Math 56: Computational and Experimental Math

Final project

Computation of Riemann ζ function

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Contents

1 Riemann ζ function and its properties

1.1 Definition

The Riemann Zeta function $\zeta(s)$ is the analytic function defined by

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \prod_{p \in \mathcal{P}} \frac{1}{1 - \frac{1}{p^s}} \tag{1}$$

for $\mathrm{Re}\,(s) > 1$ and by analytic continuation for all $s \in \mathbb{C}, s \neq 1$.

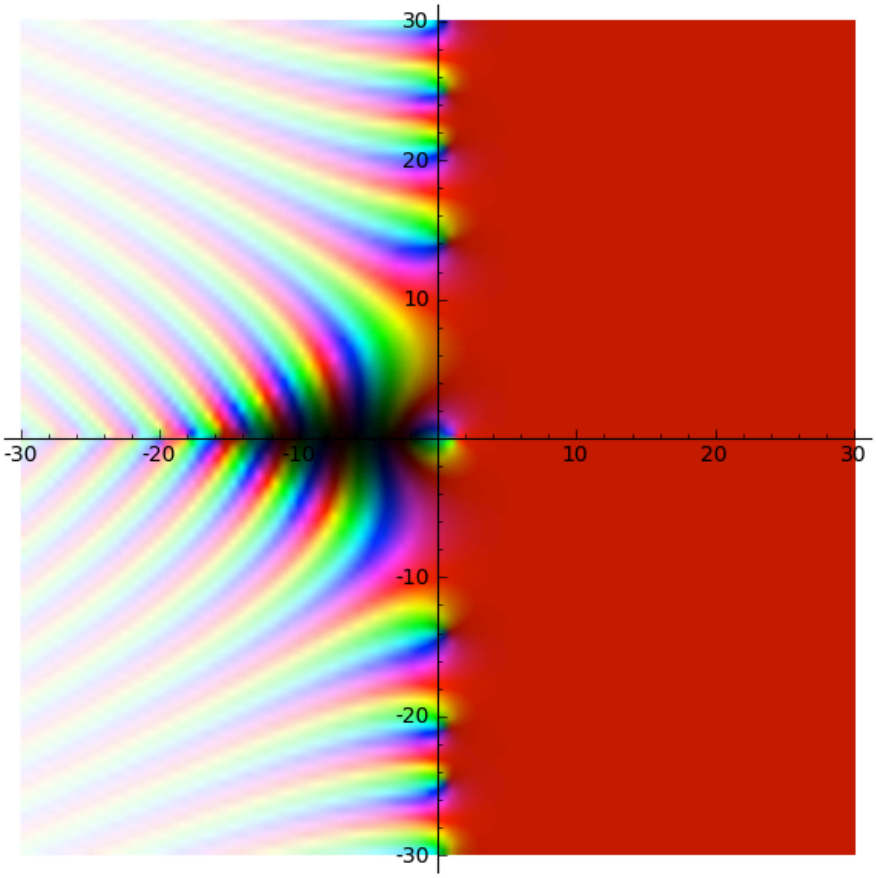

Figure 1.1: Riemann ζ function: $\{\zeta(a + bi) : -30 \leq a, b \leq 30\}$

The magnitude of the output is indicated by the brightness (with zero being black and infinity being white), and the argument is represented by the hue (with red being positive real, and increasing through orange, yellow, . . . as the argument increases).

Riemann himself, however, does not speak of the analytic continuation of ζ beyond the halfplane $\mathrm{Re}\,(s) > 1$, but instead defines ζ by the formula

$$\zeta(s) = \frac{\Gamma(1-s)}{2\pi i} \oint_{\gamma} \frac{x^{s-1}}{e^{-x} - 1} dx \tag{2}$$

where Γ is an analytic extension of factorial function with simple poles at negative integers, and γ is a contour starting and ending at $+\infty$ and wrapping around the origin once.

1.2 Functional equation and the function ξ

The Riemann ζ function satifies the functional equation

$$\zeta(s) = 2^s \pi^{s-1} \sin\left(\frac{\pi s}{2}\right) \Gamma(1-s)\zeta(1-s) \tag{3}$$

Riemann defines a variant of ζ function:

$$\xi(s) = \frac{1}{2} s(s-1)\pi^{-\frac{s}{2}}\Gamma\left(\frac{s}{2}\right)\zeta(s) \tag{4}$$

The function ξ is an entire function on the complex plane, and the functional equation is equivalent to

$$\xi(s) = \xi(1-s) \tag{5}$$

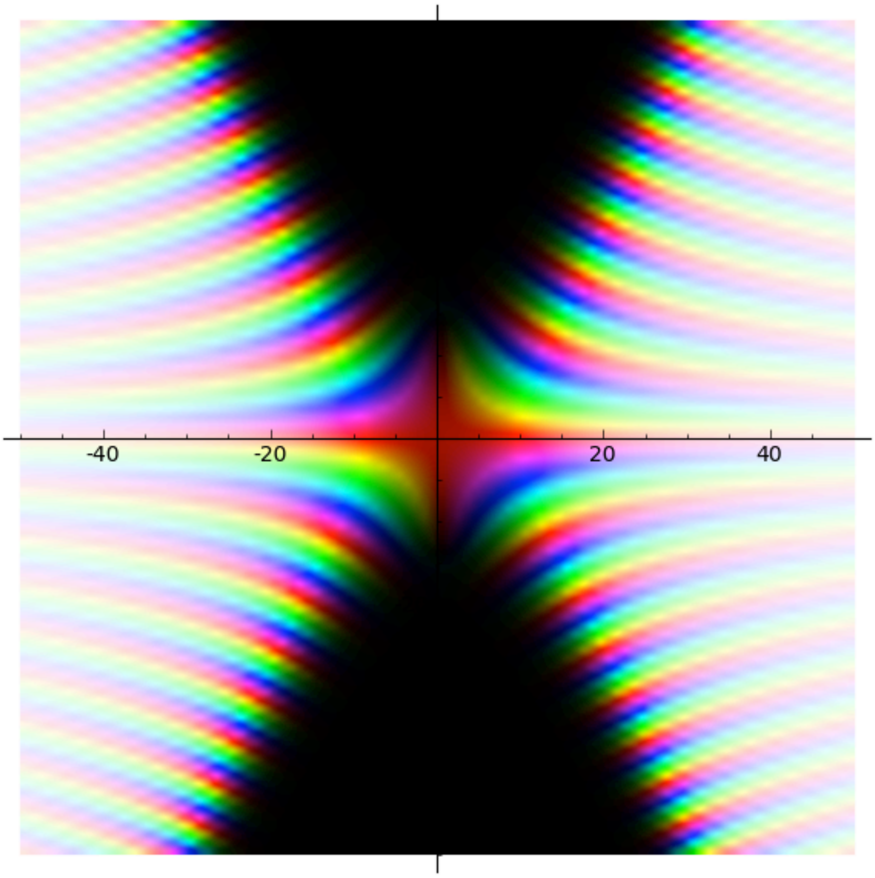

Figure 1.2: Riemann ξ function: $\{\xi(a+bi) : -50 \leq a, b \leq 50\}$

1.3 Riemann Hypothesis

The Riemann ζ function has two types of zeros: even negative integers – see the functional equation (3) – usually refered to as the trivial zeros, and non-trivial complex zeros. It is proved that any non-trivial zero lies in the open strip $\{s \in \mathbb{C} : 0 < \text{Re}\ (s) < 1\}$, called the *critical strip*.

Riemann hypothesis: All the complex zeros of the function ζ lie in the line $\{s \in C : \text{Re}\ (s) = \frac{1}{2}\}$, called the critical line.

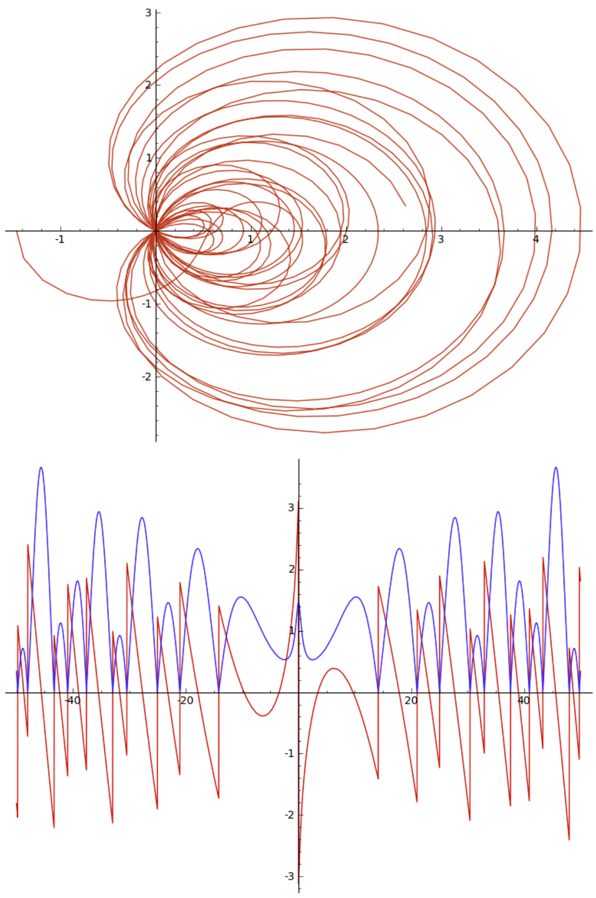

Figure 1.3: $\zeta\left(\frac{1}{2} + it\right)$: [1] Re and Im , [2] norm and phase

Proposed by Riemann in 1859, Riemann hypothesis has remained unresolved and is considered by many mathematicians to be the most important problem in pure mathematics. It is part of Hilbert's eighth problem and also one of the Clay Mathematics Institute Millennium Problems. Since the very beginning of $20th$ century, many computational efforts have taken place to support Riemann hypothesis. In the next sections, we will discuss different computational methods and how they have been used to investigate Riemann ζ function and its roots.

2 Computational Methods

In this report, we focus on two schemes to evaluate ζ function: Euler-Maclaurin summation, which is used for general value $s \in \mathbb{C}$, and Riemann Siegel formula, which is used to approximate ζ more efficiently on the critical line.

2.1 Euler-Maclaurin Summation

Euler-Maclaurin summation is a powerful tool, which can be used to evaluate integrals by finite sums, or conversely infinite series by integrals.

$$\sum_{n=M}^{N} f(n) = \int_{M}^{N} f(x)dx - B_1(f(N) + f(M)) + \sum_{k=1}^{\infty} \frac{B_{2k}}{(2k)!}(f^{(2k-1)'}(N) - f^{(2k-1)'}(M))$$

where B_k is the k-th Bernouli number.

Directly applying Euler-Maclaurin summation to evaluate $\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}$ yields large remainders; however, the series $\sum_{n=N}^{\infty} \frac{1}{n^s}$ can be approximated reasonably well by Euler-Maclaurin summation. This scheme to evaluate $\zeta(s)$ as following:

$$\begin{aligned}\sum_{n=1}^{\infty} n^{-s} &= \sum_{n=1}^{N-1} n^{-s} + \sum_{n=N}^{\infty} n^{-s} \\ &= \sum_{n=1}^{N-1} n^{-s} + \frac{N^{1-s}}{s-1} + \frac{N^{-s}}{2} + \sum_{k=1}^{\nu} \frac{B_{2k}}{(2k)!} \left(\prod_{j=0}^{2k-2} (s+j) \right) N^{-s-2k+1} + R_{N,\nu}\end{aligned}$$

where $R_{N,\nu}$ is the error tern bounded by:

$$R_{N,\nu} \leq \left| \frac{s+2\nu+1}{\text{Re }(s)+2\nu+1} \right| \left| \frac{B_{2\nu+2}}{(2\nu+2)!} \left(\prod_{j=0}^{2\nu} (s+j) \right) N^{-s-2\nu-1} \right| \qquad (6)$$

It follows from (6) that to obtain a given precision, N has to be of order $O(|s|)$.

I implement `zetaEMS(s,N,v)` in Sage, using built-in library for Bernoulli constants, to evluate $\zeta(s)$ with truncated N-term sum and ν Bernoulli terms. The error of `zetaEMS` is evaluated by cross-checking with the multiprecision built-in ζ function in `mpmath` package.

Figure 2.1 shows the linear relationship between N and $|s|$ for any given precision: each gray-level error lines up in a straight line in the $T-N$ plane.

Despite its runtime, EMS works consistently for every value of $s \in \mathbb{C}, s \neq 1$, and is used in standard algorithm for arbitrary precision computation of ζ in major symbolic algebra packages such as Maple, Mathematica, and Pari.

```
def zetaEMS(s,N,v):
    sum = 0
    for j in range(1,N):
        sum = sum + j**(-s)

    sum = sum + N**(1-s)/(s-1) + N**(-s)/2

    sprod = s
    fact = 1
    Npower = N**(1-s)
    for k in range(1,v):
        b = bernoulli(2*k)
        fact = fact*(2*k-1)*2*k
        Npower = Npower/(N**2)
        sum = sum + b/fact*sprod*Npower
        sprod = sprod*(s+2*k-1)*(s+2*k)
    return sum
```

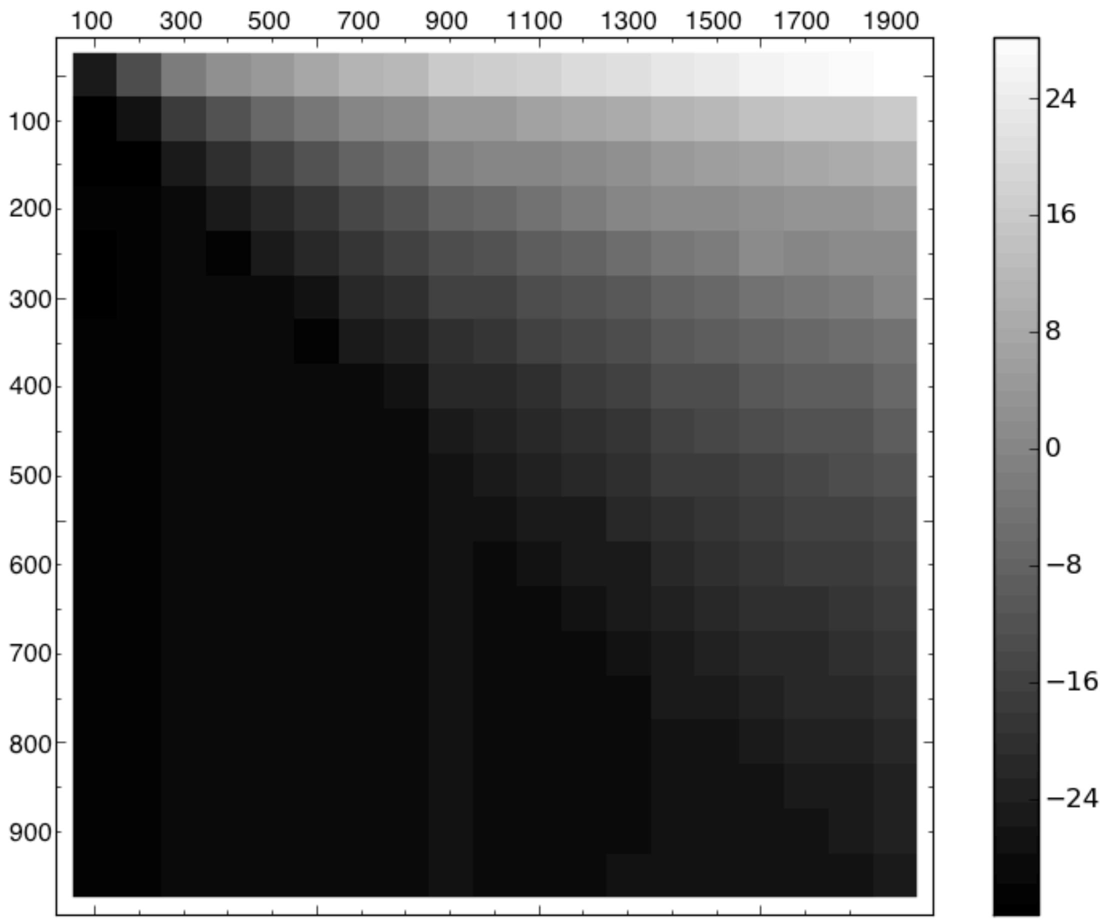

Figure 2.1: Error by EMS in estimating $\zeta(0.3 + iT)$ fixing $\nu = 10$
Horizontal axis – T Vertical axis – N

2.2 Riemann Siegel Formula

An important part of evaluation of ζ is along the critical line. The Riemann Siegel method involes estimates of the Rieman Siegel Z-function, which is defined as

$$Z(t) = e^{i\theta(t)}\zeta\left(\frac{1}{2} + it\right) \tag{7}$$

where θ is the Riemann-Siegel θ function:

$$\theta(t) = \arg\left(\Gamma\left(\frac{2it+1}{4}\right)\right) - \frac{\log\pi}{2}t \tag{8}$$

Both $Z(t)$ and $\theta(t)$ can be estimated relatively fast, which yields an efficient algorithm to calculate ζ on the critical line.

Riemann-Siegel θ function has an asymtotic expansion

$$\theta(t) = \frac{t}{2}\log\frac{t}{2\pi} - \frac{t}{2} - \frac{\pi}{8} + \frac{1}{48t} + \frac{7}{5760t^3} + \dots$$

which is not convergent, but the terms decrease very rapidly for t at all large.

Let $\tau = \frac{t}{2\pi}$, $m = \lfloor \tau^{1/2} \rfloor$ and $z = 2(\tau^{1/2} - m) - 1$, then

$$Z(t) = \sum_{k=1}^{m} 2k^{-1/2}\cos[\theta(t) - t\log k] + (-1)^{m+1}\tau^{-1/4}\sum_{j=0}^{n}\Phi_j(z)(-1)^j\tau^{-j/2} + R_n(\tau).$$

where Φ_j are entire functions which may be expressed in terms of derivatives of

$$\begin{aligned}
\Phi_0(z) = \Phi(z) &= \frac{\cos\left(\frac{(4z^2+3)\pi}{8}\right)}{\cos(\pi z)} \\
\Phi_1(z) &= \frac{\Phi^{(3)}(z)}{12\pi^2} \\
\Phi_2(z) &= \frac{\Phi^{(2)}(z)}{16\pi^2} + \frac{\Phi^{(6)}(z)}{288\pi^4}
\end{aligned}$$

The error term $R_n(\tau)$ is bounded above by $O\left(\tau^{-(2n+3)/4}\right)$. Typically, mathematicians have chosen $n = 2$, and use some conservative bound for their calculation. For example, Brent used $|R_2(\tau)| < 3\tau^{-7/4}$ for $\tau > 2000$.

3 General scheme to investigate Riemann's hypothesis by computation

Even though Riemann hypothesis remains unproved, many computational efforts have yielded strong evidences supporting it. Let $\{\rho_n\}$ be the list of zeros of ζ sorted in ascending order with respect to Im (ρ), and let $H(n)$ be the statement that the first n roots are on the critical line. As of 2004, $H(n)$ has been confirmed for $n = 10^{13}$.

3.1 Techniques for locating roots on the line

Roots of ζ on the line $\{s \in C : \text{Re}\ (s) = \frac{1}{2}\}$ is found via the Riemann-Siegel Z-function defined in (7). Because Riemann-Siegel Z function is real-valued on the line Re $(s) = \frac{1}{2}$, its number of zeros can be counted by the number of changes sign.

Gram's law:
For $n \in \mathbb{Z}^+$, the nth Gram point g_n is the solution of the equation $\theta(t) = n\pi$. Gram's law is the tendency of the zeros of Z to alternate with the Gram point g_n.

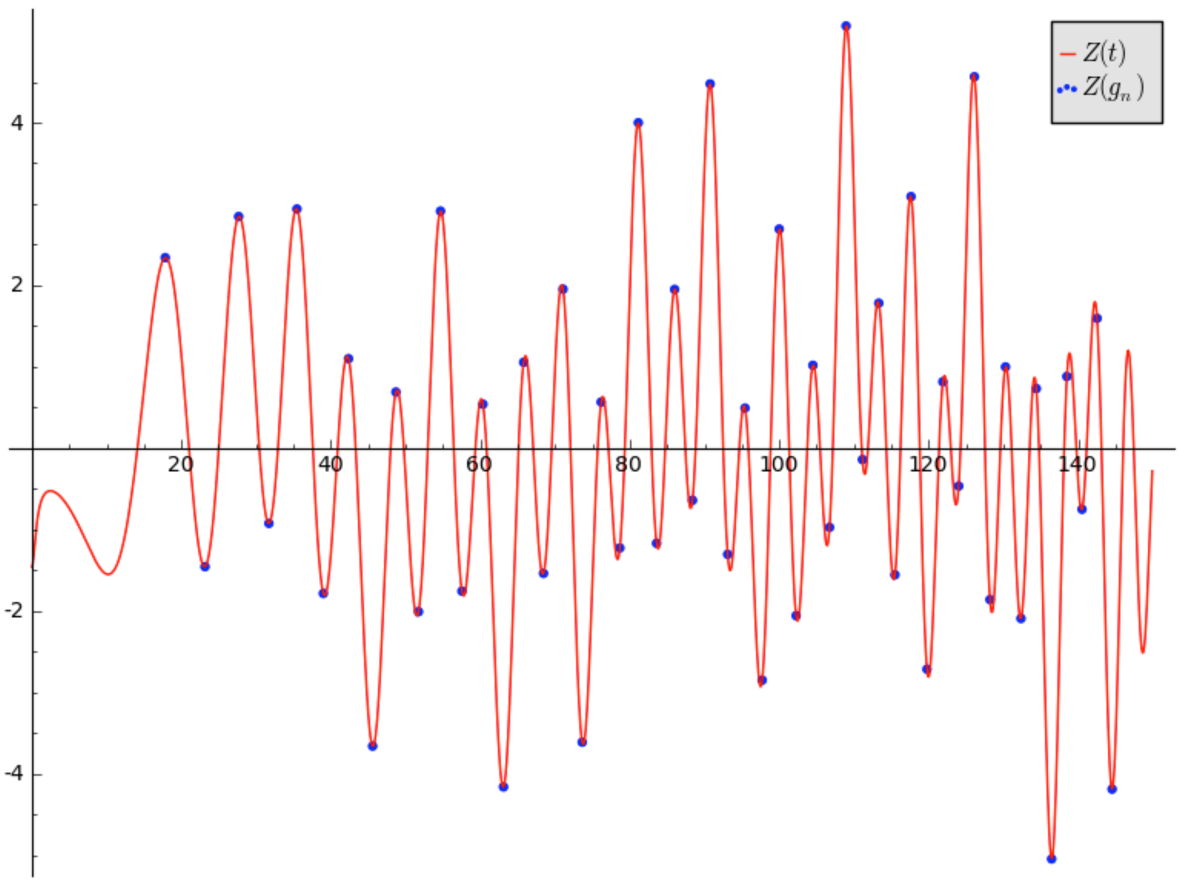

Figure 3.1: Riemann Siegel $Z(t)$'s tendency to change sign with Gram points

Even though Gram's law fails for infinitely many g_n, it provides a helpful starting points for finding roots of Z.

3.2 Techniques for counting the number of roots in given range

In order to count the number of roots of the ζ function, we turn to the entire function ξ defined in equation (4). Let $N(T)$ be the number of roots of ζ such that $0 < \text{Im } s < T$, then $N(T)$ is also the number of roots of ξ in the same portion of the critical strip. Therefore,

$$N(T) = \frac{1}{2\pi i} \int_{\delta R} \frac{\xi'(s)}{\xi(s)} ds \tag{9}$$

where R is the rectangle $\{-\epsilon \leq \text{Re } s \leq 1+\epsilon, 0 \leq \text{Im } s \leq T\}$ and δR its boundary, assuming that there are no roots of ξ on the line Im $s = T$.
By symmetry of ξ given by the functional equation and the fact that $\xi(s) \in \mathbb{R}$ for $s \in \mathbb{R}$, we can write

$$N(T) = \frac{1}{2\pi} \cdot 2 \text{ Im } \left[\int_C \frac{\xi'(s)}{\xi(s)} ds\right] = \frac{\theta(T)}{\pi} + 1 + \frac{1}{\pi} \text{Im } \int_\gamma \frac{\zeta'(s)}{\zeta(s)} ds \tag{10}$$

where γ is the path from $1+\epsilon$ to $\frac{1}{2} + Ti$. Equation (10) allows us to evaluate $N(T)$ accurately as $N(T) \in \mathbb{Z}^+$.

An alternative method is to bound $N(T)$ using the following result. We call a Gram point g_j *good* if $(-1)^j g_j > 0$, and *bad* otherwise. A *Gram block of length k* is an interval $[g_j, g_{j+k})$ such that g_j and g_{j+k} are good and $g_{j+1}, \ldots, g_{j+k-1}$ are bad.

Littlewood-Turing Theorem:
Define $S(T) = N(t) - 1 - \theta(t)/\pi$. If $A = 0.114, B = 1.71, C = 168\pi$ and $C < u < v$, then

$$\left|\int_u^v S(t)dt\right| < A \ln(v) + B$$

If $A = 0.114, B = 1.71, C = 168\pi$ and $C < u < v$, then

$$\left|\int_u^v S(t)dt < A \ln(v) + B\right|$$

Consequently, if K consecutive Gram blocks with union $[g_n, g_p)$ satisfy Rosser's rule, where $K \geq 0.0061(\ln(g_p))^2 + 0.08 \ln(g_p)$, then $N(g_n) \leq n+1$ and $N(g_p) \geq p+1$.

3.3 History of Calculation

The following table shows the achievement of computational methods to verify Riemann hypothesis, proving $H(n)$ is true for $n = 10^{13}$.

Year	n	Author
1903	15	J. P. Gram
1914	79	R. J. Backlund
1925	138	J. I. Hutchinson
1935	1 041	E. C. Titchmarsh
1953	1 104	A. M. Turing
1956	15 000	D. H. Lehmer
1956	25 000	D. H. Lehmer
1958	35 337	N. A. Meller
1966	250 000	R. S. Lehman
1968	3 500 000	J. B. Rosser, J. M. Yohe, L. Schoenfeld
1977	40 000 000	R. P. Brent
1979	81 000 001	R. P. Brent
1982	200 000 001	R. P. Brent, J. van de Lune, H. J. J. te Riele, D. T. Winter
1983	300 000 001	J. van de Lune, H. J. J. te Riele
1986	1 500 000 001	J. van de Lune, H. J. J. te Riele, D. T. Winter
2001	10 000 000 000	J. van de Lune (unpublished)
2004	900 000 000 000	S. Wedeniwski
2004	10 000 000 000 000	X. Gourdon and P. Demichel

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