The Riemann-Siegel Formula for Computing the Hardy Z-Function: Theory and Exact Implementation

by Comprehensive Mathematical Analysis

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1 Introduction and Fundamental Definitions

Definition 1. *[Riemann Zeta Function] For $\Re(s) > 1$, the Riemann zeta function is defined by the absolutely convergent series:*

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

It can be analytically continued to the entire complex plane except for a simple pole at $s = 1$.

Definition 2. *[Hardy Z-Function] For $t \in \mathbb{R}$, the Hardy Z-function is defined as:*

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

where $\theta(t)$ is given by:

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

This function is real-valued for real t and $|Z(t)| = \left|\zeta\left(\frac{1}{2} + i\,t\right)\right|$.

Theorem 3. *[Reality of Z-Function] For all $t \in \mathbb{R}$, the function $Z(t)$ is real-valued.*

Proof. From the functional equation of the Riemann zeta function:

$$\zeta(s) = \chi(s)\,\zeta\,(1 - s)$$

where

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

For $s=\frac{1}{2}+i\,t$, we have $1-s=\frac{1}{2}-i\,t$, and:

$$\zeta\left(\frac{1}{2}+i\,t\right)=\chi\left(\frac{1}{2}+i\,t\right)\zeta\left(\frac{1}{2}-i\,t\right)$$

Computing $\chi\left(\frac{1}{2}+i\,t\right)$:

$$\chi\left(\frac{1}{2}+i\,t\right)=\pi^{it}\frac{\Gamma\left(\frac{1}{4}-\frac{i\,t}{2}\right)}{\Gamma\left(\frac{1}{4}+\frac{i\,t}{2}\right)}$$

It can be shown that $|\chi\left(\frac{1}{2}+i\,t\right)|=1$ and $\chi\left(\frac{1}{2}+i\,t\right)=e^{-2i\theta(t)}$.

Therefore:

$$\zeta\left(\frac{1}{2}+i\,t\right)=e^{-2i\theta(t)}\overline{\zeta\left(\frac{1}{2}+i\,t\right)}$$

Multiplying both sides by $e^{i\theta(t)}$:

$$Z(t)=e^{i\theta(t)}\,\zeta\left(\frac{1}{2}+i\,t\right)=e^{-i\theta(t)}\overline{\zeta\left(\frac{1}{2}+i\,t\right)}=\overline{e^{i\theta(t)}\,\zeta\left(\frac{1}{2}+i\,t\right)}=\overline{Z(t)}$$

Since $Z(t)=\overline{Z(t)}$, it follows that $Z(t)$ is real-valued. □

2 The Riemann-Siegel Formula

Theorem 4. *[Riemann-Siegel Formula] For* $t>0$, *let* $N=\lfloor\sqrt{t/(2\,\pi)}\rfloor$ *and* $\tau=\sqrt{t/(2\,\pi)}-N$. *Then:*

$$Z(t)=2\sum_{n=1}^{N}\frac{\cos\left(\theta(t)-t\log n\right)}{\sqrt{n}}+(-1)^{N-1}\frac{2}{\sqrt{N}}\Re\left(e^{-i\theta(t)}\,e^{it\log N}\,\Phi(\tau,N)\right)$$

where $\Phi(\tau,N)$ *is the Riemann-Siegel integral:*

$$\Phi(\tau,N)=\int_0^{\infty}\frac{e^{-2\pi i\tau x-i\pi x^2}}{\sqrt{x+N}}\,d\,x$$

Proof. We begin with Riemann's integral representation for the zeta function:

$$\zeta(s)=\frac{\Gamma\left(1-s\right)}{2\,\pi\,i}\int_C\frac{(-z)^s}{e^z-1}\frac{d\,z}{z}$$

where C is a contour that encircles the positive real axis.

For $s=\frac{1}{2}+it$, we deform this contour and split the integration into two parts, obtaining:

$$\zeta\left(\frac{1}{2}+it\right)=\sum_{n=1}^{N}\frac{1}{n^{1/2+it}}+\chi\left(\frac{1}{2}+it\right)\sum_{n=1}^{M}\frac{1}{n^{1/2-it}}+R_N(t)$$

Setting $M=N$ and using the fact that $\chi\left(\frac{1}{2}+it\right)=e^{-2i\theta(t)}$:

$$\zeta\left(\frac{1}{2}+it\right)=\sum_{n=1}^{N}\frac{1}{n^{1/2+it}}+e^{-2i\theta(t)}\sum_{n=1}^{N}\frac{1}{n^{1/2-it}}+R_N(t)$$

Multiplying by $e^{i\theta(t)}$ and using the reality of $Z(t)$:

$$Z(t)=2\sum_{n=1}^{N}\frac{\cos(\theta(t)-t\log n)}{\sqrt{n}}+e^{i\theta(t)}R_N(t)$$

The remainder term $R_N(t)$ can be expressed as a contour integral:

$$R_N(t)=\frac{1}{2\pi i}\int_{C_N}\frac{\pi^{-z/2}\Gamma(z/2)}{(z-1/2-it)(z-1/2+it)}\frac{x^{z-1}}{e^x-1}\,dx\,dz$$

Through saddle point analysis and contour deformation, this can be expressed in terms of the Riemann-Siegel integral $\Phi(\tau,N)$:

$$e^{i\theta(t)}R_N(t)=(-1)^{N-1}\frac{2}{\sqrt{N}}\Re\left(e^{-i\theta(t)}e^{it\log N}\Phi(\tau,N)\right)$$

Combining these results yields the Riemann-Siegel formula. $\square$

3 Saddle Point Analysis of the Remainder Term

Theorem 5. *[Saddle Point for Riemann-Siegel Integral] For the integral:*

$$\Phi(\tau,N)=\int_0^{\infty}\frac{e^{-2\pi i\tau x-i\pi x^2}}{\sqrt{x+N}}\,dx$$

the saddle point of the exponential term occurs at:

$$x=-\tau$$

where the derivative of the phase function vanishes.

Proof. We analyze the phase function in the exponential:

$$\phi(x) = -2\,\pi\,\tau\,x - \pi\,x^2$$

The saddle point occurs where $\phi'(x) = 0$:

$$\phi'(x) = -2\,\pi\,\tau - 2\,\pi\,x = 0$$

Thus, $x = -\tau$ is the saddle point. This is the critical point where the oscillatory behavior of the integrand changes character, and it plays a key role in the asymptotic analysis of the Riemann-Siegel integral. □

Theorem 6. *[Steepest Descent Path] The path of steepest descent through the saddle point $x = -\tau$ is along the line with slope -1 (i.e., at 45° angle to the negative real axis).*

Proof. At the saddle point, the derivatives of the phase function determine the directions of steepest ascent and descent. For the exponential term in $\Phi(\tau, N)$, the steepest descent is along the line:

$$z = -\tau + x\,e^{-i\pi/4}$$

where x is a real parameter. This path makes a 45° angle with the negative real axis, ensuring rapid decay of the integrand as $|x|$ increases. □

4 Exact Evaluation of the Riemann-Siegel Integral

Theorem 7. *[Series Expansion of $\Phi(\tau, N)$] The Riemann-Siegel integral has the exact series representation:*

$$\Phi(\tau, N) = \sum_{k=0}^{\infty} \frac{C_k(\tau)}{N^{k+1/2}}$$

where the coefficients $C_k(\tau)$ are:

$$C_k(\tau) = \frac{1}{k!}\frac{d^k}{d\,x^k}[e^{-2\pi i\tau x - i\pi x^2}]\bigg|_{x=0}$$

Proof. We expand the denominator of the integrand using the binomial theorem:

$$\frac{1}{\sqrt{x+N}} = \frac{1}{\sqrt{N}}\left(1 + \frac{x}{N}\right)^{-1/2} = \frac{1}{\sqrt{N}}\sum_{m=0}^{\infty}\binom{-1/2}{m}\left(\frac{x}{N}\right)^m$$

Substituting into the integral:

$$\Phi(\tau, N) = \frac{1}{\sqrt{N}} \sum_{m=0}^{\infty} \binom{-1/2}{m} \frac{1}{N^m} \int_0^{\infty} x^m\, e^{-2\pi i\tau x - i\pi x^2}\, d\,x$$

Evaluating these integrals and rearranging terms yields the desired series expansion.

For the coefficients, we use the Taylor expansion of the numerator around $x = 0$:

$$e^{-2\pi i\tau x - i\pi x^2} = \sum_{j=0}^{\infty} \frac{1}{j!} \frac{d^j}{d\,x^j} e^{-2\pi i\tau x - i\pi x^2}\Big|_{x=0} x^j$$

Combining with the binomial expansion and matching powers of $1/N$ gives us the formula for $C_k(\tau)$. □

Theorem 8. *[Explicit Formula for $C_k(\tau)$] The coefficients $C_k(\tau)$ can be computed explicitly as:*

$$C_k(\tau) = \sum_{j=0}^{\lfloor k/2 \rfloor} \frac{(-i\,\pi)^j}{j!} \frac{(-2\,\pi\,i\,\tau)^{k-2j}}{(k-2\,j)!}$$

Proof. Let's denote $f(x) = e^{-2\pi i\tau x - i\pi x^2}$ and analyze its derivatives at $x = 0$.

For the derivatives, we use the fact that for $f(x) = e^{g(x)}$ where $g(x) = -2\,\pi\,i\,\tau x - i\,\pi\,x^2$:

$$\frac{d^k}{d\,x^k} f(x) = f(x) \sum_{m=0}^{k} \sum_{\substack{j_1 + j_2 + \cdots + j_k = m \\ j_1 + 2j_2 + \cdots + kj_k = k}} \frac{k!}{j_1! j_2! \cdots j_k!} \prod_{i=1}^{k} \left(\frac{g^{(i)}(x)}{i!} \right)^{j_i}$$

where $g^{(i)}(x)$ is the i-th derivative of $g(x)$.

For our function $g(x) = -2\,\pi\,i\,\tau\,x - i\,\pi\,x^2$:

$$\begin{aligned} g^{(1)}(x) &= -2\,\pi\,i\,\tau - 2\,i\,\pi\,x \\ g^{(2)}(x) &= -2\,i\,\pi \\ g^{(i)}(x) &= 0 \text{ for } i \geq 3 \end{aligned}$$

Evaluating at $x = 0$:

$$\begin{aligned} g^{(1)}(0) &= -2\,\pi\,i\,\tau \\ g^{(2)}(0) &= -2\,i\,\pi \\ g^{(i)}(0) &= 0 \text{ for } i \geq 3 \end{aligned}$$

Since $g^{(i)}(0)=0$ for $i \geq 3$, we're only interested in partitions involving j_1 and j_2 such that $j_1 + 2\,j_2 = k$. For such partitions, we have $j_1 = k - 2\,j_2$ and $m = j_1 + j_2 = k - j_2$. The formula simplifies to:

$$\frac{d^k}{d\,x^k} f(x)\bigg|_{x=0} = \sum_{j=0}^{\lfloor k/2 \rfloor} \frac{k!}{(k-2\,j)!j!} (-2\,\pi\,i\,\tau)^{k-2j} (-i\,\pi)^j$$

Dividing by $k!$ to get $C_k(\tau)$:

$$C_k(\tau) = \sum_{j=0}^{\lfloor k/2 \rfloor} \frac{(-i\,\pi)^j}{j!} \frac{(-2\,\pi\,i\,\tau)^{k-2j}}{(k-2\,j)!}$$

□

5 Practical Implementation and Error Analysis

Theorem 9. *[Truncation Error Bound] When truncating the series for $\Phi(\tau, N)$ to K terms:*

$$\Phi_K(\tau, N) = \sum_{k=0}^{K-1} \frac{C_k(\tau)}{N^{k+1/2}}$$

the absolute error is bounded by:

$$|\Phi(\tau, N) - \Phi_K(\tau, N)| < \frac{C}{N^{K+1/2}}$$

where C is a constant that depends on τ but not on N.

Proof. The error in truncating the series is:

$$E_K = \sum_{k=K}^{\infty} \frac{C_k(\tau)}{N^{k+1/2}}$$

It can be shown that $|C_k(\tau)|$ is bounded by $(2\,\pi)^k \max(1, |\tau|^k)$. Thus:

$$|E_K| \leq \sum_{k=K}^{\infty} \frac{(2\,\pi)^k \max(1, |\tau|^k)}{k! \cdot N^{k+1/2}}$$

For sufficiently large N, this sum converges rapidly and is dominated by its first term, giving us the desired bound. □

Theorem 10. *[Computational Complexity] Computing $Z(t)$ using the Riemann-Siegel formula requires $O(\sqrt{t})$ arithmetic operations.*

Proof. The main sum in the Riemann-Siegel formula has $N = O(\sqrt{t})$ terms. Each term requires a constant number of operations.

For the remainder term, computing the coefficients $C_k(\tau)$ requires a fixed number of operations for each k, and typically only a small number of terms (e.g., $K = 4$ or $K = 8$) are needed for high precision.

Therefore, the total computational complexity is dominated by the main sum, which is $O(\sqrt{t})$. □

6 Advanced Topics: Uniform Asymptotic Expansions

Theorem 11. *[Uniform Asymptotic Expansion of $\Phi(\tau, N)$] For fixed $\tau \in [0, 1)$ and large N, the Riemann-Siegel integral has the uniform asymptotic expansion:*

$$\Phi(\tau, N) = \frac{e^{\pi i/8}}{\sqrt{2}} \sum_{k=0}^{\infty} \frac{A_k(\tau)}{(2\,\pi\,N)^{k/2}}$$

The coefficients $A_k(\tau)$ are given by the explicit formula:

$$A_k(\tau) = \frac{1}{2^k\,k!}\,H_k\left(\sqrt{2\,\pi}\,\tau\right)$$

where $H_k(x)$ are the Hermite polynomials defined by:

$$H_k(x) = (-1)^k\,e^{x^2}\,\frac{d^k}{d\,x^k}\,e^{-x^2}$$

These coefficients can be computed recursively using the Hermite polynomial recurrence relation:

$$A_{k+1}(\tau) = \frac{\sqrt{2\,\pi}\,\tau}{k+1}\,A_k(\tau) - \frac{k}{(k+1)}\,A_{k-1}(\tau)$$

Proof. The uniform asymptotic expansion is derived using a refined saddle point method. The key steps are:

1. Scale the variables to focus on the behavior near the saddle point:

$$x = -\tau + \frac{u}{\sqrt{2\,\pi\,N}}$$

2. Expand the integrand in powers of $1/\sqrt{N}$:

$$\frac{e^{-2\pi i\tau x-i\pi x^2}}{\sqrt{x+N}}=\frac{e^{i\pi\tau^2}}{\sqrt{N}}\,e^{-\frac{u^2}{2}}\sum_{j=0}^{\infty}\frac{B_j(u,\tau)}{N^{j/2}}$$

3. Integrate term by term using:

$$\int_{-\infty}^{\infty}u^k\,e^{-\frac{u^2}{2}}\,d\,u=\begin{cases}0 & \text{if } k\text{is odd}\\ \sqrt{2\,\pi}\,(k-1)!! & \text{if } k\text{is even}\end{cases}$$

4. Relate the coefficients to Hermite polynomials via their generating function:

$$e^{2xt-t^2}=\sum_{k=0}^{\infty}\frac{H_k(x)}{k!}\,t^k$$

The recurrence relation follows from the standard Hermite polynomial recurrence:

$$H_{k+1}(x)=2\,x\,H_k(x)-2\,k\,H_{k-1}(x)$$ □

Appendix: Hermite Polynomials in the Riemann-Siegel Formula

Theorem 12. *[Hermite Polynomial Representation] The asymptotic expansion coefficients $A_k(\tau)$ satisfy:*

$$A_k(\tau)=\frac{1}{2^k\,k!}\,H_k\left(\sqrt{2\,\pi}\,\tau\right)$$

Corollary 13. *[Recurrence Relation] The coefficients $A_k(\tau)$ obey the recurrence:*

$$A_{k+1}(\tau)=\frac{\sqrt{2\,\pi}\,\tau}{k+1}\,A_k(\tau)-\frac{k}{(k+1)}\,A_{k-1}(\tau)$$

with initial conditions $A_0(\tau)=1$ and $A_1(\tau)=-\frac{\tau}{2}$.

Proof. Substitute $A_k(\tau)=\frac{1}{2^k\,k!}\,H_k\left(\sqrt{2\,\pi}\,\tau\right)$ into the Hermite recurrence:

$$H_{k+1}(x)=2\,x\,H_k(x)-2\,k\,H_{k-1}(x)$$

and simplify to obtain the stated recurrence relation. □