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Article

On the Approximation of the Hardy Z-Function via High-Order Sections

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Abstract: The Z-function is the real function given by $Z(t) = e^{i\theta(t)}\zeta\left(\frac{1}{2}+it\right)$, where $\zeta(s)$ is the Riemann zeta function, and $\theta(t)$ is the Riemann–Siegel theta function. The function, central to the study of the Riemann hypothesis (RH), has traditionally posed significant computational challenges. This research addresses these challenges by exploring new methods for approximating $Z(t)$ and its zeros. The sections of $Z(t)$ are given by $Z_N(t) := \sum_{k=1}^{N} \frac{\cos(\theta(t)-\ln(k)t)}{\sqrt{k}}$ for any $N \in \mathbb{N}$. Classically, these sections approximate the Z-function via the Hardy–Littlewood approximate functional equation (AFE) $Z(t) \approx 2Z_{\widetilde{N}(t)}(t)$ for $\widetilde{N}(t) = \left[\sqrt{\frac{t}{2\pi}}\right]$. While historically important, the Hardy–Littlewood AFE does not sufficiently discern the RH and requires further evaluation of the Riemann–Siegel formula. An alternative, less common, is $Z(t) \approx Z_{N(t)}(t)$ for $N(t) = \left[\frac{t}{2}\right]$, which is Spira's approximation using higher-order sections. Spira conjectured, based on experimental observations, that this approximation satisfies the RH in the sense that all of its zeros are real. We present a proof of Spira's conjecture using a new approximate equation with exponentially decaying error, recently developed by us via new techniques of acceleration of series. This establishes that higher-order approximations do not need further Riemann–Siegel type corrections, as in the classical case, enabling new theoretical methods for studying the zeros of zeta beyond numerics.

Keywords: Riemann zeta function; Hardy Z-function; approximate functional equation; Spira's approximation; series acceleration; Riemann hypothesis; numerical analysis; analytic number theory

MSC: 11M06; 11Y35; 30E10; 65H10

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1. Introduction

1.1. Riemann's Analytic Extension of Zeta

The Riemann zeta function is given by $\zeta(s) := \sum_{n=1}^{\infty} n^{-s}$ in the range $Re(s) > 1$. In his revolutionary 1859 work [1], Riemann extended the zeta function $\zeta(s)$ analytically to a meromorphic function on the entire complex plane with a single pole at $s = 1$. This extension allowed him to explore the zeta function from a complex analytic perspective, uncovering its profound connection to the distribution of prime numbers. Riemann's analytic continuation of $\zeta(s)$ is given by the integral representation:

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

Although the integral representation outlined in Equation (1) was of tremendous importance for Riemman's theoretical explorations in his manuscript, it is not amenable for direct computations. To practically compute $\zeta(s)$, asymptotic techniques are required.

1.2. The Approximate Functional Equation (AFE) and the Riemann–Siegel Formula

The development of the AFE for the Z-function due to Hardy and Littlewood, marks a cornerstone in the computation methods of zeta [2–5]. The Hardy Z-function, denoted as $Z(t)$, is the real function defined by

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

where $\theta(t)$ is the Riemann–Siegel θ-function, given by the equation

$$\theta(t) = \arg\left(\Gamma\left(\frac{1}{4} + \frac{it}{2}\right)\right) - \frac{t}{2}\log(t), \tag{3}$$

see [6,7]. The Hardy–Littlewood approximation is encapsulated in the formula

$$Z(t) = 2\sum_{k=1}^{\widetilde{N}(t)} \frac{cos(\theta(t) - ln(k)t)}{\sqrt{k}} + R(t), \tag{4}$$

where $\widetilde{N}(t) = \left[\sqrt{\frac{t}{2\pi}}\right]$, and the error term is given by

$$R(t) = O\left(\frac{1}{\sqrt{t}}\right). \tag{5}$$

This representation, while powerful, for many purposes, requires further refinement of the error term $R(t)$ to enhance the level of precision.

In the 1930's, C. L. Siegel uncovered previously unpublished notes by Riemann which revealed that, remarkably, Riemann not only knew the Hardy–Littlewood Formula (4) but also developed complex asymptotic saddle point techniques which enable the required further evaluation of its error term $R(t)$ for any order [6,8]. For instance, expanded to first-order, the Riemann–Siegel formula gives

$$R(t) = (-1)^{N(t)-1}\left(\frac{t}{2\pi}\right)^{-\frac{1}{4}} \frac{cos(2\pi(p^2 - p - \frac{1}{16}))}{cos(2\pi p)} + O\left(\frac{1}{t^{\frac{3}{4}}}\right), \tag{6}$$

where $p = \sqrt{\frac{t}{2\pi}} - \widetilde{N}(t)$. As an asymptotic formula, for a given specific value of t, indefinitely increasing the order of the expansion does not guarantee improved approximation. It is conjectured by Berry and Keating [9] that, when expanded to its optimal order, the Riemann–Siegel formula can reach the accuracy level of exponentially decaying error $O(e^{-\pi t})$.

Since its introduction, the Riemann–Siegel formula, especially when enhanced with the Odlyzko–Schönhage algorithm [10], has been the main method for numerical verification of the RH, see [11–17]. The most comprehensive verification to date, achieved by Platt and Trudigian, confirms the RH up to $3 \cdot 10^{12}$, see [18]. However, it can be argued that one of the great challenges in the Riemann hypothesis is the fact that while the Riemann–Siegel formula gives efficient methods for the numerical estimation of $R(t)$ to any given order, it offers little analytical insight on its structure, crucial for the understanding of the properties of the zeros in general, especially as the order of its expansion increases due to the complexity of the expressions involved. It should be noted that recently, various alternative methods have been suggested, see [19–21].

1.3. Sections of the Z-Function and Spira's Approximation

In [22,23], Spira introduced the notion of sections of the AFE of $Z(t)$, which are essentially defined by

$$Z_N(t) := \sum_{k=1}^{N} \frac{cos(\theta(t) - ln(k)t)}{\sqrt{k}}, \tag{7}$$

and conducted a study of their zeros for any $N \in \mathbb{N}$. In particular, Spira noted that the sections of $Z(t)$ give an additional approximation of the function to that of the AFE

$$Z(t) = Z_{N(t)}(t) + O\left(\frac{1}{\sqrt{t}}\right), \tag{8}$$

at the higher range $N(t) = \left[\frac{t}{2}\right]$.

This approximation and its proof most certainly pre-date Spira and were probably already known to Riemann, see Theorem 1.8 of [24] for a variant. For instance, Figure 1 shows the values of the sections $Z_N(t)$ for the fixed value of $t = 3000$ and $N = 1, \ldots, 1500$ (blue), the Hardy–Littlewood approximation of $\frac{1}{2}Z(3000)$ (green) and Spira approximation $Z(3000)$ (brown):

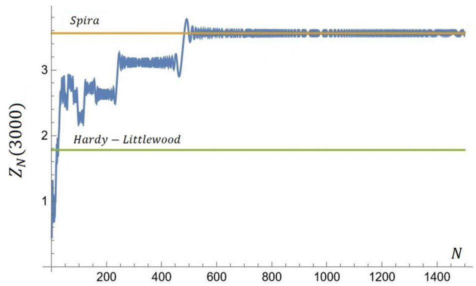

Figure 1. Values of the sections $Z_N(t)$ for the fixed value of $t = 3000$ and $N = 1, \ldots, 1500$ (blue), the Hardy-Littlewood approximation of $\frac{1}{2}Z(3000)$ (green) and the Spira approximation $Z(3000)$ (brown).

For numerical computations, employing (4) coupled with the Riemann–Siegel formula is clearly more efficient than utilizing Spira's approximation, for the following reasons:

1. The number of terms required for Spira's approximation, $N(t) = \left[\frac{t}{2}\right]$, increases quadratically compared to $\widetilde{N}(t) = \left[\sqrt{\frac{t}{2\pi}}\right]$ required by (4), making it far more costly for numerical calculations. This alone likely made (8), even if folklorically known, impractical for computational use, particularly before the advent of computers.
2. The theoretical asymptotic estimation of Spira's approximation error, obtained by classical means, is $O\left(\frac{1}{\sqrt{t}}\right)$, which is similar to that of the Hardy–Littlewood formula, before the application of the Riemann–Siegel expansion of the error whose first term already gives an error of order $O\left(t^{-\frac{3}{4}}\right)$. It should be noted, however, that these are approximate results, and hence, this seemingly superior asymptotic bound does not necessarily ensure greater practical accuracy over Spira's approximation.

A particularly noteworthy aspect of this additional approximation (8), however, is its unique properties when compared to the classical AFE.

1.4. Spira's Conjecture and the Absence of Theoretical Justification

Despite being far more costly, Spira, through his empirical investigations, suggested that (8) might have a critical significance, see S.6 of [22]. Remarkably, contrary to the Hardy–Littlewood formula, this higher-range approximation does not seem to admit zeros off the real line. That is, it is sensitive enough to observe the RH without the need for the expansion of the error term, as in the classical Riemann–Siegel formula. Although not explicitly stated by Spira in the following form, this can be formalized as follows:

Conjecture (Spira's RH for sections)**.** *All the non-trivial zeros of $Z_{N(t)}(t)$ are real.*

Figure 2 shows $ln|Z(t)|$ (orange) and compares between the Spira approximation $ln|Z_N(t)|$ with $N = N(t) = 205$ (blue-left) and the classical Hardy-Littlewood approximation $ln|2Z_N(t)|$ with $N = \widetilde{N}(t) = 8$ (blue-right) in the range $412 < t < 419$:

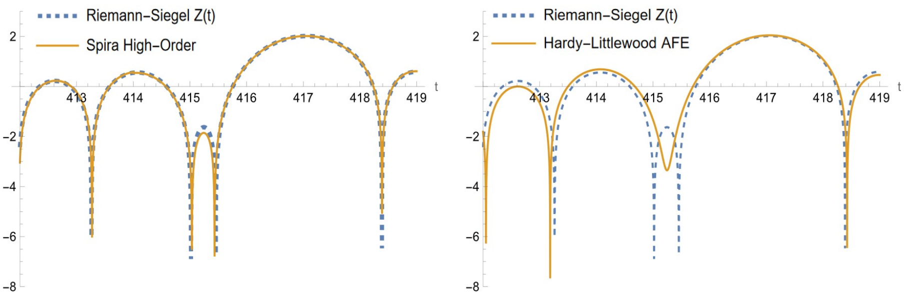

Figure 2. Graphs of $ln|Z(t)|$ (orange) and the Spira approximation $ln|Z_N(t)|$ with $N = N(t) = 205$ (blue-left) and the classical Hardy–Littlewood approximation $ln|2Z_N(t)|$ with $N = \widetilde{N}(t) = 8$ (blue-right) in the range $412 < t < 419$.

Figure 2 illustrates an instance of two real zeros accurately predicted by Spira's formula, as anticipated, but missed by the Hardy–Littlewood formula (highlighted here in red), which actually erroneously identifies them as complex zeros.

Spira's conjecture, while grounded in empirical and experimental observations, lacks direct theoretical underpinnings. Our aim in this work is to present a theoretical justification for the phenomena observed in Spira's conjecture of the advantage of the higher-order section $Z_{N(t)}(t)$ over the Hardy–Littlewood sections $Z_{\widetilde{N}(t)}(t)$, via our new techniques of accelerated approximations.

2. Spira's Approximation and Accelerated Approximations

In [25], we have developed an AFE based on the accelerated global series for $\zeta(s)$ due to Hasse–Sondow, which admits an error of exponential decay, see also [26] for a further study of this formula. For the Z-function, we have the following variant of our accelerated formula:

$$Z(t) = \widetilde{Z}_{N(t)}(t) + O\left(e^{-\omega t}\right), \tag{9}$$

where

$$\widetilde{Z}_N(t) := \sum_{n=0}^{N} \frac{1}{2^{n+1}} \sum_{k=0}^{n} \binom{n}{k} \frac{cos(\theta(t) - ln(k+1)t)}{\sqrt{k+1}}, \tag{10}$$

with $\omega > 0$ a certain positive constant computed in [25] and $N(t) = \left[\frac{t}{2}\right]$ is the same order as in Spira's approximation. The following Figure 3 shows $ln|Z(t)|$ (orange) and our approximation $ln|\widetilde{Z}_{N(t)}(t)|$ with $N = N(t) = 205$ (blue) in the range $412 < t < 419$:

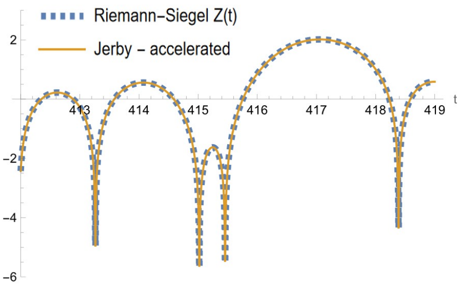

Figure 3. Graphs of $ln|Z(t)|$ (orange) and our accelerated approximation $ln|\widetilde{Z}_{N(t)}(t)|$ of [25] with $N = N(t) = 205$ (blue) in the range $412 < t < 419$.

Figure 4 illustrates the content of formula (9) by displaying $\ln|R(t)|$ (blue) and the line $-\omega \cdot t$ (orange), where $R(t) = Z(t) - \widetilde{Z}_{N(t)}(t)$ is the error of (9), for the range $0 \le t \le 350$:

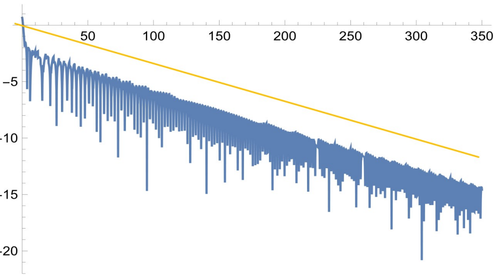

Figure 4. The graph of $ln|R(t)|$ (blue) and the line $-\omega \cdot t$ (orange), where $R(t) = Z(t) - \widetilde{Z}_{N(t)}(t)$ is the error of formula (9), for the range $0 \le t \le 350$.

It should be noted that our approximation via the accelerated $\widetilde{Z}_{N(t)}(t)$ actually achieves the superior accuracy expected to be attained by the Hardy–Littlewood AFE coupled with the Riemann–Siegel formula when evaluated at the optimal order, according to the Berry and Keating conjecture. Our main result is the following reformulation:

Proposition 1. *The Hardy Z-function can be approximated via*

$$Z(t) = \widetilde{Z}_{N(t)}(t) + O\left(e^{-\omega t}\right), \tag{11}$$

where

$$\widetilde{Z}_{N(t)}(t) = \sum_{k=1}^{N(t)} \widetilde{\alpha}_k^{acc}(t) \frac{\cos(\theta(t) - \ln(k)t)}{\sqrt{k}} \tag{12}$$

is the accelerated N-th section with the coefficients $\alpha_k^{acc}(t)$ given by

$$\widetilde{\alpha}_k^{acc}(t) := \sum_{n=k-1}^{N(t)} \frac{1}{2^{n+1}} \binom{n}{k-1}. \tag{13}$$

Proof. Denote by

$$\beta_{n,k}(t) := \beta_{n,k}^0 \frac{cos(\theta(t) - ln(k+1)t)}{\sqrt{k+1}}, \tag{14}$$

where

$$\beta_{n,k}^0 := \frac{1}{2^{n+1}} \binom{n}{k}. \tag{15}$$

The accelerated formula is given as the sum of all the coefficients $\beta_{n,k}(t)$ within the triangle $0 \le n \le N(t)$ and $0 \le k \le n$. In particular, summing first along the k indices leads to the definition of

$$A(n,t) = \sum_{k=0}^{n} \beta_{n,k}(t). \tag{16}$$

The accelerated Formula (9) is thus given by the summation of $A(n,t)$ for $0 \le n \le N(t)$. Figure 5 illustrates the triangle of coefficients $\beta_{n,k}(t)$ and their possible summation orders:

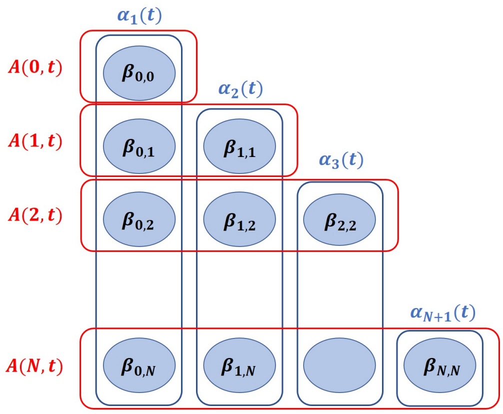

Figure 5. The triangle of coefficients $\beta_{n,k}(t)$ with $A(n,t)$ arising from the horizontal order of summation (red) and $\widetilde{\alpha}_k(t)$ arising from the vertical order of summation (blue).

On the other hand, changing the order of summation to be first along $k-1 \leq n \leq N(t)$ for given k and then along $1 \leq k \leq N(t)$ leads to the definition of $\widetilde{\alpha}_k(t)$ and the required formula. $\square$

It should be noted that our new Formula (17) is far more cost-efficient than the original accelerated Formula (10). Spira's section can be written as

$$Z_{N(t)}(t) = \sum_{k=1}^{N(t)} \alpha_k^{step}(t) \frac{\cos(\theta(t) - \ln(k)t)}{\sqrt{k}}, \tag{17}$$

where the coefficients $\alpha_k^{step}(t)$ are given by the step function:

$$\alpha_k^{step}(t) := \begin{cases} 1 & 1 \leq k \leq N(t) \\ 0 & \text{otherwise} \end{cases}. \tag{18}$$

Figure 6 shows a comparison between the accelerated coefficients $\widetilde{\alpha}_k^{acc}(t)$ (blue) and the step coefficients $\alpha_k^{step}(t)$ (orange) of Spira's section for $t = 400$ and $k = 1, \ldots, 400$:

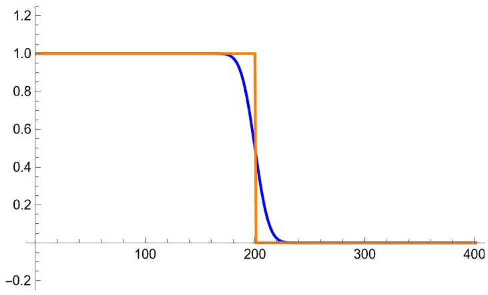

Figure 6. The accelerated coefficients $\widetilde{\alpha}_k^{acc}(t)$ (blue) and the step coefficients $\alpha_k^{step}(t)$ (orange) of Spira's section for $t = 400$ and $k = 1, \ldots, 400$.

We thus have

Corollary 1. *The accelerated section $\widetilde{Z}_{N(t)}(t)$ is related to Spira's section $Z_{N(t)}(t)$ via a smoothing of the step coefficients $\alpha_k^{step}(t)$ to obtain $\widetilde{\alpha}_k^{acc}(t)$. Moreover,*

$$lim_{t\to\infty} ||\widetilde{\alpha}_k^{acc}(t) - \alpha_k^{step}(t)|| = 0 \tag{19}$$

in the ℓ_2 norm.

3. Discussion and Conclusions

Sections of the Hardy Z-function are known to approximate the Hardy Z-function in two different ways: (a) The classical Hardy–Littlewood AFE given by $2Z_{\widetilde{N}(t)}(t)$ in (4) and (b) Spira's approximation given by $Z_{N(t)}(t)$ in (8). Although the AFE is more efficient and theoretically expected to be superior, Spira suggested, based on his numerical experimentations, that, in practice, his approximation might consistently satisfy the RH for any $t \in \mathbb{R}$, in the sense that all of its zeros are real. This is in striking contrast to the properties of the AFE, which requires the further evaluation of the Riemann–Siegel formula for this purpose.

In this work, we have presented theoretical justification for this mysterious observation, based on our new techniques of the asymptotic analysis of series acceleration, developed in [25], where we introduced a new accelerated approximation satisfying

$$Z(t) = \widetilde{Z}_{N(t)}(t) + O(e^{-\omega t}), \tag{20}$$

where $\omega > 0$ is a certain positive constant. This approximation achieves the superior accuracy expected to be attained by the Hardy–Littlewood AFE coupled with the Riemann–Siegel formula when evaluated at the optimal order, according to the Berry and Keating conjecture. In general, for any sequence $\alpha_k = (\alpha_1, \alpha_2, \dots) \in \ell_2$, set

$$Z(t;\alpha_k) := \sum_{k=1}^{\infty} \alpha_k \frac{cos(\theta(t) - ln(k)t)}{\sqrt{k}}. \tag{21}$$

In a unified manner, we have shown in Proposition 1 that both Spira's sections and our accelerated sections can be expressed as elements in this space

$$\widetilde{Z}_{N(t)}(t) = Z(t;\widetilde{\alpha}_k^{acc}(t)) \quad ; Z_{N(t)}(t) = Z(t;\alpha_k^{step}(t)), \tag{22}$$

where $\alpha_k^{step}(t)$ is defined in (18), and the definition of $\alpha_k^{acc}(t)$ is defined in (13). Furthermore, Corollary 1 shows that

$$lim_{t\to\infty}||\widetilde{\alpha}_k^{acc}(t) - \alpha_k^{step}(t)|| = 0. \tag{23}$$

This essentially implies that Spira's section $Z_{N(t)}(t)$ asymptotically coincides with our accelerated sections $\widetilde{Z}_{N(t)}(t)$ as $t \to \infty$.

In conclusion, our results provide the required theoretical justification to the numerical phenomena observed by Spira. Indeed, the fact that the difference between the accelerated sections $\widetilde{Z}_{N(t)}$ and the Hardy Z-function $Z(t)$ itself is imperceptible, coupled with the convergence of $Z_{N(t)}(t)$ to $\widetilde{Z}_{N(t)}$ at large t, establishes that Spira's RH for sections is essentially equivalent to RH for $Z(t)$ itself. Moreover, our results further motivate the definition of the new parametrized space of sections $Z(t;\alpha_k)$ and the study of the properties of their zeros with respect to variation in the parameters $\alpha_k \in \ell_2$, suggesting a promising direction for further exploration.

Finally, let us note that one of the features responsible for the notorious difficulty of the Riemann hypothesis is the fact that the Riemann–Siegel formula includes terms of the form (6) beyond the main Hardy–Littlewood sum (4). These correcting terms, while computationally feasible, present significant analytical challenges. We argue that the results of this work, showing that Spira's higher-order sections, which do not require any further correction terms, already capture the location of the zeros, represent a substantial theoretical development, potentially enabling innovative approaches to studying the zeros of the Riemann zeta function.

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