Calculating zeros of the Riemann zeta function

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Introduction

Let $s = \sigma + it$. Then the Riemann zeta function is defined by [Tit+86; Ivi13]

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \prod_p \left(1 - \frac{1}{p^s}\right)^{-1}, \quad \text{for } \sigma > 1.$$

By analytic continuation we can extend the Riemann zeta function to the whole complex plane with a simple pole at $s = 1$. The zeta function satisfies the functional equation

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

From the definition and functional equation, it is straightforward to compute $\zeta(s)$ for $\sigma > 1$ or $\sigma < 0$.

Euler Product Formula

The zeta function we have defined encodes a lot about the primes. In particular, the zeta function admits a product formula which is essentially an analytical statement of the fundamental theorem of arithmetic. This product formula, known as the Euler product of $\zeta(s)$ is given by

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \prod_{p} \left(1 - \frac{1}{p^s}\right)^{-1}, \quad \mathrm{Re}(s) > 1, \tag{1}$$

where the product is over all primes p. It is useful to verify (1), so we sketch two brief proofs.

Euler Product Formula

Suppose M and N are positive integers such that $M > N$. Every $n \leq N$ can be uniquely written as a product of primes. These primes are obviously $\leq N$, and cannot occur more than M times in the product. So, it follows that every term in the left of the following inequality shall also be in the right of the inequality. That is,

$$\sum_{n=1}^{N} \frac{1}{n^s} \leq \prod_{p \leq N} \left(1 + \frac{1}{p^s} + \frac{1}{p^{2s}} + \cdots + \frac{1}{p^{Ms}}\right).$$

Taking first $M \to \infty$ forms

$$\sum_{n=1}^{N} \frac{1}{n^s} \leq \prod_{p} \left(\frac{1}{1 - p^{-s}}\right).$$

Euler Product Formula

Then taking $N \to \infty$ gives

$$\sum_{n=1}^{\infty} \frac{1}{n^s} \leq \prod_{p} \left(\frac{1}{1 - p^{-s}} \right).$$

For the reverse inequality, observe that if we consider all products of primes such that each prime is $\leq N$ and does not occur more than M times, we shall get finitely many distinct integers. Hence

$$\prod_{p \leq N} \left(1 + \frac{1}{p^s} + \frac{1}{p^{2s}} + \cdots + \frac{1}{p^{Ms}} \right) \leq \sum_{n=1}^{N} \frac{1}{n^s}.$$

Euler Product Formula

Again taking $N \to \infty$ followed by $M \to \infty$ forms

$$\prod_p \left(\frac{1}{1 - p^{-s}} \right) \leq \sum_{n=1}^{\infty} \frac{1}{n^s},$$

so that (1) follows from the two inequalities. Another way to verify (1) (discovered by Euler) uses ideas similar to the Sieve of Eratosthenes. Start by writing

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

Then

$$\zeta(s) \frac{1}{2^s} = \sum_{n=1}^{\infty} \frac{1}{n^s} \frac{1}{2^s} = \sum_{n=1}^{\infty} \frac{1}{(2n)^s},$$

$$\zeta(s) - \zeta(s) \frac{1}{2^s} = \sum_{n=1}^{\infty} \frac{1}{n^s} - \sum_{n=1}^{\infty} \frac{1}{(2n)^s}.$$

Euler Product Formula

Therefore

$$\zeta(s)\left(1-\frac{1}{2^s}\right)=\sum_{\substack{n=1\\n\neq 2k}}^{\infty}\frac{1}{n^s}.$$

Repeating the same procedure gives

$$\zeta(s)\left(1-\frac{1}{2^s}\right)\frac{1}{3^s}=\sum_{\substack{n=1\\n\neq 2k}}^{\infty}\frac{1}{n^s}\frac{1}{3^s}=\sum_{\substack{n=1\\n\neq 2k}}^{\infty}\frac{1}{(3n)^s},$$

$$\zeta(s)\left(1-\frac{1}{2^s}\right)\left(1-\frac{1}{3^s}\right)=\sum_{\substack{n=1\\n\neq 2k\\n\neq 3k}}^{\infty}\frac{1}{n^s}.$$

Euler Product Formula

Continuing for every prime

$$\zeta(s)\left(1-\frac{1}{2^s}\right)\left(1-\frac{1}{3^s}\right)\left(1-\frac{1}{5^s}\right)\dots=\sum_{\substack{n=1\\ n\neq 2k\\ n\neq 3k\\ n\neq 5k\\ \dots}}^{\infty}\frac{1}{n^s}.$$

Hence we see that

$$\zeta(s)\left(1-\frac{1}{2^s}\right)\left(1-\frac{1}{3^s}\right)\left(1-\frac{1}{5^s}\right)\dots=1,$$

$$\zeta(s)=\frac{1}{\left(1-\frac{1}{2^s}\right)\left(1-\frac{1}{3^s}\right)\left(1-\frac{1}{5^s}\right)\dots}=\prod_p\left(\frac{1}{1-p^{-s}}\right).$$

If $\text{Re}(s)>1$ then the right-hand side of the sieve approaches 1 and convergence follows from the convergence of the Dirichlet series for $\zeta(s)$.

Trivial zeros

Suppose $s = -2k$ where k is a positive integer. Then we write the zeta function as

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

and observe that

$$\begin{aligned} \zeta(-2k) &= 2^{-2k}\pi^{-2k-1} \sin\left(-\pi k\right) 2k! \zeta(1+2k) \\ &= -2^{-2k}\pi^{-2k-1} \sin\left(\pi k\right) 2k! \zeta(1+2k) \\ &= 0. \end{aligned}$$

Therefore $\zeta(-2k) = 0$ where k is a positive integer. These are known as "trivial zeros" and are uninteresting. We are interested in locating the non-trivial zeros in the critical strip where $0 < \sigma < 1$.

The Critical Strip

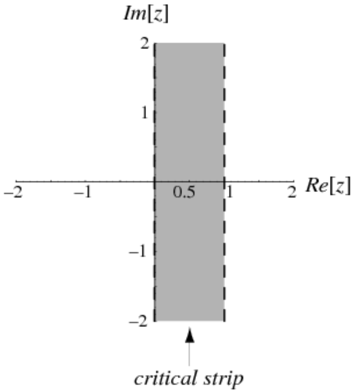


Figure 1: The region $0 < \sigma < 1$ where $\sigma = \mathrm{Re}(s)$ for $s = \sigma + it$. It is known that all nontrivial zeros (excluding negative even integers) lie inside this strip. Furthermore, it is also known that the non-trivial zeros are symmetric about the real axis and the critical line $\sigma = 1/2$.

The Critical Line

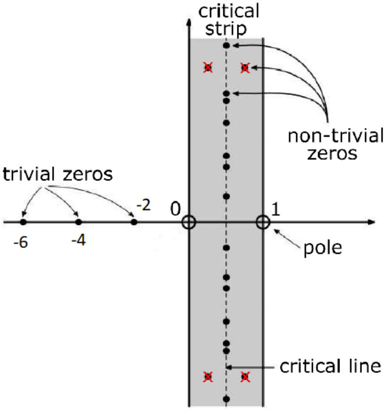


Figure 2: The critical line where $\text{Re}(s) = \frac{1}{2}$ for $s = \sigma + it$. For $0 < \sigma < 1$, the Riemann hypothesis states that the zeta function does not have any non-trivial zeros lying off the critical line. These "invalid zeros" are crossed out in the figure.

Bernhard Riemann

Figure 3: Photo of Bernhard Riemann in 1863. Riemann published a paper in 1859 [Rie59] which first introduced the Riemann hypothesis. He was a student of Carl Friedrich Gauss who was interested in the distribution of prime numbers.

The Riemann Hypothesis

Riemann makes his famous conjecture.

Conjecture (Riemann Hypothesis)

Let $s = \sigma + it$. *Then* $Re(s) = 1/2$ *for every nontrivial zero of the Riemann zeta function.*

If the conjecture is true then every nontrivial zero in the critical strip $0 < \sigma < 1$ lies on the critical line consisting of the complex numbers $\frac{1}{2} + it$.

Hardy's Theorem

G. H. Hardy then finds a lot of zeros on the critical line.

Theorem (Hardy, 1915)

There are infinitely many nontrivial zeros on the critical line where $Re(s) = 1/2$.

Methods to Find Zeros

There are three common techniques used to find nontrivial zeros of the Riemann zeta function. They are the

1. Euler-Maclaurin Summation Formula
2. Riemann–Siegel Formula
3. Odlyzko–Schönhage Algorithm

More modern techniques expand upon ideas presented in these three methods.

Setup of Euler-Maclaurin Summation Formula

Suppose that f and its derivative are continuous functions on the closed interval $[a, b]$. Let

$$\psi(x) = \{x\} - \frac{1}{2},$$

where $\{x\} = x - [x]$ is the fractional part of x.

Lemma 1

If $a < b$ and $a, b \in \mathbb{Z}$, then

$$\sum_{a \leq n \leq b} f(n) = \int_a^b (f(x) + \psi(x) f'(x))\, dx + \frac{1}{2}(f(b) - f(a)).$$

The proof of Lemma 1 follows from the Abel partial summation formula.

Bernoulli Polynomials

We define Bernoulli polynomials by the following three properties

$$B_0(x) = 1,$$

$$B_k'(x) = kB_{k-1}(x), \quad k = 1, 2, \dots \, ,$$

$$\int_0^1 B_k(x)\, dx = 0, \quad k = 1, 2, \dots \, .$$

To determine the polynomials we introduce a generating function

$$F(t, x) = \sum_{k=0}^{\infty} B_k(x) \frac{t^k}{k!}.$$

Bernoulli Polynomials

Using this generating function we can find the first few Bernoulli polynomials:

$$
\begin{aligned}
B_0(x) &= 1, \\
B_1(x) &= x - \frac{1}{2}, \\
B_2(x) &= x^2 - x + \frac{1}{6}, \\
B_3(x) &= x^3 - \frac{3}{2}x^2 + \frac{1}{2}x, \\
B_4(x) &= x^4 - 2x^3 + x^2 - \frac{1}{30}, \\
B_5(x) &= x^5 - \frac{5}{2}x^4 + \frac{5}{3}x^3 - \frac{1}{6}x, \\
B_6(x) &= x^6 - 3x^5 + \frac{5}{2}x^4 - \frac{1}{2}x^2 + \frac{1}{42}.
\end{aligned}
$$

Bernoulli Numbers

The Bernoulli numbers are defined by

$$B_n = B_n(0),$$

that is, the value of the Bernoulli polynomial at $x = 0$. The generating function for the Bernoulli numbers is

$$F(t) := \sum_{n \geq 0} B_k \frac{t^k}{k!} = \frac{t}{e^t - 1}.$$

It is straightforward to verify $F(-t) = F(t) + t$ so that $F(-t) - F(t) = t$. The last equality implies $B_{2k+1} = 0$ for $k = 1, 2, \ldots$.

The function $\psi_k(x)$

Define

$$\psi_k(x) = B_k(\{x\})$$

where $\{x\} = x - [x]$ is the fractional part of x. Observe that

$$\psi(x) = \psi_1(x) = \{x\} - \frac{1}{2},$$

as in Lemma 1. Since $\{x\}$ is periodic with a period 1, so too are the functions $\psi_k(x)$ and they have the generating function

$$\sum_{k\geq 0} \psi_k(x) \frac{t^k}{k!} = \frac{te^{t\{x\}}}{e^t - 1}.$$

Setup of Euler-Maclaurin Summation Formula

We now assume that f is twice continuously differentiable in $[a, b]$. Applying integration by parts to the term $\psi = \psi_1$ in Lemma 1 yields

Lemma 2

Let f be twice continuously differentiable on $[a, b]$ where $a < b$ and $a, b \in \mathbb{Z}$. Then

$$\sum_{a \le n \le b} f(n) = \int_a^b \left\{ f(x) - \frac{1}{2}\psi_2(x) f''(x) \right\} dx + \sum_{\ell=1}^{2} \frac{(-1)^\ell}{\ell!} (f^{\ell-1}(b) - f^{\ell-1}(a)) B_\ell .$$

Repeating this process and integrating by parts k times gives the Euler-Maclaurin summation formula.

Method 1: Euler-Maclaurin Summation Formula

Theorem (Euler-Maclaurin Summation Formula)

Suppose f is k-times continuously differentiable on the interval $[a, b]$ with $a < b$, $a, b \in \mathbb{Z}$. Then

$$\sum_{a<n\leq b} f(n) = \int_a^b \left\{ f(x) - \frac{(-1)^k}{k!}\psi_k(x) f^{(k)}(x) \right\} dx + \sum_{\ell=1}^{k} \frac{(-1)^\ell}{\ell!} \left(f^{(\ell-1)}(b) - f^{(\ell-1)}(a) \right) B_\ell.$$

Method 1: Euler-Maclaurin Summation Formula

Theorem (Euler-Maclaurin Summation Formula (continued))

Suppose f and all its derivatives go to zero as $x \to \infty$. Then we obtain by letting $b \to \infty$ (and adding $f(a)$ to both sides)

$$\sum_{n=a}^{\infty} f(n) = \int_a^{\infty} f(x)\,dx + \frac{1}{2}f(a) - \sum_{\ell=2}^{k} \frac{(-1)^{\ell}}{\ell!} f^{(\ell-1)}(a)B_{\ell} - \frac{(-1)^k}{k!}\int_a^{\infty} f^{(k)}(x)\psi_k(x)\,dx. \tag{2}$$

Here

$$B_n = B_n(0)$$

are the *Bernoulli numbers* and are the value of the Bernoulli polynomial at $x = 0$.

Analytic Continuation

To see how this applies to the Riemann zeta function, let $s = \sigma + it$ where σ is the real part of s and t is the imaginary part of s. For $\sigma > 1$ we define the Riemann zeta function as

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}, \quad \mathrm{Re}(s) > 1. \tag{3}$$

The series converges absolutely and uniformly in the half-plane $\sigma = \mathrm{Re}(s) \geq 1 + \varepsilon$ for small $\varepsilon > 0$. We then observe that

$$\left|n^{-s}\right| = \left|n^{-\sigma - it}\right| = n^{-\sigma} \leq n^{-1-\varepsilon}.$$

Now apply the Weiestrass M-test to the series

$$\sum_{n=1}^{\infty} \frac{1}{n^{1+\varepsilon}},$$

which is convergent for all $\varepsilon > 0$. The series (3) diverges at $s = 1$.

Analytic Continuation

Then apply the Euler-Maclaurin summation formula (2) with $k = 1$ to (3). Choosing $f(x) = 1/x^s$, we observe that for $Re(s) > 1$

$$\int_1^\infty \frac{1}{x^s}\,dx = \frac{1}{s-1}.$$

The summation formula then becomes

$$\zeta(s) = \frac{1}{s-1} + \frac{1}{2} - s\int_1^\infty \frac{1}{x^{s+1}}\psi_1(x)\,dx,$$

where we once again assume $\sigma > 1$. We then observe that if we write

$$\zeta(s) - \frac{1}{s-1} = \frac{1}{2} - s\int_1^\infty \frac{1}{x^{s+1}}\psi_1(x)\,dx, \tag{4}$$

then the right-hand side of the above equation defines a holomorphic function for $\sigma > 0$.

Analytic Continuation

This follows from bounding the integral on the right-hand side by

$$\left| \int_1^\infty \frac{1}{x^{s+1}} \psi_1(x)\, dx \right| \leq \int_1^\infty \frac{1}{x^{\sigma+1}}\, dx < \infty, \tag{4}$$

since $|\psi_1(x)| \leq 1/2$. We now use the *right-hand side* (4) to define the left-hand side of (4) for $0 < \sigma \leq 1$. The two sides agree for $\sigma > 1$. This is an example of *analytic continuation*. We have made sense out of the Riemann zeta function for $\text{Re}(s) > 0$. We see that it has a simple pole at $s = 1$ and is holomorphic for all other points $\text{Re}(s) > 0$.

If we apply the Euler-Maclaurin summation formula (2) to (3) for an arbitrary positive integer k and do a lot of computation we obtain

$$\zeta(s) = \frac{1}{s-1} + \frac{1}{2} + \sum_{\ell=2}^{k} \frac{B_\ell}{\ell!} s(s+1)\cdots(s+\ell-2) -$$
$$\frac{(-1)^k}{k!} \int_1^\infty s(s+1)\cdots(s+k-1) x^{-s-k} \psi_k(x)\, dx$$

As ψ_k is 1-periodic and equal to the polynomial $B_k(x)$ on $[0,1)$, $\psi_k(x)$ is a bounded function on all of $\mathbb{R}$. Thus the integral on the right-hand side is convergent for all $\sigma + k > 1$ and thus defines a holomorphic function for $\sigma > 1 - k$. By repeating the above argument we see that we have analytically continued the Riemann zeta function to the right-half plane $\sigma > 1 - k$, for all $k = 1, 2, 3, \ldots$. We summarize our findings as

Analytic Continuation

Theorem (Analytic Continuation)

The Riemann zeta function $\zeta(s)$ *defined by* (3) *for* $Re(s) > 1$ *can be analytically continued to* $\mathbb{C} \setminus \{1\}$ *where it is holomorphic and at* $s = 1$, $\zeta(s)$ *has a simple pole.*

Euler-Maclaurin Formula

It is more practical to choose a number N [BH16] and write

$$\zeta(s) = \sum_{1}^{N} \frac{1}{n^s} + \int_{N}^{\infty} \frac{1}{y^s} \lfloor dy \rfloor = \sum_{1}^{N} \frac{1}{n^s} + s \int_{N}^{\infty} \frac{\{y\}}{y^{s+1}} + c(N) \frac{s}{1-s},$$

which converges for $\sigma > 0$ by analytical continuation.

If we choose N properly then $\zeta(s) - \sum_{1}^{N} \frac{1}{n^s}$ won't be too large and we can compute the difference through the Euler-Maclaurin summation formula. It requires $O(t)$. Thankfully, the other methods are faster.

The Functional Equation of $\zeta(s)$

The functional equation of the Riemann zeta function is

$$\zeta(s) = \Pi(-s)(2\pi)^{s-1} 2 \sin\left(\frac{\pi s}{2}\right) \zeta(1-s). \tag{5}$$

Riemann derived this from the familiar

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \prod_p (1 - p^{-s})^{-1},$$

which is valid for $\mathrm{Re}(s) > 1$. Using contour integration (i.e., Cauchy's theorem) he was able to extend $\zeta(s)$ to all points $s \in \mathbb{C} \setminus \{1\}$.

The Function $\xi(s)$

Let $s \in \mathbb{R}$ and $s > 1$. We define

$$\Pi(s-1) := \int_0^\infty e^{-x} x^{s-1}\, dx, \quad s > 1,$$

where $\Pi(s-1)$ is used in place of the more familiar $\Gamma(s)$. Then define the function $\xi(s)$ by

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

The $(s-1)$ term in the ξ-function eliminates the simple pole of $\zeta(s)$ as $s = 1$ so that $\xi(s)$ is an entire function. By the functional equation (5) for the zeta function we see that

$$\xi(s) = \xi(s-1).$$

The Function $\xi(s)$

An important fact about $\xi(s)$ is that it is real when s lies on the line $1/2 + it$, $t \in \mathbb{R}$, (the set of points called the *critical line*). This can be deduced as follows:

For $s \in \mathbb{R}$, $\xi(s) \in \mathbb{R}$. By the Schwartz reflection principle, $\overline{\xi(\overline{s})} = \xi(s)$, so that $\xi(\overline{s}) = \overline{\xi(s)}$. If $s = 1/2 + it$, $t \in \mathbb{R}$, we may then use the functional equation (5) to write

$$\xi(1/2 + it) = \xi(1 - (1/2 + it)) = \xi(\overline{1/2 + it}) = \overline{\xi(1/2 + it)}.$$

Therefore locating roots on the critical line reduces to locating sign changes of $\xi(1/2 + it)$. We then observe

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

The Function $\xi(s)$

Substituting $s = 1/2 + it$ yields

$$\xi\left(\frac{1}{2}+it\right) = \left(e^{\mathrm{Re}\left[\log \Pi\left(\frac{it}{2}-\frac{3}{4}\right)\right]}\pi^{-1/4}\frac{-t^2-1/4}{2}\right)\times$$
$$\left(e^{i\cdot \mathrm{Im}\left[\log \Pi\left(\frac{it}{2}-\frac{3}{4}\right)\right]}\pi^{-it/2}\zeta\left(\frac{1}{2}+it\right)\right).$$

The point is that the first term is always negative, so sign changes in $\xi(1/2+it)$ correspond to sign changes in the second term. The second term is denoted $Z(t)$ and is called the Riemann-Siegel Z function.

Method 2: Riemann–Siegel Formula

Another prominent mathematician named Carl Siegel worked on computing zeros in the critical strip. Painstakingly going through Riemann's notes, he defined the Z function (around 1932) as

$$Z(t) := e^{i\theta(t)}\zeta(1/2 + it),$$

where

$$\theta(t) = \operatorname{Im}\left(\log \Pi\left(\frac{it}{2} - \frac{3}{4}\right)\right) - \frac{t}{2}\log\pi = \arg\left(\Pi\left(\frac{it}{2} - \frac{3}{4}\right)\right) - \frac{t}{2}\log\pi.$$

The Riemann-Siegel formula is an approximation formula for $Z(t)$. Once $Z(t)$ is known, a straightforward approximation of $\theta(t)$ can be used to compute $\zeta(s)$.

The Z function is important because $Z(t)$ is real when t is real and it has the same absolute value as $\zeta(1/2 + it)$. $Z(t)$ has sign changes at zeros on the critical line where $s = 1/2 + it$, so it can be used to locate zeros.

Method 2: Riemann–Siegel Formula

The function $\theta(t)$ is known as the Riemann–Siegel theta function and is defined in terms of the Π function as

$$\theta(t) := \arg\left(\Pi\left(\frac{it}{2} - \frac{3}{4}\right)\right) - \frac{t}{2}\log\pi,$$

for real values of t. The argument is chosen so that a continuous function is obtained and $\theta(0) = 0$ holds, analogously to the way that the principal branch of the log-gamma function is defined. It has an asymptotic expansion

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

which doesn't converge, but whose first few terms give a good approximation for $t \gg 1$.

Riemann-Siegel Z Function

The Riemann-Siegel Z function is purely real and the equality $|Z(t)| = |\zeta(1/2 + it)|$ holds. So we can think of the Z function as a kind of real-valued version of the Riemann zeta function on the critical strip. We will use Gram points to locate zeros of the Z function (and therefore zeros of the Riemann zeta function on the critical line).

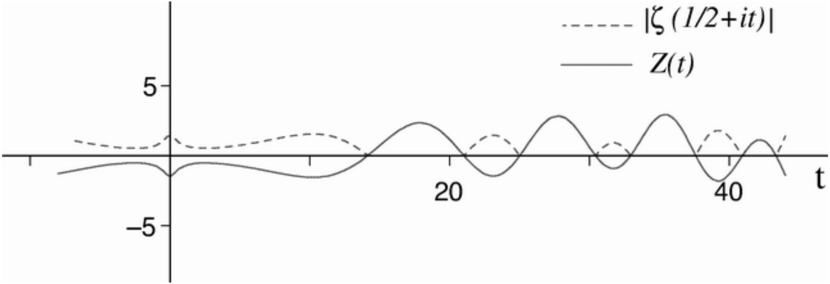


Figure 4: The Riemann-Siegel Z function for small values of t near 0. In dashed, the value of $|\zeta(1/2 + it)|$.

Riemann-Siegel Z Function

Glossing over some of the fine points, Siegel was able to show that we can rewrite the Z function as

$$Z(t) = 2 \sum_{n^2 < t/2\pi} n^{-1/2} \cos\left(\theta(t) - t \log n\right) + R_t,$$

where the remainder R_t is

$$R(t) \sim (-1)^{N-1} \left(\frac{t}{2\pi}\right)^{-1/4} \times \left[C_0 + C_1 \left(\frac{t}{2\pi}\right)^{-1/2} + C_2 \left(\frac{t}{2\pi}\right)^{-2/2} + C_3 \left(\frac{t}{2\pi}\right)^{-3/2} + C_4 \left(\frac{t}{2\pi}\right)^{-4/2} \right].$$

Most computer implementations of Riemann-Siegel are designed to calculate a combination of C_0, C_1, C_2, C_3, and C_4.

Through a bit more analysis, we find

$$C_0 = \Psi(p) = \frac{\cos 2\pi(p^2 - p - 1/16)}{\cos 2\pi p},$$

and set $N = \left\lfloor \frac{t}{2\pi} \right\rfloor^{1/2}$ and $p = \left(\frac{t}{2\pi}\right)^{1/2} - \left\lfloor \frac{t}{2\pi} \right\rfloor^{1/2}$. This gives

$$C_1 = -\frac{\Psi^3(p)}{96\pi^2}, \quad C_2 = \frac{\Psi^2(p)}{64\pi^2} + \frac{\Psi^6(p)}{18432\pi^4},$$

$$C_3 = -\frac{\Psi'(p)}{64\pi^2} - \frac{\psi^5(p)}{3840\pi^4} - \frac{\Psi^9(p)}{5308416\pi^6},$$

$$C_4 = \frac{\Psi(p)}{128\pi^2} + \frac{19\Psi^4(p)}{24576\pi^4} + \frac{11\Psi^8(p)}{5898240\pi^6} + \frac{\Psi^{12}(p)}{2038431744\pi^8}.$$

Zeros of the zeta function

The Z function and the coefficients C_0, C_1, C_2, C_3, and C_4 from the remainder term allow us to find nontrivial zeros of the Riemann zeta function. Writing $\rho = \frac{1}{2} + i\alpha_j$, the first 12 nontrivial zeros are

$$\alpha_1 = 14.134725142, \quad \alpha_2 = 21.022039639, \quad \alpha_3 = 25.010857580,$$

$$\alpha_4 = 30.424876126, \quad \alpha_5 = 32.935061588, \quad \alpha_6 = 37.586178159,$$

$$\alpha_7 = 40.918719012, \quad \alpha_8 = 43.327073281, \quad \alpha_9 = 48.005150881,$$

$$\alpha_{10} = 49.7738324781, \quad \alpha_{11} = 52.970321478, \quad \alpha_{12} = 56.446247697.$$

All of these roots are where $Z(t)$ changes sign. A paper from Haselgrove [Fle61] (in the 1960s) makes finding the coefficients easier (to be discussed later with code).

Gram's Law

Definition: Gram's law is a direct observation that zeros of the Riemann-Siegel $Z(t)$ function tend to alternate between what are known as Gram points. Gram predicted that that there is exactly one zero of the zeta function between any two Gram points.

This is not an actual law and can be shown to fail indefinitely. Recall that Siegel defined the Z function as

$$Z(t) = e^{i\theta(t)}\zeta(1/2 + it).$$

Therefore

$$\zeta(1/2 + it) = e^{-i\theta(t)}Z(t),$$

and by Euler's identity $e^{i\theta} = \cos(\theta) + i\sin(\theta)$, the equation can be divided into

$$\zeta(1/2 + it) = \cos(\theta(t))Z(t) - i\sin(\theta(t))Z(t).$$

Gram's Law

Provided $t \in \mathbb{R}$, the equation can be further simplified to

$$\text{Re } \zeta(1/2 + it) = \cos(\theta(t))Z(t).$$

Therefore a zero of a real value of the zeta function on the critical line is directly related to both $\cos(\theta(t))$ and $Z(t)$. Alternatively, we see that $\text{Im } \zeta(1/2 + it) = -i \sin(\theta(t))Z(t)$ which implies that a sign change of $\text{Im } \zeta(s)$ corresponds to a sign change of either $Z(t)$ or $\sin(\theta(t))$.

Therefore, one can think of the Riemann-Siegel formula as a direct relationship between a sign change of $Z(t)$ and a root where $\text{Re}(s) = 1/2$. Further analysis shows that $\text{Re } \zeta(1/2 + it)$ is generally positive while $\text{Im } \zeta(1/2 + it)$ alternates between positive and negative values.

Gram Points

So the zeros of $Z(t)$ tend to alternate with the zeros of $\sin(\theta(t))$. This is known as Gram's law. A Gram point is a point on the critical line $1/2 + it$ where the zeta function is real and non-zero. We know that $\sin(\theta(t))$ is zero at integer multiples of π. Positive values of t where this occurs are known as Gram points. Matching Gram's notation, we replace the t in the Riemann-Siegel theta function $\theta(t)$ by g_n so that a Gram point occurs where

$$\theta(\mathrm{g}_n) = n\pi, \quad \text{for all } n \geq -1.$$

It can then be shown that

$$\zeta\left(\frac{1}{2} + i\mathrm{g}_n\right) = \cos(\theta(\mathrm{g}_n))Z(\mathrm{g}_n) = (-1)^n Z(\mathrm{g}_n),$$

where

$$(-1)^n Z(\mathrm{g}_n) > 0$$

Gram Block

if and only if g_n is a Gram point. All the points where $(-1)^n Z(g_n) > 0$ are "good" and all the points where $(-1)^n Z(g_n) \leq 0$ are "bad." A process to handle the bad points uses what is known as a Gram block. A Gram block is an interval $g_n \leq t \leq g_{n+k}$ in which

$$g_n \text{ and } g_{n+k} \text{ are good}$$

but

$$g_{n+1}, g_{n+2}, g_{n+3}, \cdots, g_{n+k-1}$$

are bad. The total number of Gram points, both good and bad, give the number of zeros of $Z(t)$ in the interval $0 \leq t \leq g_n$. To find the number of roots on the critical line we can count the number of Graham points where Gram's law is satisfied. We can then count the number of zeros of $Z(t)$ in each Gram block.

Number of Roots up to Height T

Once we find all of the roots on the critical line up to some height T (using Gram blocks or a different technique), we need to verify that these are all the roots in the critical strip up to this height.

Let $N(T)$ denote the number of roots of $\zeta(\sigma + it)$ in the region $0 < \rho < 1$ and $0 \leq \tau \leq T$. We would like to have a method of evaluating $N(T)$ in order to verify the result of our root finding algorithm based on Gram's law. A method that is widely used was developed by A. Turing and is based on results by J. Littlewood and R. Backlund.

Number of Roots up to Height T

Riemann found that

$$N(T) = \frac{1}{2\pi i} \int_C \frac{\xi'(s)}{\xi(s)} \, ds,$$

where C is the contour

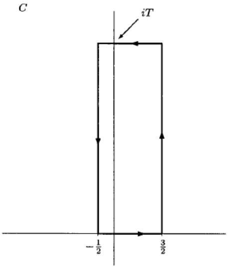


Figure 5: The contour C created by Riemann.

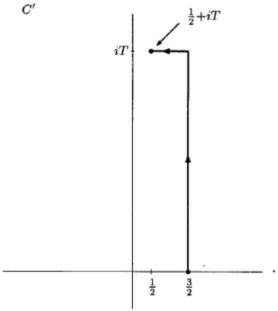
provided that there are no zeros of ξ on the contour itself.

Number of Roots up to Height T

This can be verified through the Residue theorem and the fact that ξ is entire. Using properties of $\xi(s)$ and the functional equation, we can write

$$N(T) = \frac{1}{\pi}\theta(T) + 1 + \frac{1}{\pi}\text{Im}\left(\int_{C'} \frac{\zeta'(s)}{\zeta(s)}\, ds\right).$$

Here the contour C' is



where Re(ζ) is non-zero on the contour C'.

Number of Roots up to Height T

Backlund then found that

$$\left| \frac{1}{\pi} \mathrm{Im} \left(\int_{C'} \frac{\zeta'(s)}{\zeta(s)} \, ds \right) \right| < 2,$$

which implies that $N(T)$ is bounded. Under the condition that $\mathrm{Re}(\zeta)$ is non-zero on the contour C', $N(T)$ is the nearest integer to $\frac{1}{\pi}\theta(T) + 1$.

Therefore, in order to find the number of roots up to height T, one must explicitly show that no zeros of $\zeta(s)$ lie on the contour C'. Alternatively, consider the function

$$S(T) = N(T) - \frac{\theta(T)}{\pi} - 1.$$

Then

$$N(T) = S(T) + \frac{\theta(T)}{\pi} + 1 = S(T) + N_0(T).$$

Since we already know how to compute $\theta(T)$, finding $N_0(T)$ is easy. However, computing $S(T)$ is harder.

In general, $S(T)$ is typically small and is zero on average. Littlewood, Turing, and many others have already done a lot of work bounding and finding estimates for $S(T)$. We will use their results.

Number of Roots up to Height T

Littlewood proved

$$S(t) = O(\log(t)), \quad \int_0^T S(t)\,dt = O(T).$$

Then Turing found that

$$\left| \int_{t_1}^{t_2} S(t)\,dt \right| \leq 2.30 + 0.128 \log\left(\frac{t_2}{2\pi}\right),$$

when $168\pi < t_1 < t_2$. For certain Gram points g_n, this expression can be used to bound $S(g_n)$ so that $N(g_n) = n + 1$. A. Turing then showed that we can use the Gram blocks to verify the RH up to height $t = g_n$ (I have omitted most of the details, but a good exposition can be found in the book by Edwards [Edw01]).

Number of Roots up to Height T

Another way to analyze $N(T)$ is to use the asymptotic expansion of $\theta(T)$ to write

$$N(T) = \frac{T}{2\pi}\log\frac{T}{2\pi} - \frac{T}{2\pi} + O(\log(T)).$$

where Backlund used Jensen's inequality to show that the inequality

$$\left| N(T) - \left(\frac{T}{2\pi}\log\frac{T}{2\pi} - \frac{T}{2\pi} + \frac{7}{8} \right) \right| < 0.137\log T + 0.443\log\log T + 4.350$$

holds for all $T \geq 2$. Therefore both

$$N(T) \approx \frac{\theta(T)}{\pi} + 1, \quad N(T) \approx \frac{T}{2\pi}\log\frac{T}{2\pi} - \frac{T}{2\pi} + \frac{7}{8},$$

can be used as crude estimates to find the number of roots of $\zeta(\sigma + it)$ in the region $0 < \rho < 1$ and $0 \leq \tau \leq T$.

Lehmer's phenomenon

Lehmer's phenomenon was originally discovered by D. H. Lehmer while computing non-trivial zeros of the zeta function in 1956. In his own estimates of the zeros of $\zeta(s)$, Lehmer was only able to estimate the C_0 term in the Riemann-Siegel formula above. While performing these calculations, he noticed that some of the sign changes between consecutive roots of $Z(t)$ appeared to be extremely small. This is now known as Lehmer's phenomenon. The phenomenon is a direct observation that $|Z'(t)|$ can be extremely small at consecutive t-values between two zeros.

It is important to describe Lehmer's observations in detail as someone could use this to (numerically) disprove the Riemann hypothesis. However, this seems extremely unlikely given the amount of numerical evidence supporting the Riemann hypothesis.

Lehmer's phenomenon

A direct application of the RH states that if the RH is true, then the graph of $Z'(t)/Z(t)$ must be monotonically decreasing between the zeros of $Z(t)$ for all $t \geq t_0$ (WLOG, we can take $t_0 = 0$). This can be proved by contradiction. Stated in a different format, the function $Z(t)$ must have a positive local maximum followed by a negative local minimum (or vice versa). Two consecutive zeros, ρ_n and ρ_{n+1}, must have a local maximum or minimum between them which crosses the t-axis of the Riemann-Siegel $Z(t)$ function.

Lehmer's phenomenon

As I calculated around 10^7 zeros of the Riemann zeta function, I was interested in observing Lehmer's phenomenon on my laptop. An instance of the phenomenon occurred on $17143 \leq t \leq 17144$.

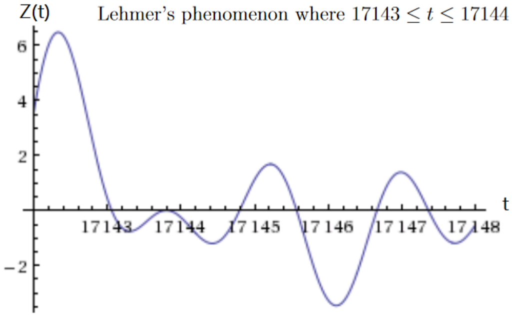


Figure 6: The function $Z(t)$ where $17142 \leq t \leq 17148$. At around the t-value of 17143.8, the vertical height above the t-axis is roughly 0.00397. Subtracting -0.00398 from the value of $Z(t)$ would contradict the Riemann hypothesis.

Lehmer's phenomenon

The phenomenon also occurs when $7005 \leq t \leq 7006$.

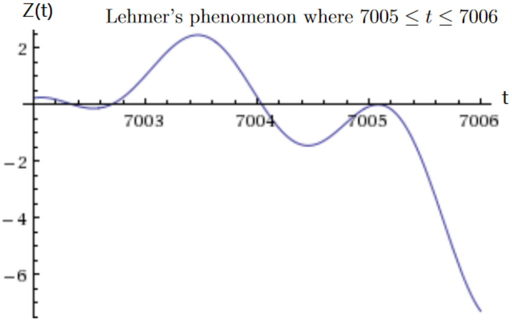


Figure 7: The function $Z(t)$ where $7005 \leq t \leq 7006$. At around the t-value of 7005.1, the $Z(t)$ function is slightly above the t-axis.

And when $13,999,997 \leq t \leq 13,999,998$.

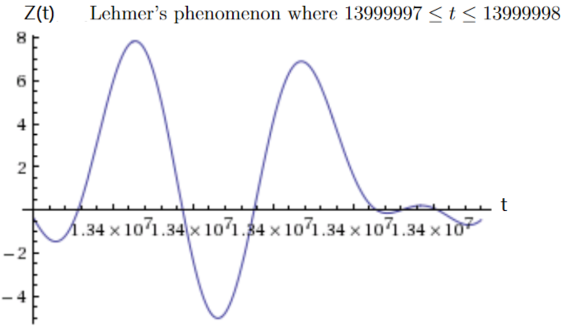


Figure 8: The function $Z(t)$ where $13,999,997 \leq t \leq 13,999,998$. Near the t-value $13,999,997.3$ a pair of zeros vary by only 4.4×10^{-4}.

Lehmer's phenomenon

Other people have observed the phenomenon. In particular, Ghaith Hiary (a student of Andrew Odlyzko) verified the RH at large t-values.

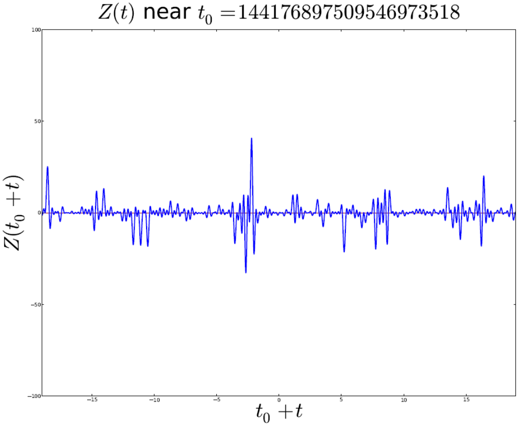


Figure 9: The function $Z(t)$ near $t_0 = 144,176,897,509,546,973,518$.

Lehmer's phenomenon

Hiary found a lot of t-values which "almost contradicted" the Riemann hypothesis. However, none of them violated the rule.

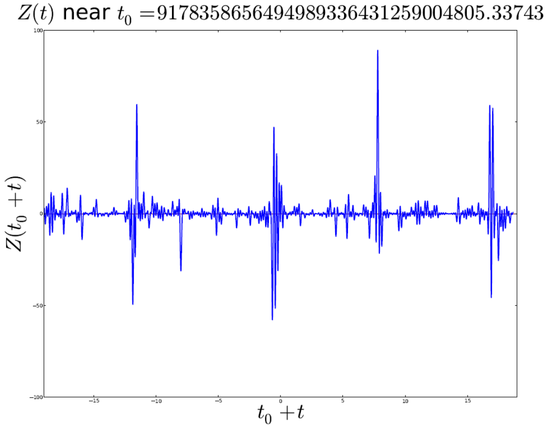


Figure 10: The function $Z(t)$ at a large value of t_0.

Lehmer's phenomenon

In 2004, Gourdon and Demichel [Gou04] verified the Riemann hypothesis for the first 10^{13} nontrivial zeros. They then verified the Riemann hypothesis at very large heights of $10^{13}, 10^{14}, \ldots, 10^{24}$. Later in 2020, Platt and Trudgian [PT20] showed that Riemann hypothesis is true up to the height of $3 \cdot 10^{12}$. So, all zeros of the Riemann zeta-function in the height $0 < t \leq 3 \cdot 10^{12}$ have $\sigma = 1/2$.

Lehmer's phenomenon would have been a major concern before Odlyzko verified the Riemann hypothesis near the height of 10^{12} [Odl87] in the 1980s. Up to the most recent work in 2020, all research has verified the Riemann hypothesis and no violations have been found.

Montgomery's Pair Correlation Conjecture

As many people calculated many zeros of the Riemann zeta function, it is natural to use statistical tools to find relationships between these zeros. In 1973, Hugh Montgomery and Freeman Dyson discovered that there is an interesting relationship between the spaces of consecutive zeros of the Riemann zeta function and the spaces of eigenvalues generated from a random matrix. This is known as Montgomery's pair correlation conjecture. The conjecture states that the pair correlation between pairs of zeros of the Riemann zeta function (normalized to have unit average spacing) is

$$1 - \left(\frac{\sin(\pi u)}{(\pi u)} \right) + \delta(u).$$

Here $\delta(u)$ represents the normalized spacing between zeros.

Montgomery's Pair Correlation Conjecture

In the 1980s, Andrew Odlyzko started investigating the statistics of the zeros of $\zeta(s)$. He investigated the distribution of the spacings between non-trivial zeros using detailed numerical calculations. This work was a motivating factor to create a more powerful algorithm named the Odlyzko-Schönhage algorithm which is based off of the Riemann Siegel formula. Odlyzko found that distribution of zeros agrees with the distribution of spacings of GUE random matrix eigenvalues in random matrix theory. All of his calculations were performed on the Cray X-MP supercomputer.

Montgomery's Pair Correlation Conjecture

Writing a nontrivial zero as $\rho = \frac{1}{2} + i\gamma_n$, Odlyzko let the normalized spacings be

$$\delta_n = \frac{\gamma_{n-1} - \gamma_n}{2\pi} \log\left(\frac{\gamma_n}{2\pi}\right).$$

Given that the Odlyzko-Schönhage algorithm can compute $\zeta(1/2 + it)$ in an average time of t^ε steps, Odlyzko was able to compute millions of zeros around heights of 10^{20}. This provided evidence supporting the relationship between the distribution of zeros of the Riemann zeta function and the distribution of spacings of GUE random matrix eigenvalues. In particular, Odlyzko noticed that as more zeros are sampled, the more closely their distribution approximates the shape of the GUE random matrix.

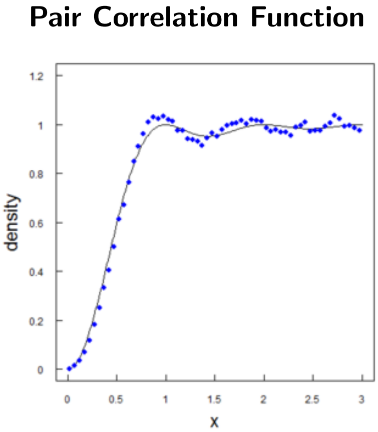


Figure 11: The real line describes the two-point correlation function of the random matrix of type GUE. Blue dots describe the normalized spacings of the non trivial zeros of Riemann zeta function, for the first 10^5 zeros.

Riemann–Siegel Formula

Returning back to the Riemann-Siegel formula. Let t be a real number. Then we find [BH16]

$$Z(t) = 2\mathrm{Re}\left\{ e^{i\theta(t)} \sum_{n \leq \left(\frac{t}{2\pi}\right)^{1/2}} \frac{1}{n^{1/2+it}} \right\} + O(t^{-1/4}).$$

We conclude that it is possible to compute $\zeta(1/2 + it)$ to sufficient accuracy in $O(t^{1/2})$ time.

Method 3: Odlyzko–Schönhage Algorithm

Following [OS88] and [Gou04] we recall that the Riemann-Siegel theta function is

$$\theta(t) = \arg\left(\pi^{-it/2}\Pi(it/2 - 3/4)\right),$$

where the argument is defined by continuous variation of t starting with the value 0 at $t = 0$. As a consequence, the Riemann-Siegel Z function is real-valued

$$Z(t) = e^{i\theta(t)}\zeta(1/2 + it),$$

and $|Z(t)| = |\zeta(1/2 + it)|$ so the zeros of $Z(t)$ are the imaginary part of the zeros of $\zeta(s)$ which lie on the critical strip. We are lead to find sign changes of a real valued function to find zeros on the critical strip, and this is a very convenient property in numerical verification of the RH.

Setup of the Odlyzko–Schönhage Algorithm

Therefore on the critical line $\sigma = 1/2$, the Riemann zeta function satisfies

$$\zeta(1/2 + it) = e^{-i\theta(t)} Z(t),$$

where $\theta(t)$ is a real-valued function and as t approaches infinity, $\theta(t)$ satisfies the asymptotic formula

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

The Riemann-Siegel Z function is a real valued function of the real variable t which satisfies the Riemann-Siegel expansion

$$Z(t) = 2 \sum_{n=1}^{m} \frac{\cos(\theta(t) - t \log n)}{\sqrt{n}} + R(t).$$

Setup of the Odlyzko–Schönhage Algorithm

We now write the remainder term $R(t)$ as

$$R(t) = (-1)^{m+1}\tau^{-1/2}\sum_{j=0}^{M}(-1)^j\tau^{-j}\Phi_j(z) + R_M(t), \tag{6}$$

where $R_M(t) = O(t^{-(2M+3)/4})$ and the other terms are defined by

$$\tau = \sqrt{\frac{t}{2\pi}}, \quad m = \lfloor \tau \rfloor, \quad z = 2(t-m) - 1.$$

Similar to the Riemann-Siegel formula, we have explicit forms for the first few functions of $\Phi_j(z)$.

These are

$$\Phi_0(z) = \frac{\cos\left(\frac{1}{2}\pi z^2 + \frac{3}{8}\pi\right)}{\cos(\pi z)}, \quad \Phi_1(z) = \frac{1}{12\pi^2}\Phi_0^{(3)}(z),$$

$$\Phi_2(z) = \frac{1}{16\pi^2}\Phi_0^{(2)}(z) + \frac{1}{288\pi^4}\Phi_0^{(6)}(z).$$

The general expression of $\Phi_j(z)$ for $z > 2$ is quite involved and is therefore omitted. As exposed in [BBC00], Borwein and Bradley obtained explicit bounds on the error term $R_M(t)$. In particular, for $t \geq 200$

$$|R_0(t)| \leq 0.127t^{-3/4}, \quad |R_1(t)| \leq 0.053t^{-5/4}, \quad |R_2(t)| \leq 0.011t^{-7/4}.$$

In practice one can compute zeros of $Z(t)$ above the 10^{10}-th zero by choosing $M = 1$. This choice obtains an absolute precision of $Z(t)$ smaller than 2×10^{-14} and is more than sufficient to locate zeros.

The Odlyzko–Schönhage Algorithm

The Odlyzko–Schönhage algorithm admits efficient evaluations of $Z(t)$ in a range of the form $T \le t \le T + \Delta$, where $\Delta = O(\sqrt{T})$. For t in this range, we write

$$Z(t) = \sum_{n=1}^{k_0 - 1} \frac{\cos(\theta(t) - t \log n)}{\sqrt{n}} + \mathrm{Re}(e^{-i\theta(t)} F(t)) + \sum_{n=k_1+1}^{m} \frac{\cos(\theta(t) - t \log n)}{\sqrt{n}} + R(t).$$

Here $R(t)$ is the remainder term defined by (6) and $F(t)$ is a complex function defined by

$$F(t) = F(k_0 - 1, k_1; t) := \sum_{k=k_0}^{k_1} \frac{1}{\sqrt{k}} e^{it \log k},$$

with $k_1 = \left\lfloor \sqrt{T/2\pi} \right\rfloor$ and k_0 a fixed, small integer.

In practice, given an interval $[T, T+\Delta]$ and t in this range, the values of k_0 and k_1 are fixed in the computation of $Z(t)$. We choose k_0 to be small compared to the value of $T^{1/2}$. As $m-k_1$ is bounded (since $\Delta = O(\sqrt{T})$), the most time consuming part of the evaluation of $Z(t)$ is the computation of $F(k_0-1, k_1; t)$. To this end, Odlyzko and Schönhage developed a technique dedicated to a fast evaluation of this sum.

The Odlyzko–Schönhage Algorithm

To obtain fast evaluations of $F(t) = F(k_0 - 1, k_1; t)$ in the range $[T, T + \Delta]$, the Odlyzko–Schönhage algorithm is divided into two steps :

1. Multiple evaluations of $F(t)$ are handled on a well chosen regular grid of abscissa for t.
2. From these values, an interpolation formula obtains efficiently any value of $F(t)$ at a certain accuracy provided that t stays in our range.

In particular, Odlyzko handles multi-evaluations of $F(t)$ and multi-evaluations of derivatives of $F(t)$ on the regular grid. His implementation uses an interpolation formula (based on Chebyshev polynomials) for multi-evaluations of $F(t)$.

Fast multi-evaluation of $F(t)$ on a regular grid

The Odlyzko–Schönhage algorithm approximates values of $F(t)$ at evenly spaced values

$$t = T_0, \quad T_0 + \delta, \quad \ldots, \quad T_0 + (R-1)\delta,$$

where both δ and R are to be determined. Instead of computing $F(T_0), F(T_0+\delta), \ldots, F(T_0+(R-1)\delta)$ directly, the key idea is to compute their discrete Fourier transform. This transform is defined by

$$u_k = \sum_{j=0}^{R-1} F(T_0 + j\delta)\omega^{-jk}, \quad \omega = \exp\left(\frac{2\pi i}{R}\right),$$

for $0 \le k < R$.

Fast multi-evaluation of $F(t)$ on a regular grid

Using the inverse Fourier transform, we obtain

$$F(T_0 + j\delta) = \frac{1}{R} \sum_{k=0}^{R-1} u_k \omega^{jk}.$$

In the algorithm, the value of R is chosen to be a power of two, so the values $F(T_0 + J\delta)$ are efficiently obtained from the (u_k) with an FFT transform. Both the FFT and IFFT take a small portion of the total computation time. It is harder to efficiently compute the (u_k).

Different research groups apply different methods to calculate (u_k). This is an active area of research today.

The Odlyzko–Schönhage Algorithm

Using a preconditioner of time $O(T^{1/2+\varepsilon})$, the Odlyzko–Schönhage algorithm can evaluate a single value of $\zeta(1/2+it)$ for any $T < t < T + T^{1/2}$ to within $\pm t^{-c}$ in $O(t^{\varepsilon})$ operations on numbers of $O(\log t)$ bits for any $\varepsilon > 0$.

However, it is difficult to implement the Odlyzko–Schönhage algorithm. Hiary has stored a portion of his code in a Github repository.

History: Verification of RH

A history of the verification of the Riemann hypothesis up to n zeros is shown below [Gou04].

Table 1: Verification of Riemann Hypothesis

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

History: Verification of RH

Table 2: Verification of Riemann Hypothesis

Year	n	Author
1966	250,000	R. S. Lehman
1968	3,502,500	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
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
1987	Near ($\sim 10^{12}$)	A. M. Odlyzko
1992	Near ($\sim 10^{20}$)	A. M. Odlyzko
1998	Near ($\sim 10^{21}$)	A. M. Odlyzko

History: Verification of RH

Table 3: Verification of Riemann Hypothesis

Year	n	Author
2001	10,000,000,000	J. van de Lune
2003	250,000,000,000	S. Wedeniwsk
2004	10,000,000,000,000	X. Gourdon, Patrick Demichel
2020	12,363,153,437,138	Platt, Trudgian

The work of Platt and Trudgian verified the Riemann hypothesis up to the height of $3 \cdot 10^{12}$.

Computer Implementation

Java code and C code. Time permitting, also talk about Hiary's implementation.

Future Work/Projects

An interested student could work on a variety of different projects involving calculations of the Riemann zeta function. The projects would involve implementing (preferably C or Fortran) code to calculate zeros of the Riemann zeta function. Alternatively, one can analyze the distribution of spaces between zeros of the zeta function[Odl87]. Some ideas are:

1. Calculate nontrivial zeros through the Euler-Maclaurin Summation formula (see chapter 6 of [Edw01]).
2. Calculate nontrivial zeros by the Riemann-Siegel formula (see [Pug98] and [Tak]).
3. Calculate nontrivial zeros by the Odlyzko-Schönhage algorithm (see [Odl89] and [OS88]).
4. Parallelize the code for items (1)-(2).
5. Investigate Montgomery's pair correlation conjecture in more detail (see [Gol05] and [Li]).
6. Analyze the distribution of spaces between zeros (see [FW12] and [BMN09]).

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