

Computational methods for evaluating the Riemann zeta function

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Abstract

We introduce the Riemann Zeta function, $\zeta(s)$, and a few well known theoretical results. The rest of this paper explores numerical techniques which allow us to approximate $\zeta(s)$ and its zeros. We investigate which methods are best suited for evaluating $\zeta(s)$ at various domain, for example the integers, complex arguments, and arguments near the critical line. We present some well known algorithms for evaluating complex arguments such as the Euler-Maclaurin method, a few algorithms based on convergent alternating series (which are simple to implement), and the Riemann-Siegel formula, a powerful algorithm for evaluating the Riemann zeta function near the critical line.

Contents

1	Introduction	6
1.1	Background Material	6
1.1.1	Behavior of the Riemann zeta function in various domains	6
1.1.2	Introducing zeros	8
1.1.3	Connection to the prime numbers	10
1.2	Aim, Overview, and Structure	11
2	Numerical Evaluations of $\zeta(s)$	13
2.1	Euler Maclaurin Method	13
2.2	Alternating Series Method	15
2.2.1	The method of convergence of alternating series	18
2.3	Riemann-Siegel formula	20
2.3.1	Riemann-Siegel formula on the critical line $Re(s) = \frac{1}{2}$	21
2.4	Evaluations of $\zeta(s)$ at integer arguments	31
2.4.1	Even integers	32
2.4.2	Odd integers	35

3	Conclusion	48
4	Various Code	50
5	Bibliography	56

1 Introduction

Definition: The Riemann zeta function is defined as follows

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = 1 + \frac{1}{2^s} + \frac{1}{3^s} + \frac{1}{4^s} + \dots = \prod_p \frac{1}{1 - p^{-s}} \quad (1.1)$$

where $s = a + bi \in \mathbb{C}$ and p are primes . The second equality is a well known result called the Euler Product Expansion of $\zeta(s)$. This formula, perhaps famous because it can be used to investigate properties of the prime numbers, was first expressed by Riemann in 1859. He used it to construct an explicit formula for the number of primes up to any preassigned limit. This proved to be an improvement of the approximation given by the prime number theorem which will be discussed in the next section. His formula approximation depended on knowing the zeros of the formula (1), instances of s where (1) is equal to zero. The investigation for these zeros is an important endeavor as we see later on in this introduction.

1.1 Background Material

1.1.1 Behavior of the Riemann zeta function in various domains

It can easily be shown that the summation diverges for $s = 1$. It is slightly more difficult to show that it also diverges for $s \neq 1$ if we have $Re(s) = 1$. For $s > 1$, $\zeta(s)$ converges absolutely to an analytic function, in fact this is true also for $Re(s) > 1$. The Riemann

zeta function is defined for complex valued s where $Re(s) > 1$, however through analytic continuation, $\zeta(s)$ extends to the whole complex plane (except for a simple pole at $s = 1$) as a meromorphic function.

Although $\zeta(s)$ diverges for $s = 1$, we can still describe the behavior of the function as $s \searrow 1$, that is as s approaches 1 from above.

Proposition 1.1

$$\lim_{s \searrow 1} (s - 1) \cdot \zeta(s) = 1$$

proof: Consider the inequality

$$(n + 1)^{-s} < \int_n^{n+1} x^{-s} dx < n^{-s}$$

for $n \geq 1$. Summing the inequality, we obtain

$$\zeta(s) - 1 < \int_1^\infty x^{-s} dx = (s - 1)^{-1} < \zeta(s)$$

and so we have $1 < (s - 1)\zeta(s) < s$. If we now let $s \searrow 1$ we obtain the desired result.

[19]□

It should be noted that, in this proof, we use the upper and lower Riemann sums for the estimate. It should also be mentioned that this proposition implies that the Riemann zeta function has a simple pole with residue 1 at $s=1$.

1.1.2 Introducing zeros

Numerical evaluations of $\zeta(s)$ “have been used to establish theoretical bounds...There is Euler’s rigorous deduction of the infinitude of primes from the appearance of the pole at $s = 1$; in fact he deduced a stronger result that the sum of the reciprocals of the primes diverges.” [5] Another instance of when numerical evaluations facilitated the development of theory is when Te Riele and Odlyzko approximated the first two thousand critical zeros of $\zeta(s)$ and used them to disprove Mertens conjecture, “thanks to a massive evaluation of the zeta-function” [3]. Their results can be found in [1] and [2].

The zeros for $\zeta(s)$ are interesting. Their intrigue comes from their connection to the distribution of prime numbers. Zeros are instances of s where $\zeta(s) = 0$. We know $\zeta(s)$ has two types of zeros, namely trivial and non-trivial. Trivial zeros are “trivial” in the sense that we know they all occur at the negative numbers. So we have that $\zeta(s) = 0$ for $s = -2, -4, -6, \dots$

The non-trivial zeros are even more interesting. This is partly due to the fact that their distribution is far less understood. More importantly, the study of the non-trivial zeros has yielded magnificent results pertaining to the prime numbers, which have mysterious and far reaching connections to seemingly countless results in different fields of mathematics. We know that all non-trivial zeros are contained in $\{s \in \mathbb{C} : 0 < \operatorname{Re}(s) < 1\}$. This is called the critical strip. We refer to the set $\{s \in \mathbb{C} : \operatorname{Re}(s) = \frac{1}{2}\}$ as the critical line. One of the most important open problems in number theory today is concerned with these zeros, the Riemann Hypothesis, conjectures that all non-trivial zeros s of $\zeta(s)$ have $\operatorname{Re}(s) = \frac{1}{2}$, that

is that they occur on the critical line. This conjecture has been standing since Riemann stated it in 1859. In 1900, Hilbert added it to his list of 23 unsolved problems. Hardy proved that on the critical line there exist infinitely many zeros. The first 1.5 billion non-trivial zeros were proved to be on the critical line by 1915. The exploration which has been fueled by this conjecture has certainly enriched the fields of number theory and complex numbers.

Let us take a look at an illustration concerning the first few non-trivial zeros.

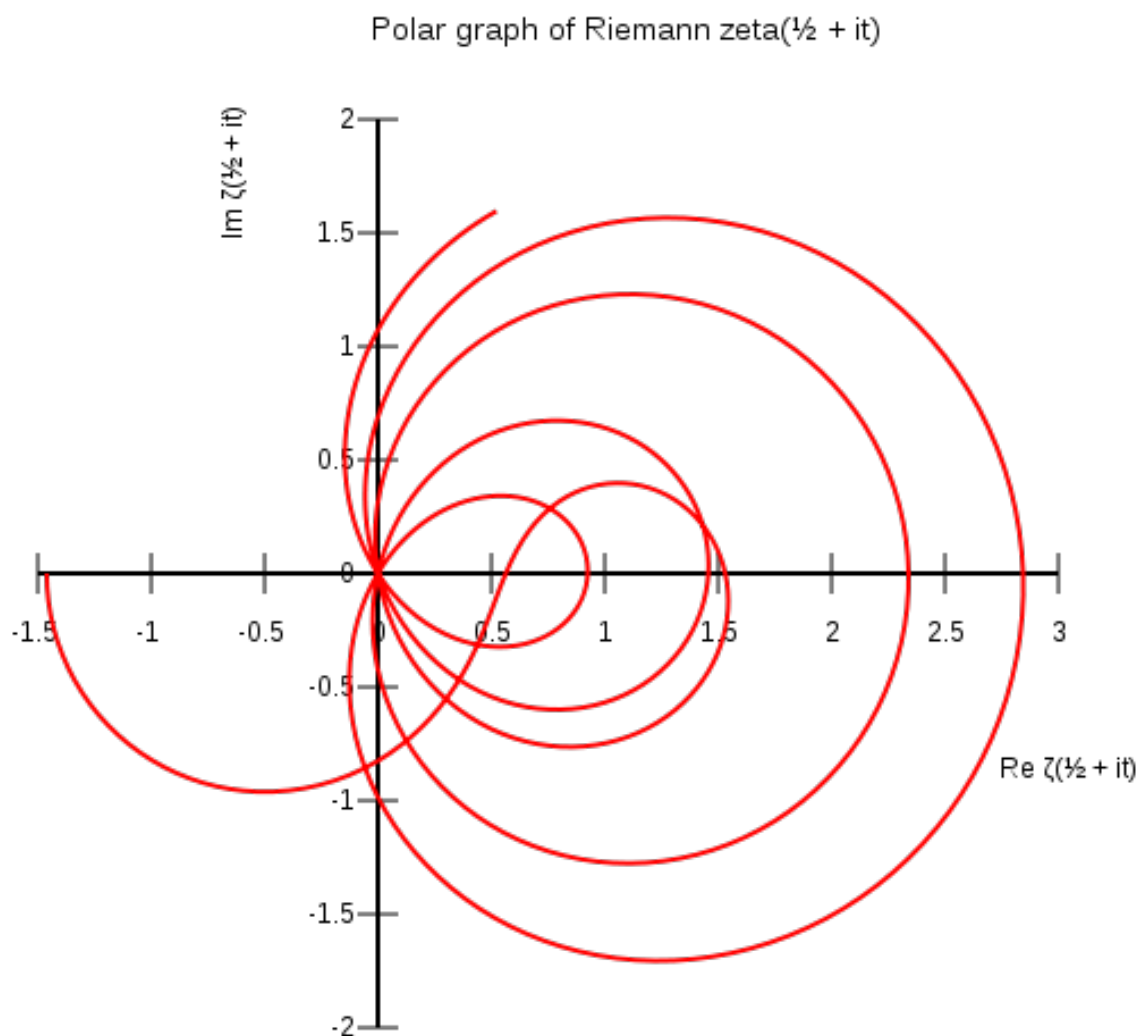


Figure A. This plot shows the real and imaginary parts of $\zeta(\frac{1}{2} + it)$, that is the values of the Riemann zeta function along the critical line, as t is varied from 0 to 35. [18, Derbyshire 2004, p. 221] Notice the spirals, passing through the origin, represent the first five zeros in the critical strip.

1.1.3 Connection to the prime numbers

The prime number theorem (PNT) describes the asymptotic distribution of the primes among the positive integers. It is a formalization of the intuitive idea that the prime numbers occur less and less often as they grow in size. This is done through constructing a precise quantification of the rate of occurrence. The PNT has been shown to be equivalent to “the non-vanishing of the Riemann Zeta function on the line $Re(s) = 1$ in the complex plane” [4]. The PNT states:

$$\pi(x) \sim li(x) := \int_0^x \frac{du}{\log u} \sim \frac{x}{\log x} \quad (1.2)$$

Another way, according to Borwein [5], to “witness the connection between the prime numbers and the Riemann zeta function is the following.” He states that “the behavior of $\zeta(s)$ on a line such as $Re(s) = 2$ in principle determines $\pi(x)$. In fact for any non-integer $x > 1$ ” we have

$$\pi^*(x) := \pi(x) + \frac{1}{2}\pi(x^{1/2}) + \frac{1}{3}\pi(x^{1/3}) + \dots = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{x^s}{s} \log \zeta(s) ds$$

for any real $c > 1$. After performing the contour integral to sufficient precision, we have a value for π^* and may “peel off” the terms with $\pi(x^{1/n})$ one by one, for example by recursive appeal to the same integral formula with reduced x . Through this sort of scheme, experimental calculations of $\pi(x)$ have been done using standard 64-bit floating point arithmetic for $\zeta(s)$ evaluations for quadrature of the contour integral, with Gaussian decay specified for the integrand. These calculations can reach up to $x \sim 10^{14}$.

1.2 Aim, Overview, and Structure

The rest of this paper is primarily concerned with presenting and briefly discussing numerical techniques for evaluating the Riemann zeta function in different context. It is emphasized that this paper has more of an experimental and computational focus than a pure theoretical one. We aim to discuss the purpose for which each method is best used, for example we find that for simplicity and efficiency the alternating series methods in section 2.1 are best suited. However, if we are interested more in computing zeros (evaluations of the Riemann zeta function near $Re(s) = \frac{1}{2}$), then the Riemann-Siegel formula is best suited. This method is found in section 2.3.

Section two presents the numerical methods. In the first subsection we discuss the formula derived from the famous classical Euler-Maclaurin method. This was the original algorithm presented by Euler, it is generally not used in modern day computations due to its slow speed because of the computation of Bernoulli numbers involved in the algorithm. In section 2.2 we present some efficient algorithms which are simple to imple-

ment and based on formula (2.3) and convergent alternating series. These are faster algorithms than the traditional Euler-Maclaurin method because of the computation of “Bernoulli-Like” numbers as opposed to Bernoulli numbers. These methods are best suited for middle or high precision evaluations of $\zeta(s)$, for low precision calculations (near the critical line) section 2.3 is best suited. We investigate why the Riemann-Siegel Z-function is convenient for exploring $\zeta(s)$ near or on the critical line. In the investigation, code was written in Python to generate a graph of the Riemann-Siegel Z-function. This code can be found at the end of this paper in an appendix called Various Codes, refer to the Table of Contents.

In Section 2.4 we present some well known and a relatively new algorithm for evaluating the Riemann zeta function at integer valued arguments. Here, we find that the studying the odd-valued integer arguments are much more difficult to study than the even-valued arguments. This is primarily due to the fact that, unlike for the even integers in formula (2.23), a closed form expression representing the Riemann zeta function evaluated at odd integers has not yet been discovered. We present a proof for formula (2.23). The rest of the section, namely subsection 2.4.2, discusses various techniques for evaluating the Riemann zeta function for odd-valued integer arguments, all of which involve integral representations.

2 Numerical Evaluations of $\zeta(s)$

In this section we discuss methods for numerically evaluating $\zeta(s)$ for complex numbers $s = a + bi$ as well as for integers. The most desirable method depends on the purpose for which the method is being employed. Normally, a specific method is geared to a particular domain, such as the positive integers, arguments in arithmetic progression, or the critical strip. [5] For example, for high or medium precision the alternating series method is best and for low precision the best method is the Riemann-Siegel method. This method is better suited for evaluations on the critical strip and hence for computations of zeros. [3]

2.1 Euler Maclaurin Method

“Until the 1930’s the workhorse for the evaluation art for the Riemann zeta function was Euler-Maclaurin expansion.” [5]

We can apply the standard Euler-Maclaurin formula not to $\zeta(s)$, but to the remainders $\sum_{n>N} \frac{1}{n^{-s}}$ of $\zeta(s)$. Before we state the result, let us state the standard Euler-Maclaurin summation formula in its most general form.

$$\sum_{n=a}^b f(n) = \int_a^b f(t)dt + \frac{1}{2}(f(b)+f(a)) + \sum_{i=2}^k \frac{b_i}{i!}(f^{(i-1)}(b)-f^{(i-1)}(a)) - \int_a^b \frac{B_k(\{1-t\})}{k!} f^{(k)}(t)dt$$

where a and b are arbitrary real numbers where $b - a$ is a positive integer. B_n and b_n are Bernoulli polynomials and Bernoulli numbers, respectively and k is a positive integer. The function f should have continuous k -th derivatives. The notation $\{t\}$ for real numbers

t denotes the fractional part of t . The remainder term is given by the last integral in the formula above. Generally speaking, this formula gives an approximation of $\sum_{i=0}^n f(i)$ through the integral $\int_0^n f(t)dt$ with an error term involving an integral with Bernoulli numbers. The result is

$$\zeta(s) = \sum_{n=1}^N \frac{1}{n^{-s}} + \frac{N^{1-s}}{s-1} + \frac{N^{-s}}{2} + \sum_{r=1}^{q-1} \frac{B_{2r}}{(2r)!} s(s+1) \cdots (s+2r-2) N^{-s-2r+1} + E_{2q}(s) \quad (2.1)$$

for any complex $s = a + bi$ with $a = \text{Re}(s) > -2q + 1$. Where B_{2r} are the Bernoulli numbers. [3] It should be noted that N and q are fixed. The error term is approximated in the form

$$|E_{2r}(s)| < \left| \frac{s(s+1) \cdots (s+2q-1) B_{2q} N^{-s-2q+1}}{(2q)!(a+2q-1)} \right| \quad (2.2)$$

There are difficulties presented in using this method since it requires the computation of Bernoulli numbers and the error term expansion is non-convergent. The expansion is of asymptotic character and when trying a new precision, rescaling the cutoff parameters is required

Furthermore, even if we were to choose q and N carefully, the expansion would still converge at a slower rate than the expansion obtained from simpler techniques based on the acceleration of alternating series. [3].

2.2 Alternating Series Method

We present the following extension of the Riemann zeta function

$$\zeta(s) = \frac{1}{(1 - 2^{1-s})} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^s} \quad (2.3)$$

where, here, we have $\operatorname{Re}(s) > 0$ and $s \neq 1$. We present some algorithms from [6].

Algorithm 1. Let $p_n(x) := \sum_{k=0}^n a_k x^k$ be a polynomial of degree n such that it does not vanish at -1 . Let

$$c_j := (-1)^j \cdot \sum_{k=0}^j (-1)^k a_k - p_n(-1) \quad (2.4)$$

then we have

$$\zeta(s) = \frac{1}{(1 - 2^{1-s})p_n(-1)} \cdot \sum_{j=0}^{n-1} \frac{c_j}{(1+j)^s} + \xi_n(s) \quad (2.5)$$

where

$$\xi_n(s) = \frac{1}{p_n(-1)(1 - 2^{1-s})} \frac{1}{\Gamma(s)} \int_0^1 \frac{p_n(x) |\log x|^{s-1}}{1+x} dx \quad (2.6)$$

Here Γ is the gamma function. For a proof of (2.4) see [6], where it is also observed that the c_j in (2.4) are the coefficients of $\frac{p_n(x) - p_n(-1)}{1+x}$ which is a polynomial of degree $n-1$.

The difficulty here is to pick p_n such that the error in the integral for ξ_n over $p_n(-1)$ is as small as possible. Borwein suggests (in [6]) that since for polynomials of comparable supremum norm on $[0, 1]$, the Chebychev polynomials, when shifted to $[0, 1]$ and also normalized, maximize the value of $p_n(-1)$. They are an obvious choice for p_n and they

provide us with the next result.

Algorithm 2. Let

$$d_k := n \cdot \sum_{i=0}^k \frac{(n+i-1)!4^i}{(n-i)!(2i)!} \quad (2.7)$$

then

$$\zeta(s) = \frac{-1}{d_n(1-2^{1-s})} \cdot \sum_{k=0}^{n-1} \frac{(-1)^k(d_k - d_n)}{(k+1)^s} \quad (2.8)$$

where for $s = \sigma + it$ with $\sigma \geq \frac{1}{2}$ we have

$$|\gamma_n(s)| \leq \frac{2}{(3 + \sqrt{8})^n} \frac{1}{|\Gamma(s)|} \frac{1}{|(1-2^{1-s})|} \leq \frac{3}{(2 + \sqrt{8})^n} \frac{(1+2|t|)e^{\frac{|t|\pi}{2}}}{|(1-2^{1-s})|} \quad (2.9)$$

We see that approximately $1.3n$ terms are required for n digit accuracy, given we are close enough to the real axis.

Algorithm 3. This algorithm is even simpler than the previous, though not as fast.

Take $p_n(x) := x^n(1-x)^n$ and let

$$e_j = (-1)^j \left[\sum_{k=0}^{j-n} \frac{n!}{k!(n-k)!} - 2^n \right]$$

then

$$\zeta(s) = \frac{-1}{2^n(1-2^{1-s})} \sum_{j=0}^{2n-1} \frac{e_j}{(j+1)^s} + \gamma_n(s) \quad (2.10)$$

where for $s = \sigma + it$ with $\sigma > 0$ we have

$$|\gamma_n(s)| \leq \frac{1}{8^n} \frac{(1 + |\frac{t}{\sigma}|) e^{\frac{|t|\pi}{2}}}{|1 - 2^{1-s}|}.$$

If $-(n-1) \leq \sigma < 0$ then

$$|\gamma_n(s)| \leq \frac{1}{8^n |1 - 2^{1-s}|} \frac{4^{|\sigma|}}{|\Gamma(s)|}$$

Note that for $s = -1, 2, \dots, -n+1$ we have $\gamma_n(s) = 0$.

“The fact that convergence persists into the part of the half plane $\{re(s) < 0\}$ is a consequence of the fact that

$$\int_0^1 \frac{x^n(1-x)^n}{1+x} |\log x|^{s-1} dx$$

converges provided $re(s) > -n$.” [6] Therefore, this algorithm gives a proof of the analytic continuation of $\zeta(s)(1-s)$.

For any computations based on Euler-Maclaurin, Bernoulli numbers will need to be computed. If these Bernoulli numbers are stored then subsequent evaluations will be faster, however this still makes the method “storage intensive” and “computationally expensive” for large precision computations. “Roughly speaking, order of n Bernoulli numbers are required for n -digit precision and this requires in excess of order of n^2 storage.” [6]

The sum of Algorithm 2 computes Bernoulli numbers for $s = -1, \dots, -n+1$. “The Bernoulli-Like coefficients of Algorithms 2 and 3 are much easier to compute and if done

sequentially require only one additional binomial coefficient per term which computes by a single multiplication and division.” [6]

Another method, by Gourdon and Sebah [3], is based on the alternating series convergence we saw above. This method is also efficient and easy to implement.

2.2.1 The method of convergence of alternating series

Let $s = \sigma + it$ be a complex number with $\sigma = \text{Re}(s) > 0$. We begin with the “Zeta alternating series”

$$\zeta_a(s) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n^s} = (1 - 2^{1-s})\zeta(s). \quad (2.11)$$

”We apply the general technique of convergence of alternating series of [7] described in Acceleration of the Convergence of Series.” [7] Let $P_n(x) = \sum_{k=0}^n p_k(-x)^k$ be a polynomial with $P_n(-1) \neq 0$. Define S_n as

$$S_n = \frac{1}{P_n(-1)} \sum_{k=0}^{n-1} c_k \frac{(-1)^k}{(k+1)^s},$$

$$c_k = \sum_{j=k+1}^n p_j$$

Now we have the identity

$$\zeta_a(s) - S_n = \xi_n \quad (2.12)$$

where

$$\xi_n = \frac{1}{P_n(-1)\Gamma(s)} \int_0^1 \frac{P_n(x)(\log(1/x))^{s-1}}{1+x} dx \quad (2.13)$$

As we saw before, polynomials P_n are chosen such that the supremum of the norm is small, that is $\sup_{x \in [0,1]} |P_n(x)/P_n(-1)|$ is small making ξ_n small. This identity can be used with the Chebyshev polynomials shifted to $[0, 1]$ as before, can be used with Algorithm 2 to compute $\zeta(\sigma + it)$ with d decimals of accuracy, which requires n number of terms approximately equal to $1.3d + 0.9|t|$.

The approach we present next is based on the choice of polynomial $x^n(1 - x)^n$. This approach, although less efficient, is simpler. The integral in (2.13) is convergent if $\sigma = \operatorname{Re}(s) > -(n - 1)$, so we may use Algorithm 3 and let

$$e_k = \sum_{j=k}^n \binom{n}{j}$$

then

$$\zeta(s) = \frac{1}{(1 - 2^{1-s})} \left[\sum_{k=1}^n \frac{(-1)^{k-1}}{k^s} + \frac{1}{2^n} \sum_{k=n+1}^{2n} \frac{(-1)^{k-1} e_{k-n}}{k^s} \right] + \gamma_n(s)$$

where for $s = \sigma + it$ with $\sigma > 0$ we have

$$|\gamma_n(s)| \leq \frac{1}{8^n} \frac{(1 + |\frac{t}{\sigma}|) e^{\frac{|t|\pi}{2}}}{|1 - 2^{1-s}|}.$$

If $-(n - 1) \leq \sigma < 0$ then

$$|\gamma_n(s)| \leq \frac{1}{8^n |1 - 2^{1-s}|} \frac{4^{|\sigma|}}{|\Gamma(s)|}$$

Note that for $s = -1, 2, \dots, -n + 1$ we have $\gamma_n(s) = 0$.

These techniques are easy to implement and efficient to compute $\zeta(s)$ with high or middle

accuracy, that is for $s = \sigma + it$ where t is small. In practice, terms are computed sequentially, with a fixed number of multiplication and addition per term. For integer values of s , the “binary-splitting technique can be used making these formula suitable for huge computations in quasi-linear time.” [3]. For large values of t , to compute $\zeta(\frac{1}{2} + it)$ requires a number of terms proportional to $|t|$. As such, we will see, the Riemann-Siegel formula is better suited.

2.3 Riemann-Siegel formula

The Riemann-Siegel formula and its variants “amount to the most powerful evaluation scheme known for s possessed of large imaginary part.” [5] This allows us to estimate $\zeta(\sigma + it)$ in the critical strip for large values of t with a number of terms proportional to $\sqrt{|t|}$. Note this is better than previous methods which require a number of terms proportional to $|t|$. Another fact about the Riemann-Siegel formula is it is difficult to implement, and different variants are best suited in different regions of the complex plane with different error-bounding formula.

Theorem 1 (Riemann-Siegel formula) Let x and y be positive real numbers such that $2\pi xy = |t|$. Then for $s = \sigma + it$ with $0 \leq \sigma \leq 1$, we have

$$\zeta(s) = \sum_{n \leq x} \frac{1}{n^s} + \chi(s) \sum_{n \leq y} \frac{1}{n^{1-s}} + O(x^{-\sigma}) + O(|t|^{\frac{1}{2}-\sigma} y^{\sigma-1}) \quad (2.14)$$

where the O holds uniformly for $x > h$ and $y > h$ for any $h > 0$. [3] Here, $\chi(s)$ is the functional equation

$$\chi(s) = 2^s \pi^{s-1} \sin\left(\frac{\pi s}{2}\right) \Gamma(1-s). \quad (2.15)$$

We can use these formula when $x = y = \sqrt{\frac{|t|}{2\pi}}$ which gives the form

$$\zeta(s) = \sum_{n=1}^m \frac{1}{n^s} + \chi(s) \sum_{n=1}^m \frac{1}{n^{1-s}} + E_m(s) \quad (2.16)$$

where

$$m = \sqrt{\frac{|t|}{2\pi}}$$

and the error term satisfies

$$E_m(s) = O(|t|^{\frac{-\sigma}{2}}).$$

We may write an explicit asymptotic expansion of the error term, however in its general form it is complicated and messy. Although this error term depends in a complicated way on the particular domain of s which is of interest, it can be explicitly bounded for computations in regions of the complex- s plane which are useful. [8] We will focus on presenting the first few terms in the case when $\sigma = \frac{1}{2}$.

2.3.1 Riemann-Siegel formula on the critical line $Re(s) = \frac{1}{2}$

The Riemann-Siegel formula present interesting results on the critical line $\sigma = \frac{1}{2}$, in order to study these results we first define the Riemann-Siegel Z -function as in [3]. This function

allows for a convenient study of $\zeta(s)$ in the critical strip.

The Riemann-Siegel Z-function

We begin with the function $\chi(s)$ which satisfies $\chi(s)\chi(1-s) = 1$, we see that for $s = \frac{1}{2} + it$ we have

$$\chi\left(\frac{1}{2} + it\right)\chi\left(\frac{1}{2} - it\right) = 1$$

and therefore

$$|\chi\left(\frac{1}{2} + it\right)| = 1.$$

We can now implicitly define the function $\theta(t)$ as

$$e^{i\theta(t)} = \chi\left(\frac{1}{2} + it\right)^{-1/2} \tag{2.17}$$

with $\theta(0) = 0$.

As shown in [3], it can equivalently be shown that $\theta(t)$ also satisfies

$$\theta(t) = \arg(\pi^{-it/2}\Gamma(\frac{1}{4} + i\frac{t}{2})) \tag{2.18}$$

where they define the argument by continuous variation of t starting with the value 0 at $t = 0$.

The Riemann-Siegel Z-function (as referred to in [3], also referred to as the Hardy Z-

function in [5]) is defined for real valued t by

$$Z(t) = e^{i\theta(t)} \zeta\left(\frac{1}{2} + it\right). \quad (2.19)$$

It follows from the functional equation of the Zeta function that

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

and that $\overline{Z(t)} = Z(t)$. This shows $Z(t)$ is a real valued function and that

$$|Z(t)| = \left| \zeta\left(\frac{1}{2} + it\right) \right|.$$

This remarkable property is illustrated in Figures 1, 2, and 3 below.

Figure 1 simply plots $\zeta(\frac{1}{2} + it)$, and figure 2 plots $Z(t)$. However, if we take the absolute value, both $|Z(t)|$ and $|\zeta(\frac{1}{2} + it)|$ seemingly have the exact same plot, namely figure 3.

Upon observing figure 4, and the video created from figures 5 and 6, it becomes evident that studying Riemann-Siegel Z -function makes the study of $\zeta(\frac{1}{2} + it)$ relatively convenient.

Figure 4 certainly offers inspiration for using $Z(t)$ to compute $\zeta(s)$ on and near the critical line. And we will see that it is powerful in doing so, in the sense that it can do so for arguments with large imaginary part.

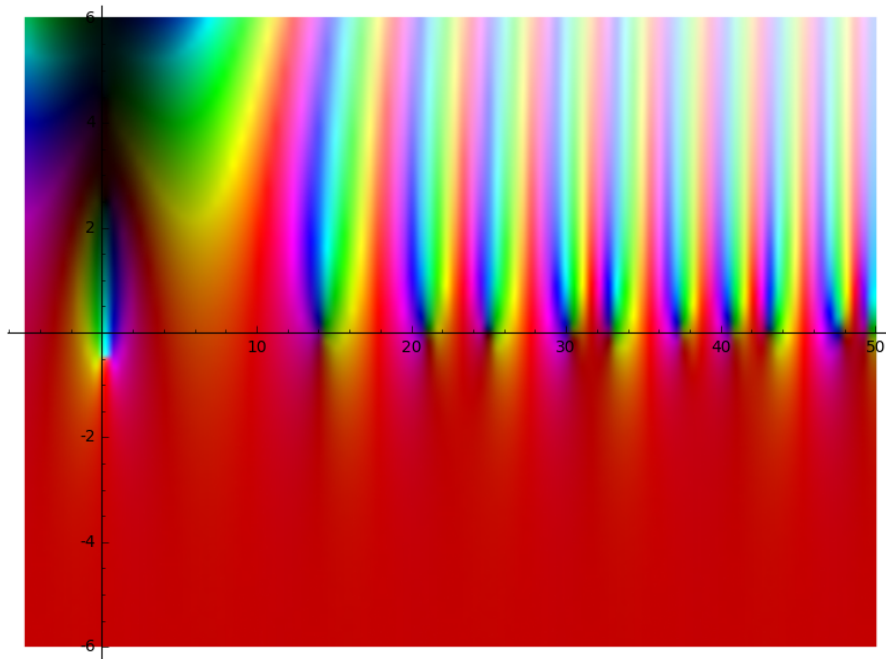


Figure 1:

The figure above (generated using a version of domain coloring) illustrates the Riemann zeta function $\zeta(s)$ evaluated at $s = \frac{1}{2} + it$ in a rectangular region of the complex plane.

It was generated in Sage using the `complex_plot()` function. The magnitude of the output is indicated by the brightness (with zero as black and infinity as white) and the argument is represented by the color or hue. Red represents positive real, increasing through orange and yellow as the argument increases.

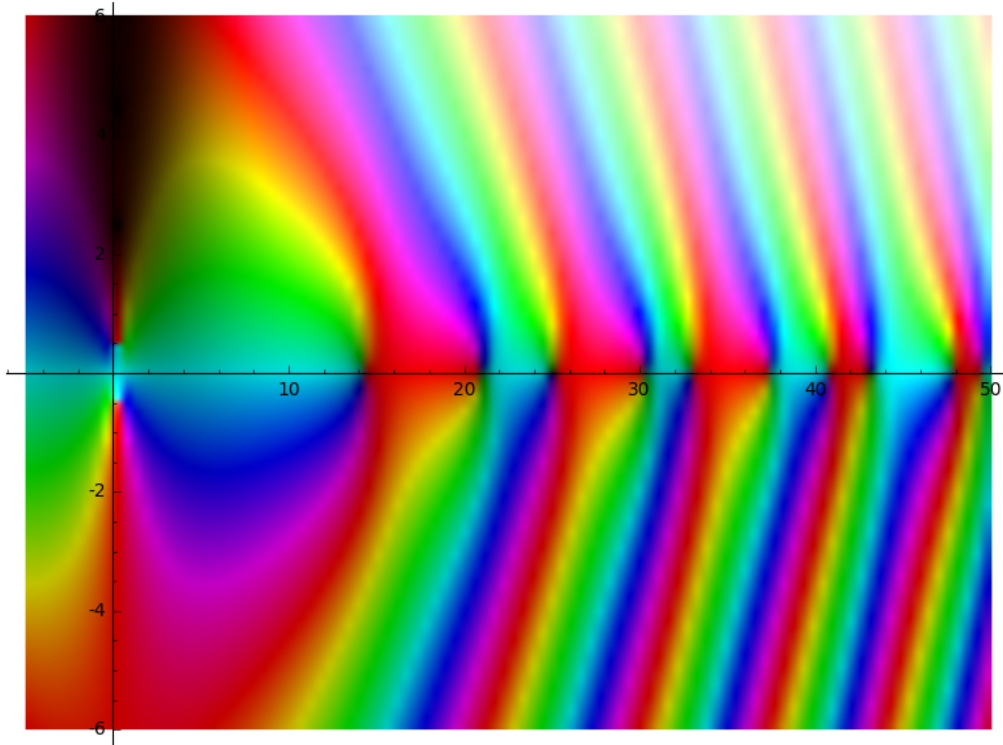


Figure 2:

The figure above illustrates the Riemann-Siegel Z-function $Z(t)$ for values of t near 0, again the color represents the argument and the brightness represents magnitude.

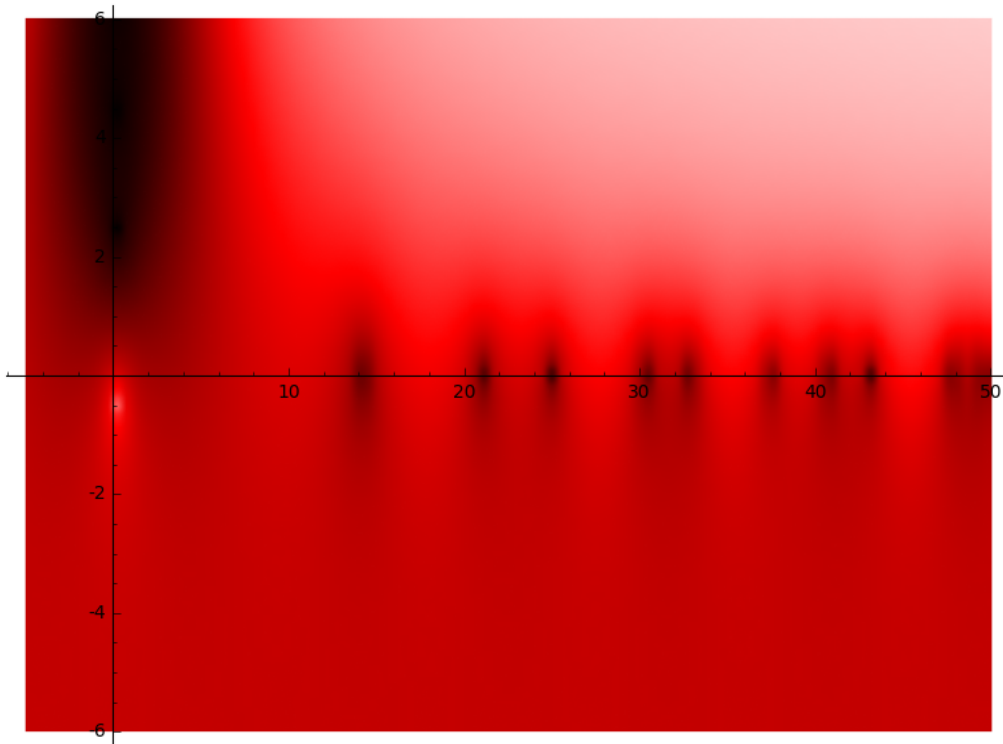


Figure 3:

The above figure illustrates the absolute value of the Riemann-Siegel Z-function $Z(t)$ for values of t near 0. As it turns out, this is also the plot representing $|\zeta(\frac{1}{2} + it)|$.

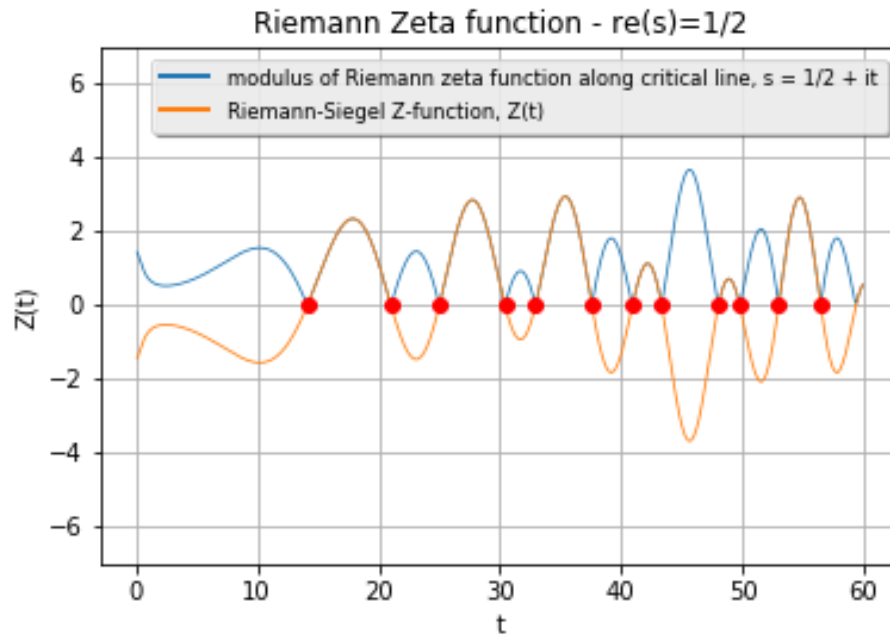


Figure 4:

Here we see the values of $|\zeta(\frac{1}{2} + it)|$ in blue and the values for the Riemann-Siegel Z-function $Z(t)$ in orange for t near zero. Notice that above the horizontal axis, the two paths conveniently overlap. This graph was it was generated using Python. The code used to generate these figures is including at the end of this paper. This code is original and was made for this project.

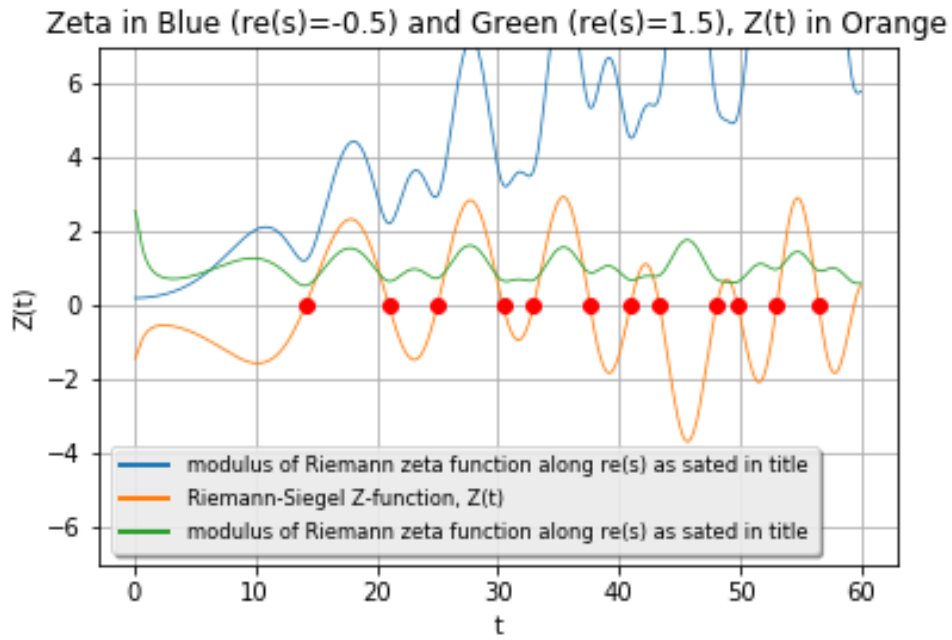


Figure 5:

Here we see the values for $|\zeta(-\frac{1}{2} + it)|$ in blue and the values for $|\zeta(\frac{3}{2} + it)|$ in green. From here, we used the second code in the section Various Codes to loop through an array of inputs for the real part of s and generate the same plot as in figure 5 for each input. A video was then created to show the green and blue paths meeting. This can be seen in figure 6. The video can be found at github page, <https://github.com/danerf/Riemann-zeta>, the video name is output.mp4. Alternatively, it can be accessed at the URL:
<https://raw.githubusercontent.com/danerf/Riemann-zeta/master/output.mp4>

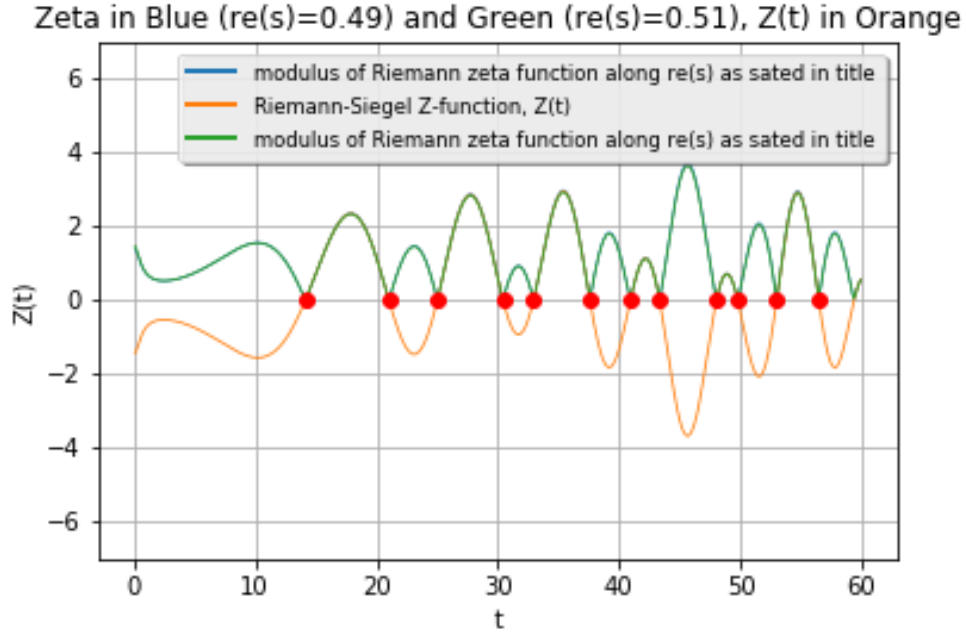


Figure 6:

Here we see blue and green meeting, again illustrating that on the critical line the application of the Riemann-Siegel formula is convenient.

The Riemann-Siegel formula and the Z-function

As done in [3], let us multiply (2.16) by $e^{i\theta(t)}$ and set $s = \frac{1}{2} + it$. We get

$$Z(t) = e^{i\theta(t)} \sum_{n=1}^m n^{-\frac{1}{2}-it} + e^{-i\theta(t)} \sum_{n=1}^m n^{-\frac{1}{2}+it} + O(t^{-\frac{1}{4}}) = 2 \sum_{n=1}^m \frac{\cos(\theta(t) - t \log n)}{\sqrt{n}} + O(t^{-\frac{1}{4}}). \quad (2.20)$$

This formula is well suited for large computations of t , and this is required for computations of zeros of the zeta function. Using the formulation of [5], asymptotic formula for the error term can be derived. For positive t we have

$$Z(t) = 2 \sum_{n=1}^m \frac{\cos(\theta(t) - t \log n)}{\sqrt{n}} + (-1)^{m+1} \tau^{-1/2} \sum_{j=0}^M (-1)^j \tau^{-j} \Phi_j(z) + R_m(t) \quad (2.21)$$

with $R_M(t) = O(t^{-(2M+3)/4})$ where $\tau = \sqrt{\frac{t}{2\pi}}$, $m = \lfloor \tau \rfloor$, and $z = 2(t - m) - 1$.

We present the first few $\Phi_j(z)$ as presented in [3]

$$\Phi_0(z) = \frac{\cos(\frac{1}{2}\pi z^2 + \frac{3}{8}\pi)}{\cos(\pi z)}$$

$$\Phi_1(z) = \frac{1}{12\pi^2} \Phi_0^{(3)}(z)$$

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

The general form equation for $\Phi_j(z)$ is very complicated. It can be seen in [9].

Although this notation and these functions seem complicated and messy, the wonderful benefit is that, as exposed in [5], the error terms R_M have been explicitly and rigorously bounded “in computationally convenient fashion.”

For $t \geq 200$ and $M \leq 10$ we have

$$|R_M(t)| < B_M t^{-(2M+3)/4}$$

and

$$\{B_0, B_1, \dots, B_{10}\} = \{0.127, 0.053, 0.011, 0.031, 0.017, 0.061, 0.661, 9.2, 130, 1837, 25966\}.$$

This gives us, for example the first few

$$|R_0(t)| \leq 0.127t^{-3/4},$$

$$|R_1(t)| \leq 0.053t^{-5/4},$$

$$|R_2(t)| \leq 0.011t^{-7/4}.$$

As mentioned in [3], to fully approximate $Z(t)$ using equation (2.21), we must first approximate $\theta(t)$. In [3], using expression (2.18), Stirling series are used to give this approximation

$$\theta(t) = \frac{t}{2} \log \frac{t}{2\pi} - \frac{t}{2} - \frac{\pi}{8} + \frac{1}{48t} + \frac{7}{5760t^3} + \dots \quad (2.22)$$

According to Goudon and Sebah in [3], for practical purposes in computations pertaining to zeros of $\zeta(s)$, it suffices to “locate” the zeros and use $M=1$ or $M=2$ in formula (2.21) instead of precisely computing every zero. For, t close to 10^{10} for example, if we choose $M = 1$ we obtain an absolute precision of $Z(t)$ which is smaller than 2×10^{-14} and with $M = 2$ it is smaller than 5×10^{-20} .

The method in [10], which is optimized, for finding and “proving” that zeros lie on the critical line reported to have never failed with the R_1 bound. The method of locating zeros is “ingenious: one uses known rigorous bounds on the number of zeros in a vertical segment of the critical strip.” [5] For example, the number of zeros which have $t \in [0, T]$

can be obtained from

$$N(T) = 1 + \pi^{-1}\theta(T) + \pi^{-1}\Delta \arg \zeta(s)$$

where Δ signifies the variation in the argument, which in [5] is defined to start from $\arg \zeta(2) = 0$ and to vary continuously to $s = 2 + iT$, then to $s = \frac{1}{2} + iT$. We proceed and count the number of sign changes of $Z(t)$, if this count “saturates” the theoretical bounds (that is if bound gives us $N(t) < 15.6$ and we obtain 15) then all of the zeros in that particular segment have been found. They must lie exactly on the critical line and since Z changed signs then these zeros must be simple.

The number of terms involved in (2.21) is proportional to \sqrt{t} , this is much better than methods previously discussed which require a number of terms of order t . For example lets take t around 10^{10} , Algorithm 2 in section 2.2 would require $\simeq 9 \times 10^9$ terms and the Riemann-Siegel formula would require only $\simeq 4 \times 10^4$ terms. The Riemann-Siegel formula with just $M = 1$ was used to compute the first 1.5 billion zeros of $\zeta(s)$.

One can derive, as stated in [5], the Riemann-Siegel formula by employing the application of saddle point methods to integral representations, and Galway [11] pointed out that these integrals are well suited for numerical integration. This means computations of $\zeta(s)$ to arbitrary accuracy can be carried out while still benefiting from other advantages of the Riemann-Siegel formula. This method also makes the error term analysis relatively simplified.

As can be seen in [5], we observe that the Riemann-Siegel formula shares properties in

common with equation (3) from the Euler-Maclaurin method. Borwein presents what the two have in common, “the Riemann-Siegel form is asymptotic in nature, at least in the sense that one chooses a set of about M correction terms depending, in principle, on *both* the range of the argument and the required accuracy.”

As we have observed the Riemann-Siegel formula is much better suited for computations near the critical line than the methods we previously discussed.

2.4 Evaluations of $\zeta(s)$ at integer arguments

We now turn our attention to evaluations of $\zeta(s)$ where s is an integer. It is easier to evaluate $\zeta(s)$ at positive even integers than positive odd integers. Euler famously argued $\zeta(s) = \frac{\pi^2}{6}$ using the sine product formula. We observe the general form below.

2.4.1 Even integers

Theorem 2 (Euler) For all positive integers n we have

$$\zeta(2n) = (-1)^{n+1} \frac{(2\pi)^{2n}}{2(2n)!} B_{2n} \quad (2.23)$$

where B_{2n} are Bernoulli numbers.

proof : From the cotangent exponential formula in [12], we have

$$\pi x \cot \pi x = i\pi x \frac{e^{i\pi x} + e^{-i\pi x}}{e^{i\pi x} - e^{-i\pi x}}$$

$$\begin{aligned}
&= i\pi x \frac{e^{2i\pi x} + 1}{e^{2i\pi x} - 1} \\
&= i\pi x \left(1 + \frac{2}{e^{2i\pi x} - 1}\right) \\
&= i\pi x + \frac{2i\pi x}{e^{2i\pi x} - 1} \\
&= i\pi x + \sum_{n=0}^{\infty} \frac{B_n(2i\pi x)^n}{n!}
\end{aligned}$$

by definition of Bernoulli numbers, now by changing summation limits and since the first two Bernoulli numbers are 1 and $-\frac{1}{2}$ respectively, we have

$$\begin{aligned}
i\pi x + \sum_{n=0}^{\infty} \frac{B_n(2i\pi x)^n}{n!} &= 1 + \sum_{n=2}^{\infty} \frac{B_n(2i\pi x)^n}{n!} \\
&= 1 - 2 \sum_{n=2}^{\infty} \left(-\frac{1}{2}\right) \frac{B_{2n}(2i\pi x)^n}{(2n)!}
\end{aligned}$$

and since odd Bernoulli numbers vanish, we have

$$1 - 2 \sum_{n=2}^{\infty} \left(-\frac{1}{2}\right) \frac{B_{2n}(2i\pi x)^n}{(2n)!} = 1 - 2 \sum_{n=1}^{\infty} \left(-\frac{1}{2}\right) \frac{B_{2n}(2i\pi x)^{2n}}{(2n)!} \quad (2.24)$$

Now, from Euler's formula for the sine function we have

$$\frac{\sin \pi x}{\pi x} = \prod_{k=1}^{\infty} \left(1 - \frac{x^2}{k^2}\right)$$

\Rightarrow

$$\ln \frac{\sin \pi x}{\pi x} = \ln \prod_{k=1}^{\infty} \left(1 - \frac{x^2}{k^2}\right)$$

\Rightarrow

$$\ln \sin \pi x = \ln \pi x + \sum_{k=1}^{\infty} \ln \left(1 - \frac{x^2}{k^2}\right)$$

\Rightarrow

$$\pi \frac{\cos \pi x}{\sin \pi x} = \frac{1}{x} + \sum_{k=1}^{\infty} \frac{1}{\left(1 - \frac{x^2}{k^2}\right)} \left(-\frac{2x}{k^2}\right)$$

by differentiating with respect to x . We know have

$$\pi x \cot \pi x = 1 + \sum_{k=1}^{\infty} \frac{1}{\left(1 - \frac{x^2}{k^2}\right)} \left(-\frac{2x^2}{k^2}\right)$$

notice if we use the geometric series we obtain

$$\begin{aligned} 1 + \sum_{k=1}^{\infty} \frac{1}{\left(1 - \frac{x^2}{k^2}\right)} \left(-\frac{2x^2}{k^2}\right) &= 1 + \sum_{k=1}^{\infty} \sum_{n=0}^{\infty} \left(\frac{x^2}{k^2}\right)^n \left(-\frac{2x^2}{k^2}\right) \\ &= 1 - 2 \sum_{k=1}^{\infty} \sum_{n=1}^{\infty} \left(\frac{x^2}{k^2}\right)^n. \end{aligned}$$

Now we may interchange the order of summation because to get

$$\pi x \cot \pi x = 1 - 2 \sum_{n=1}^{\infty} \left(\sum_{k=1}^{\infty} \frac{1}{k^{2n}}\right) x^{2n} = 1 - 2 \sum_{n=1}^{\infty} \zeta(2n) x^{2n}. \quad (2.25)$$

Now we may equate the coefficients of formula (2.25) and formula (2.24) to obtain our desired result

$$\zeta(2n) = (-1)^{n+1} \frac{B_{2n} 2^{2n-1} \pi^{2n}}{(2n)!}$$

□

The Bernoulli numbers are defined by the generating series

$$F(t) = \frac{t}{e^t - 1} = \sum_{m=0}^{\infty} \frac{B_m}{m!} t^m \quad (2.26)$$

in which $B_{2n+1} = 0$ for $n > 0$. This series has radius of convergence of 2π . From the

above results, we can deduce

$$\zeta(-2n) = 0$$

verifying the trivial zeros. We can also deduce

$$\zeta(1 - 2n) = -\frac{B_{2n}}{2n}$$

for integers $n > 0$.

From (2.25), we can derive

$$\pi x \cot \pi x = -2 \sum_{n=0}^{\infty} \zeta(2n) x^{2n}. \quad (2.27)$$

This series converges for $|x| < 1$ and is a “computationally lucrative representation for the even-argument ζ -values” according to Borwein [5], in that it can be used in many different algorithms including recycling algorithms.

2.4.2 Odd integers

As for the positive odd integers, a general form expression as in formula (2.23) for the evens has not yet been determined. For certain values it has been calculated to whatever number of places, but an exact expression has never been found. Regarding whether a convenient generating function can be obtained for odd integer arguments, there is (according to Borwein [5]) at least one candidate, namely the following relation regarding

the logarithmic derivative of the gamma function, that is the *digamma function* $\psi(z) = d \log \Gamma(z)/dz$ for $|x| < 1$:

$$\psi(1-x) = -\gamma - \sum_{n=2}^{\infty} \zeta(n)x^{n-1} \quad (2.28)$$

It was suggested in [13] by Luo and Wang that the Riemann zeta function with odd integer arguments “produces a recurrence relation that is self-recursive.” They point out that up until now $\zeta(s)$ can only be represented for positive odd integer arguments with series and integrals. As with traditional methods seen in previous sections (i.e. Euler-Maclaurin, Alternating Series, and Riemann-Siegel), a particular numerical method for evaluating the Riemann zeta function is limited to a particular domain. As such, Luo and Wang suggest that when focusing on the Riemann zeta function at positive odd integers, “a special method should be constructed in view of the connection of Riemann zeta function values between odd and even integers.” In their paper, they construct an algorithm for evaluating $\zeta(s)$ for odd integers $s = 2n + 1$ based on a recurrence formula which they obtained for the Riemann zeta function. Before discussing their results any further, let us first focus on some integral representations.

Usually, an expression which is given for evaluating the Riemann zeta function at odd integer arguments is

$$\zeta(2n+1) = \frac{(-1)^{n+1}(2\pi)^{2n+1}}{2(2n+1)!} \int_0^1 B_{2n+1}(x) \cot(\pi x) dx \quad (2.29)$$

where $B_m(x)$ are Bernoulli polynomials.

In [14], Cvijovic and Klinowski deduce four integral representations for $\zeta(2n+1)$ for $n \in \mathbb{N}$. They recall that there is an expression for $\zeta(2n)$ which is a rational multiple of π^{2n} , however there is no analogous closed form evaluation for $\zeta(2n+1)$. In their paper titled “Integral representations of the Riemann zeta function for odd-integer arguments,” three of the four integrals they derive are new in the sense that they were not included in [15] or [16]. We present their results and summarize their method for deriving their representations. Before we do this, we present some definitions and notation.

Throughout the rest of this section, $B_n(x)$ and $E_n(x)$ will be the Bernoulli and Euler polynomials, respectively.

$$\frac{te^{tx}}{e^t - 1} = \sum_{n=0}^{\infty} B_n(x) \frac{t^n}{n!} \quad (2.30)$$

where $|t| < 2\pi$ and

$$\frac{2e^{tx}}{e^t + 1} = \sum_{n=0}^{\infty} E_n(x) \frac{t^n}{n!} \quad (2.31)$$

where $|t| < \pi$. We also define

$$\eta(s) = (1 - 2^{1-s})\zeta(s) = \sum_{k=1}^{\infty} (-1)^{k-1} \frac{1}{k^s} \quad (2.32)$$

$$\lambda(s) = (1 - 2^{-s})\zeta(s) = \sum_{k=0}^{\infty} \frac{1}{(2k+1)^s} \quad (2.33)$$

$$\beta(s) = \sum_{k=0}^{\infty} (-1)^k \frac{1}{(2k+1)^s}. \quad (2.34)$$

Now we are ready to present their results.

Theorem 3 Assume that n is a positive integer and that $\delta = 1$ and $\frac{1}{2}$. Let $\zeta(s)$, $\eta(s)$, $\lambda(s)$, $\beta(s)$ be defined as above. Also let $B_n(x)$ and $E_n(x)$ be Bernoulli and Euler polynomials as in (2.29) and (2.30), respectively. Then we have:

$$\zeta(2n+1) = (-1)^{n+1} \frac{(2\pi)^{2n+1}}{2\delta(2n+1)!} \int_0^\delta B_{2n+1}(t) \cot(\pi t) dt,$$

$$\eta(2n+1) = (-1)^{n+1} \frac{(2\pi)^{2n+1}}{2\delta(2n+1)!} \int_0^\delta B_{2n+1}(t) \tan(\pi t) dt,$$

$$\lambda(2n+1) = (-1)^n \frac{\pi^{2n}}{4\delta(2n)!} \int_0^\delta E_{2n}(t) \csc(\pi t) dt,$$

$$\beta(s) = (-1)^n \frac{\pi^{2n}}{4\delta(2n-1)!} \int_0^\delta E_{2n-1}(t) \sec(\pi t) dt.$$

We observe that since all of the integrands have removable singularities on $[0, \delta]$, then the integrals in the above expressions do indeed exist. We will demonstrate this as they did in [14] but first some basic properties regarding the Bernoulli and Euler polynomials.

It is well known that the odd-indexed Bernoulli numbers are all zero. It follows that for $F(t)$ from formula (2.26), we have $F(t) - F(-t) = -t$. A fact which can be used directly to show that $B_1 = \frac{1}{2}$ and $B_m = 0$ for all odd $m > 1$. With this in mind, Cvijovic and Klinowski present the following property

$$\begin{aligned} \lim_{t \rightarrow 1/2} B_{2n+1}(t) \tan(\pi t) &= \lim_{t \rightarrow 1/2} \frac{B_{2n+1}(t)}{\cos(\pi t)} \\ &= \lim_{t \rightarrow 1/2} \frac{(2n+1)B_{2n}(t)}{-\pi \sin(\pi t)} \end{aligned}$$

$$= (1 - 2^{1-2n})(2n + 1)B_{2n}/\pi$$

since $B_n(\frac{1}{2}) = (2^{1-n} - 1)B_n$. This property can be found in the “Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables” [16, pg. 805, Eq. 23.1.21]. Now we present the proof for Theorem 3 as stated in [14].

Proof of the results in Theorem 3 First, they show the following four results:

$$\sin(2kx) \cot x = 1 + \sum_{j=1}^{k-1} \cos(2jx) + \sum_{j=1}^k \cos(2jx), \quad (2.35)$$

$$\sin(2kx) \tan x = (-1)^{k-1} + \sum_{j=1}^{k-1} (-1)^{k-1-j} \cos(2jx) + \sum_{j=1}^k (-1)^{k-j} \cos(2jx), \quad (2.36)$$

$$\frac{\sin(2k+1)x}{\sin x} = 1 + 2 \sum_{j=1}^k \cos(2jx), \quad (2.37)$$

$$\frac{\cos(2k+1)x}{\cos x} = (-1)^k + 2 \sum_{j=1}^k (-1)^{k-j} \cos(2jx). \quad (2.38)$$

They start from

$$2 \sin x \cos(2mx) = \sin(2m+1)x - \sin(2m-1)x$$

and obtain

$$2 \sin x \sum_{j=1}^k \cos(2jx) = \sin(2k+1)x - \sin x.$$

From here, formula (2.37) follows quite easily. To obtain formula (2.38) from (2.37), simply set $x = t + \frac{\pi}{2}$. To get formula (2.35) and (2.36) from (2.37) and (2.38), respectively, they

use

$$\sin(2kx) \cot x = \frac{1}{2} \left(\frac{\sin(2k+1)x}{\sin x} + \frac{\sin(2k-1)x}{\sin x} \right),$$

$$\sin(2kx) \tan x = \frac{1}{2} \left(\frac{\cos(2k-1)x}{\cos x} - \frac{\cos(2k+1)x}{\cos x} \right).$$

Next, they use the Fourier expansions for the Bernoulli and Euler polynomials from [16, pg. 805, Eq. 23.1.17 and Eq. 23.1.17]

$$B_{2n+1}(x) = (-1)^{n+1} \frac{2(2n+1)!}{(2\pi)^{2n+1}} \sum_{k=1}^{\infty} \frac{\sin(2k\pi x)}{k^{2n+1}} \quad (2.39)$$

$$E_{2n}(x) = \frac{(-1)^n 4(2n)!}{\pi^{2n+1}} \sum_{k=0}^{\infty} \frac{\sin(2k+1)\pi x}{(2k+1)^{2n+1}} \quad (2.40)$$

$$E_{2n-1}(x) = \frac{(-1)^n 4(2n-1)!}{\pi^{2n}} \sum_{k=0}^{\infty} \frac{\cos(2k+1)\pi x}{k^{2n}}, \quad (2.41)$$

where $n = 1, 2, 3, \dots$ and $0 < x \leq 1$. From these expansions, in conjunction with formula (2.35), (2.36), (2.37), (2.38) and the definitions given earlier for $\zeta(s)$, $\eta(s)$, $\lambda(s)$, $\beta(s)$, the formula in Theorem 3 are obtained. For instance,

$$\begin{aligned} (-1)^{n+1} \frac{(2\pi)^{2n+1}}{2(2n+1)!} \int_0^\delta B_{2n+1}(t) \tan(\pi t) dt &= \sum_{k=1}^{\infty} \frac{1}{k^{2n+1}} \int_0^\delta \sin(2k\pi t) \tan(\pi t) dt \\ &= \delta \sum_{k=1}^{\infty} (-1)^{k-1} \frac{1}{k^{2n+1}} = \delta \eta(2n+1). \end{aligned}$$

Here, the inversion of the order of summation and integration is allowed due to absolute convergence. This completes the proof for Theorem 3.

□

In the concluding remarks, Cvijovic and Klinowski deduce the following representations for $\zeta(2n+1)$, where n is a natural number

$$\zeta(2n+1) = \frac{(-1)^{n+1}(2\pi)^{2n+1}}{2\delta(1-2^{-2n})(2n+1)!} \int_0^\delta B_{2n+1}(t) \tan(\pi t) dt, \quad (2.42)$$

and

$$\zeta(2n+1) = \frac{(-1)^n \pi^{2n+1}}{4\delta(1-2^{-(2n+1)})(2n)!} \int_0^\delta E_{2n}(t) \csc(\pi t) dt \quad (2.43)$$

where $\delta = 1$ and $\frac{1}{2}$.

For computational speed and efficiency, there are accelerated series for the Riemann zeta function at odd integer arguments [15] and Fast computation of the Riemann Zeta function to arbitrary accuracy [11]. Another good candidate would be the method of Luo and Wang in [13]. Let us now go back and describe their algorithm.

Consider the definition of the Bernoulli polynomial (2.30), taking the derivative with respect to x on both sides gives us

$$B'_n(x) = nB_{n-1}(x). \quad (2.44)$$

We can also express Bernoulli polynomials explicitly in terms of Bernoulli numbers

$$B_n(x) = \sum_{k=0}^n \binom{n}{k} B_k x^{n-k}. \quad (2.45)$$

Luo and Wang introduce two kinds of “reduced Bernoulli numbers (RBNs)”, one relating

to even-indexed Bernoulli numbers, denoted by $+$

$$B_n^+ = (-1)^{n+1} B_{2n}. \quad (2.46)$$

The other relates to the odd-indexed Bernoulli polynomials, denoted by $-$

$$B_n^- = (-1)^{n+1} \int_0^1 B_{2n+1}(x) \cot(\pi x) dx. \quad (2.47)$$

In their paper, they demonstrate the asymptotic representation of the two RBNs and establish their integral representation. The asymptotic expressions of the Bernoulli polynomials at even and odd index (as expressed in [17]) are given by

$$(-1)^{n+1} \frac{(2\pi)^{2n}}{2(2n)!} B_{2n}(x) \sim \cos(2\pi x) \quad (2.48)$$

and

$$(-1)^{n+1} \frac{(2\pi)^{2n+1}}{2(2n+1)!} B_{2n+1}(x) \sim \sin(2\pi x). \quad (2.49)$$

Notice that (2.49) is simply a corollary of the Fourier expansion for the odd-indexed Bernoulli polynomial (2.39) and that (2.48) is a corollary of the Fourier expansion for the even-indexed Bernoulli polynomials

$$B_{2n}(x) = (-1)^{n+1} \frac{2(2n)!}{(2\pi)^{2n}} \sum_{k=1}^{\infty} \frac{\cos(2\pi kx)}{k^{2n}}. \quad (2.50)$$

Using the fact that

$$\int_0^1 \sin(2\pi x) \cot(\pi x) dx = 1,$$

and equations (2.48) and (2.49) they obtained the asymptotic behavior of the RBNs

$$B_n^+ = (-1)^{n+1} B_{2n}(0) \sim \frac{2(2n)!}{(2\pi)^{2n}} \quad (2.51)$$

and

$$B_n^- (-1)^{n+1} \int_0^1 B_{2n+1}(x) \cot(\pi x) dx \sim \frac{2(2n+1)!}{(2\pi)^{2n+1}}. \quad (2.52)$$

Now for the integral representations of the RBNs. Consider the following integrals

$$I_c(n, m) = \int_0^1 B_{2n}(t) \cos(m\pi t) dt \quad (2.53)$$

and

$$I_s(n, m) = \int_0^1 B_{2n+1}(t) \sin(m\pi t) dt \quad (2.54)$$

where m and n are integers and $n \geq 1$. For illustration purposes, let us show the direct computation for when $n = 1$

$$I_c(1, m) = \int_0^1 (t^2 - t + \frac{1}{6}) \cos(m\pi t) dt \quad (2.55)$$

$$= \begin{cases} 0, & m = 1, 3, 5, \dots \\ \frac{2!}{(m\pi)^2}, & m = 2, 4, 6, \dots \end{cases}$$

and

$$I_s(1, m) = \int_0^1 (t^3 - \frac{3}{2}t^2 + \frac{1}{2}t) \sin(m\pi t) dt \quad (2.56)$$

$$= \begin{cases} 0, & m = 1, 3, 5, \dots \\ \frac{3!}{(m\pi)^3}, & m = 2, 4, 6, \dots \end{cases}$$

As done in [13], we utilize (2.44) and integrate by parts twice to obtain

$$I_c(n, m) = -\frac{(2n)(2n-1)}{(m\pi)^2} I_c(n-1, m) \quad (2.57)$$

and

$$I_s(n, m) = -\frac{(2n+1)(2n)}{(m\pi)^2} I_s(n-1, m). \quad (2.58)$$

Now combining (2.55) and (2.56) with (2.57) and (2.58) we find that

$$I_c(n, m) = \frac{(-1)^{n+1}(2n)!}{(m\pi)^{2n}} \quad (2.59)$$

and

$$I_s(n, m) = \frac{(-1)^{n+1}(2n+1)!}{(m\pi)^{2n+1}} \quad (2.60)$$

hold for even m . The integral representations of the RBNs B_n^+ and B_n^- immediately follow

$$B_n^+ \sim 2(-1)^{n+1} I_c(n, 2) \quad (2.61)$$

and

$$B_n^- \sim 2(-1)^{n+1} I_s(n, 2). \quad (2.62)$$

We now define the reciprocal function

$$\rho(s) = \text{frac}\left(\frac{1}{\eta(s)}\right) = \frac{1}{\eta(s)} - 1. \quad (2.63)$$

The asymptotic nature of the ratio of the reciprocal function (2.63) at odd and even integers is of key interest in their paper [13]. Motivated by the Goldbach-Euler theorem and the related results (2.64), (2.65), (2.66), Luo and Wang demonstrate a formula, the “so-called” recurrence formula, on the condition that the argument is a positive integer. Also motivated by this recurrence, they manage to construct an algorithm for computing $\zeta(s)$.

The Goldbach-Euler theorem states that

$$\sum_{n=2}^{\infty} \text{frac}(\zeta(n)) = 1 \quad (2.64)$$

where $\text{frac}(x) = x - [x]$ denotes the fractional part of the real number x . Two related

results are

$$\sum_{n=1}^{\infty} \text{frac}(\zeta(2n)) = \frac{3}{4} \quad (2.65)$$

and

$$\sum_{n=1}^{\infty} \text{frac}(\zeta(2n+1)) = \frac{1}{4}. \quad (2.66)$$

Let us now present their recurrence formula and their proof.

Theorem 4 If n is a positive integer such that $n \geq 1$, the following recurrence relation holds

$$\lim_{n \rightarrow \infty} \frac{\rho(2n+1)}{\rho(2n)} = \frac{1}{2}. \quad (2.67)$$

proof : Using (2.23) and (2.29) and definition (2.63), we have

$$\frac{\rho(2n+1)}{\rho(2n)} = \frac{(2n+1)! - (2^{2n} - 1)\pi^{2n+1}B_n^-}{(2n)! - (2^{2n-1} - 1)\pi^{2n}B_n^+} \cdot \frac{B_n^+}{\pi B_n^-} \cdot \frac{2^{2n-1} - 1}{2^{2n} - 1}. \quad (2.68)$$

Since the limit of the right-hand side expression is exactly $\frac{1}{2}$ as n goes to ∞ , it suffices to prove

$$\frac{(2n+1)! - (2^{2n} - 1)\pi^{2n+1}B_n^-}{(2n)! - (2^{2n-1} - 1)\pi^{2n}B_n^+} \cdot \frac{B_n^+}{\pi B_n^-} \sim 1 \quad (2.69)$$

or equivalently

$$\frac{(2n+1)!}{\pi^{2n+1}} \cdot \frac{1}{B_n^-} - \frac{(2n)!}{\pi^{2n}} \cdot \frac{1}{B_n^+} \sim 2^{2n-1}. \quad (2.70)$$

From formula (2.51) and (2.52), namely the formula for asymptotic behavior of the RBNs, they claim to have finished the demonstration of the recurrence formula of the Riemann

zeta function. \square

We now describe how they use this recurrence relation to construct an algorithm for evaluating the Riemann zeta function at odd integer arguments. When n is large enough, (2.67) can be written as

$$\rho^l(2n+1) \sim \frac{1}{2}\rho(2n) \quad (2.71)$$

$$\rho^r(2n+1) = 2\rho(2n+2) \quad (2.72)$$

where $\rho^l(2n+1)$ and $\rho^r(2n+1)$ are two different representations of the asymptotic behavior of $\rho(2n+1)$. Either of these can be used to compute the Riemann zeta function at odd integers, according to Luo and Wang. They claim that there can exist a map from $\zeta(2n)$ and $\zeta(2n+2)$ to $\zeta(2n+1)$, from which an approximation of the values of $\zeta(2n+1)$ can be obtained with higher precision. Before progressing in the algorithm, they give two results.

Lemma 1 (Luo,Wang, [13]) If n is a positive integer such that $n \geq 1$, the two inequalities hold

$$\frac{4}{\eta(2n+2)} - \frac{1}{\eta(2n)} > 3 \quad (2.73)$$

and

$$\eta(2n) > \frac{2^{2n-1} - 2}{2^{2n-1} - 1}. \quad (2.74)$$

By virtue of this lemma, they present the following theorem.

Theorem 5(Luo,Wang,[13]) If n is a positive integer such that $n \geq 1$, the inequality holds

$$\zeta^l(2n+1) > \zeta^r(2n+1) > 1 \quad (2.75)$$

where $\zeta^l(2n+1)$ and $\zeta^r(2n+1)$ correspond to $\rho^l(2n+1)$ and $\rho^r(2n+1)$, respectively.

Now, since $\zeta(s)$ is monotonically decreasing, then $\zeta(2n+1)$ is between $\zeta^l(2n+1)$ and $\zeta^r(2n+1)$ for any positive integer value n . Luo and Wang regard the geometric mean values of formula (73) and (74) as approximate values of the reciprocal function $\rho(2n+1)$, namely

$$\rho(2n+1) \approx \sqrt{\rho(2n)\rho(2n+2)}. \quad (2.76)$$

This proves to be invaluable in their algorithm, whose basic steps are described below.

First, the values of $\rho(2n)$ and $\rho(2n+2)$ should be computed from formula (2.23), (2.32), and (2.63) in sequence. Second, from (78) and the result from the first step, $\rho(2n+1)$ can be obtained. Now $\zeta(2n+1)$ can be computed using (2.63) and (2.32) in reverse. This method requires the computation of $\zeta(2n)$ which in turn requires the computation of Bernoulli numbers. Given the error bounds discussed in [13], this method seems like a good candidate for calculating ζ -values for large odd integers.

3 Conclusion

The Riemann zeta function is fascinating on many levels. The search for numerical methods for evaluating and computing $\zeta(s)$ is ongoing. The motivation for such a pursuit is not by any means limited to a numerical verification of the Riemann Hypothesis. As mentioned before numerical methods have inspired theoretical advancements. Our review of various numerical methods led to the conclusion that each method is specific to a domain of the complex plane, and serves a specific purpose.

Originally, for computations concerning complex arguments, the Euler-Maclaurin method and its variants were the streamlined methods for high and middle precision computations. However as we saw in section 2.2, there are simpler methods which depend on the alternating series definition (2.3). These methods are also easier to implement as they don't require the computation of the traditional Bernoulli numbers. For low precision evaluations near the critical strip, the Riemann-Siegel method and its variants stand as modern benchmarks.

As for integer values, the formula for evaluating the Riemann zeta function at even integers (2.23) involves Bernoulli numbers as well. However, since it is a closed form explicit expression, it makes the study of the Riemann zeta function at even integers easier than that of the odd integers. The odd integer case involves integral representations, there is no known closed form expression for $\zeta(2n + 1)$.

Original work done in this project, without direct help from references, include but is

not limited to 1) some of the calculations done in the proof on pages 31, 32, and 33 involving the expression for the Riemann zeta function evaluated at even integers, 2) the investigation done involving figures 1 through 6, especially the Python code written in the section Various Codes and the corresponding github repository mentioned.

For further information, [3] and [5] present brief yet comprehensive studies.

4 Various Code

The following code produced Figure 4. It is written in Python 2.7.

It can all be found at <https://github.com/danerf/Riemann-zeta>

```
import numpy as np

import matplotlib.pyplot as plt

#The next library contains the zeta(), zetazero(), and siegelz() functions
from mpmath import *

mp.dps = 25; mp.pretty = True

def graph_zeta(real, image_name):

A,B,C = [], [], []

fig = plt.figure()

ax = fig.add_subplot(111)

for i in np.arange(0.1, 60.0, 0.1):

    function = zeta(real + 1j*i)

    function1 = siegelz(i)

    A.append(abs(function))

    B.append(function1)

    C.append(i)

ax.grid(True)

ax.plot(C,A, label='modulus of Riemann zeta function along
critical line,  $s = 1/2 + it$ ', lw=0.8)
```

```

ax.plot(C,B, label='Riemann-Siegel Z-function ,  $Z(t)$ ' , lw=0.8)

ax.set_title("Riemann Zeta function -  $\text{re}(s)=1/2$ ")

ax.set_ylabel("Z(t)")

ax.set_xlabel("t")

#Include legend

leg = ax.legend(shadow=True)

#Edit font size of legend to make it fit into chart

for t in leg.get_texts():

    t.set_fontsize('small')

#Edit the line width in the legend

for l in leg.get_lines():

    l.set_linewidth(2.0)

#Plot the zeroes of zeta

for i in xrange(1, 13):

    zero = zetazero(i)

    ax.plot(zero.imag, [0.0] , "ro")

#save plot and print that it was saved

ax.set_ylim(-7, 7)

plt.savefig(image_name)

print "Successfully plotted %s !" % image_name

plt.close()

```

```
graph_zeta(0.5, "Z(t)_Plot.png")
```

Now we have the code which produced an array of plots (the same as the plot produced above) each of which correspond to an input value from an input array. The plots (in .png format) were used to create the video (using ffmpeg on a Linux machine) on the github.com page created for this project. Namely, <https://github.com/danerf/Riemann-zeta>. It is used to further illustrate the convenience of the Riemann-Siegel Z-function near the critical line. The code is as follows.

```
import numpy as np

import matplotlib.pyplot as plt

#The next library contains the zeta(), zetazero(), and siegelz() functions
from mpmath import *

mp.dps = 25; mp.pretty = True

def graph_zeta(real, image_name):

A,B,C, D = [], [], [], []

fig = plt.figure()

ax = fig.add_subplot(111)

for i in np.arange(0.1, 60.0, 0.1):

    function = zeta(real + 1j*i)

    function2 = zeta((real+((0.5-real)*2))+1j*i)

    function1 = siegelz(i)

    A.append(abs(function))
```

```

        B.append(function1)

        C.append(i)

        D.append(abs(function2))

ax.grid(True)

ax.plot(C,A, label='modulus of Riemann zeta function along
re(s) as sated in title ', lw=0.8)

ax.plot(C,B, label='Riemann–Siegel Z–function , Z(t) ', lw=0.8)

ax.plot(C,D, label='modulus of Riemann zeta function along
re(s) as sated in title ', lw=0.8)

ax.set_title("Zeta in Blue (re(s)=%s) and Green (re(s)=%s),
Z(t) in Orange"%(real , real+(0.5–real)*2))

ax.set_ylabel("Z(t)")

ax.set_xlabel("t")

#Include legend

leg = ax.legend(shadow=True)

#Edit font size of legend to make it fit into chart

for t in leg.get_texts():

    t.set_fontsize('small')

#Edit the line width in the legend

for l in leg.get_lines():

    l.set_linewidth(2.0)

```

```

#Plot the zeroes of zeta

for i in xrange(1, 13):

    zero = zetazero(i)

    ax.plot(zero.imag, [0.0], "ro")

#save plot and print that it was saved

ax.set_ylim(-7, 7)

plt.savefig(image_name)

print "Successfully plotted %s !" % image_name

plt.close()

counter = 1

for i in np.arange(-0.5, 0.5, 0.01):

    counter += 1

    graph_zeta(i, "zeta_plot1_%s.png" % counter)

```

The sage code which was used to generate figures 1, 2, and 3 is as follows.

Figure1:

```
complex_plot(zeta((1/2)+i*x), (-5,50), (-6,6))
```

Figure2:

```

theta(x)=arg((pi^(-i*x/2))*gamma((1/4)+(i*x/2)))

complex_plot((e^(i*theta(x)))*zeta((1/2)+i*x), (-5,50), (-6,6))

```

Figure3:

```
theta(x)=arg((pi^(-i*x/2))*gamma((1/4)+(i*x/2)))
```

```
complex_plot(abs((e^(i*theta(x)))*zeta((1/2)+i*x)), (-5,50), (-6,6))
```

Or

```
complex_plot(abs(zeta((1/2)+i*x)), (-5,50), (-6,6))
```


5 Bibliography

References

- [1] J. Lagarias and A. Odlyzko, “Computing $\pi(x)$: an analytic method”, *J. Algorithms* **8**, (1987), 173-191.
- [2] A. Odlyzko and H.J.J. te Riele, “Disproof of the Mertens conjecture”, *J. Reine angew. Math.* **357**, (1985), 138-160.
- [3] Xavier Gourdon and Pascal Sebah, “Numerical evaluations of the Riemann Zeta function,” *Numbers, Constants and Computations*, (2003)
- [4] H.G. Diamond, “Elementary Methods in the study of the distribution of prime numbers,” *Volume 7, Number 3* (1982)
- [5] J. Borwein, D. Bradley, R. Crandall, “Computational Strategies for the Riemann Zeta function,” (1999) available from the CECM preprint server, URL=<http://www.cecm.sfu.ca/preprints/1999pp.html>, CECM-98-118
- [6] P. Borwein, “An Efficient Algorithm for the Riemann Zeta Function” (1995) available from the CECM preprint server, URL=<http://www.cecm.sfu.ca/preprints/1999pp.html>, CECM-95-043
- [7] Henri Cohen, Fernando Rodriguez Villegas, and Don Zagier, “Convergence Acceleration of Alternating Series,” *AMS Classification 11Y40, Experimental Mathematics*, Vol. 9, No. 1, (2000)

- [8] A. Odlyzko, A. Schonhage, “Fast Algorithms for multiple evaluations of the Riemann zeta-function,” *Trans. Amer. Math. Soc.* **309** (1988), 797-809
- [9] E. C. Titchmarsh, “The theory of the Riemann Zeta Function,” Oxford Science Publications, second edition, revised by D. R. Heath-Brown (1986)
- [10] J. van de Lune, H.J.J te Riele, D.T. Winter, “On the zeros of the Riemann Zeta function in the critical strip,” *IV. Math. Comp.* **46** (1986), 667-681
- [11] W. Galway, “Fast computation of the Riemann Zeta function to arbitrary accuracy,” manuscript, 1999
- [12] George F. Simmons, *Calculus Gems: Brief Lives and Memorable Mathematics*, 2007
- [13] Qiang Luo and Zhidan Wang, “Numerical calculation of the Riemann zeta function at odd-integer arguments: a direct formula method,” Springerlink.com, (2015)
- [14] D. Cvijovic and J. Klinowski, “Integral representations of the Riemann zeta function for odd-integer arguments,” *J. Comput. Appl. Math.* **142** (2), 435-439 (2002)
- [15] I.S. Gradshteyn and I.M. Ryzhik, Table of Integrals, Series, and Products, Academic Press, New York, 1980
- [16] M .Abramowitz, I .Stegun (Eds .), Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables, Dover Publications, New York, 1972.
- [17] Dilcher, K. “Asymptotic behavior of Bernoulli, Euler, and generalized Bernoulli polynomials,” *J. Approx. Theory* 49 (4), 321-330 (1987)

- [18] Derbyshire, “Prime Obsession: Bernhard Riemann and the Greatest Unsolved Problem in Mathematics,” New York: Penguin, 2004.
- [19] G14HTN Higher Number Theory Lecture Notes, University of Nottingham, 2016/2017 Academic Year
- [20] Victor Kac, “Euler-Maclaurin formula,” Seminar in Algebraic number Theory, 2005.