and about 3300 oscillating parts of lambda, $\tilde{\lambda}_n$, both with linearly decreasing accuracy. The accuracies of $\eta_n$ and $\tilde{\lambda}_n$ decrease with $n$ due to complicated error cumulating but almost perfect linearity of their dependence is a priori not so obvious because the number of terms in (3.11) and (3.13) grows fast with increasing $n$. In particular, the fact that the accuracy of $\eta_n$ decreases faster than accuracy of $\tilde{\lambda}_n$ is rather counter intuitive.

• Figures 7a and 7b. The trend of $\lambda_n$ (7a) in comparison with the oscillating part of $\lambda_n$ (7b). Note different vertical scales. In fact, the sum of the trend and the oscillating part, i.e. full $\lambda_n$, 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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Figure 1.
Figure 2.
Figure 3
Figure 4.
