DEGREE PROJECT IN TECHNOLOGY,
FIRST CYCLE, 15 CREDITS
STOCKHOLM, SWEDEN 2018

On the Asymptotic Behaviour of Sums of Two Squares

Theoretical and Numerical Studies of the Counting Function *B(x)*

IVAR ERIKSSON

LUKAS GUSTAFSSON

KTH ROYAL INSTITUTE OF TECHNOLOGY
SCHOOL OF ENGINEERING SCIENCES

EXAMENSARBETE INOM TEKNIK,
GRUNDNIVÅ, 15 HP
STOCKHOLM, SVERIGE 2018

Asymptotiska beteendet hos summor av två kvardrater

En teoretisk och numerisk studie av räknefunktionen *B(x)*

IVAR ERIKSSON

LUKAS GUSTAFSSON

KTH
SKOLAN FÖR TEKNIKVETENSKAP

Abstract - Svenska

Att studera fördelnigen av speciella tal är en fundamental del av talteorin. Denna rapport behandlar fördelningen hos summor av två kvadrater genom användningen av analytisk talteori. I rapportens fokus ligger det asymptotiska beteendet av den motsvarande räknefunktionen, B(x). Konvergenstakten för approximationen har inte varit i fokus tidigare och underpresterar när det kommer till faktiskt evaluera B(x). Vi introducerar en Dirichletserie och använder den i Perrons formel för att ta fram de första termerna i talföljden som generear Dirichletserien. Denna integral är dessvärre otymplig och än svårare att evaluera numeriskt. Dirichletserien utvidgas därmed analytisk och en grenskärning i det komplexa talplanet introduceras. Konturen från Perron sluts och delar utav den nya konturen förkastas för att kunna likställa den sökta integralen med en enklare. Den kan då approximeras med en explicit serie med godtyckligt många termer. Resten av rapporten behandlar en numerisk implementation för att ta fram koefficienterna i serien och sedan resultaten från den nya approximationsformeln. Denna rapport är en liten fortsättning på arbetet av Daniel Shanks som beräknade de första 2 koefficienterna med bra noggrannhet. Genom att beräkna högre ordningens koefficienter uppnår vi ännu högre precision i approximationen för stora x. Det finns flera möjligheter för att utvidga detta arbete. Genom att vidare utvidga analyciteten hos Dirichletserien kan man förhoppningsvis plocka upp korrektionstermer som reducerar det asymptotiska felet till fjärderoten av x istället för det nuvarande roten ur x ifall man antar RH. Det exakta antalet korrekta värdesiffror i de uträknade koefficenterna kan även diskuteras vidare.

Abstract - English

Studying the distributions of special numbers is a fundamental area of research in number theory. This paper studies the distribution of sums of two squares using analytic number theory. The asymptotic behaviour of the corresponding counting function, B(x), is the object of study. The rate of convergence for the relative error has not been in focus previously and the current formulas underperform when used to evaluate B(x). We introduce a Dirichlet series and use Perron's formula to retrieve the first terms in the series. The integral is however unwieldy and numerically hard to calculate. Therefore the Dirichlet series is analytically extended and a branchcut is then introduced. Neglecting some parts of a new encircling contour in the complex plane allows for a simpler integral to arise. This can in turn be approximated into an explicit series formula with arbitrary many coefficients. The rest of the paper discusses a numerical method for evaluating the coefficients in the series and the results for the new formula. This paper is a small continuation of the work done by Daniel Shanks who calculated the first 2 coefficients with good precision. By calculating higher order coefficients we achieve even greater precision for large x. There also exists work that can be done to extend this report. Further extending analyticity of the Dirichlet series would allow for correction terms, hopefully reducing the asymptotic error to be close to the fourth root of x instead of the current square root error when assuming RH. Also the exact number of correct significant decimals in the calculated coefficients can be discussed further

Contents

Chapter 1

Theoretical Background

1.1 The counting function $B(x)$

We study the function

$$B(x) = \sum_{1 \le n \le x} b(n) \tag{1.1}$$

where n runs through the positive integers and $b(x) : \mathbb{R} \to \{0, 1\}$ is 1 iff $x \in \mathbb{Z}^+$ and can be written as the sum of the squares of two integers. Otherwise it is zero. Here we disregard 0 as a sum of two squares, even though it is, since it will let us bypass an index shift in the Dirichlet series we are about to introduce.

1.1.1 Reformulating $B(x)$

According to the sum of two squares theorem we have that $b(n) = 1$ if the prime decomposition of n contains no prime congruent to 3 modulo 4 raised to an odd power and otherwise it is 0 [1]. Now for all n with $b(n) = 1$ we have for the prime decomposition of n that

$$n = p_1^{m_1} p_2^{m_2} p_3^{m_3} \cdots q_1^{2n_1} q_2^{2n_2} q_3^{2n_3} \cdots 2^o \tag{1.2}$$

where $p_i \equiv_4 1$ are primes congruent to 1 mod 4 and $q_i \equiv_4 3$ primes congruent to 3 mod 4. Then for its corresponding Dirichlet series we have in the region of absolute convergence ($\mathrm{Re}(s) > 1$) that for p and q denoting primes

$$\begin{aligned} \beta(s) = \sum_{n=1}^{\infty} \frac{b(n)}{n^s} = \\ (1 + \frac{1}{2^s} + \frac{1}{2^{2s}} \cdots) \prod_{p \equiv_4 1} (1 + \frac{1}{p^s} + \frac{1}{p^{2s}} \cdots) \prod_{q \equiv_4 3} (1 + \frac{1}{q^{2s}} + \frac{1}{q^{4s}} \cdots) = \\ (1 - 2^{-s})^{-1} \prod_{p \equiv_4 1} (1 - p^{-s})^{-1} \prod_{q \equiv_4 3} (1 - q^{-2s})^{-1}. \end{aligned} \tag{1.3}$$

For details see appendix B.1 and B.2. This expression can in turn be rewritten using the Riemann Zeta function and another Dirichlet series generated by a certain Dirichlet character. We have two series, shown analogously to 1.3

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = (1 - 2^{-s})^{-1} \prod_{p \equiv_4 1} (1 - p^{-s})^{-1} \prod_{q \equiv_4 3} (1 - q^{-s})^{-1} \tag{1.4}$$

$$L(s, \chi_4) = \sum_{n=1}^{\infty} \frac{(-1)^n}{(2n+1)^s} = \prod_{p \equiv_4 1} (1 - p^{-s})^{-1} \prod_{q \equiv_4 3} (1 + q^{-s})^{-1}. \tag{1.5}$$

These equalities are proven using unique prime factorization in the integers and that the coefficients in $L(s, \chi_4)$ are determined by their prime decomposition. Proving that the products (1.4) and (1.5) converge absolutely and are analytic for $\mathrm{Re}(s) > 1$ is shown in the same way as for $\beta(s)$. Using that all factors converge absolutely in this region, allowing free rearranging of the terms and factors, we can now state that in the region $\text{Re}(s) > 1$

$$\beta(s)^2 = (1-2^{-s})^{-1}\zeta(s)L(s,\chi_4)\prod_{q\equiv_4 3}(1-q^{-2s})^{-1} \tag{1.6}$$

Observe that the right hand-side of (1.6) is analytic all the way to $\text{Re}(s) > \frac{1}{2}$, this is clearly an analytic extension of $\beta(s)^2$. From now on $\beta(s)^2$ denotes this analytic extension defined by the right hand-side of (1.6).

Let $s = \sigma + it$ be a complex number. Now use the results from appendix B.1 saying that the modulus of $\beta(s) - 1$ is bounded from above by $\frac{1}{\sigma-1}$. Study the region $\sigma > 3$ in the complex plane. This is an open connected subset of $\mathbb{C}$. Here $\beta(s)$ can be written as $\beta(s) = 1 + (\beta(s) - 1)$ where the latter term has a modulus bounded by $\frac{1}{2}$. So $|\beta(s)| \geq \frac{1}{2}$ and $Arg(\beta(s)) \in (-\frac{\pi}{4}, \frac{\pi}{4})$. Then clearly when taking the principal-branch-square root of $\beta(s)^2$ in this area we get back $\beta(s)$ and not $-\beta(s)$

$$\text{Re}(s) > 3 \implies \beta(s) = \sqrt{\beta(s)^2} \tag{1.7}$$

Now we can use that β^2 is an analytic extension given by equation (1.6) to try and extend β using the monodromy theorem for $\text{Re}(s) > \frac{1}{2}$ defining

$$\beta(s) := \sqrt{\beta(s)^2} \tag{1.8}$$

This is extension is well-defined with the exception that zeros and poles of $\beta(s)^2$ will cause branch points and therefore branch cuts for the square root. We can choose these branch cuts to be horizontal rays stretching to the left of the branch points. Along the cuts the function will not be analytic. Later we will integrate along a contour in this region and any such ray can be encircled using the classic key-hole contour. $\beta(s)^2$ is analytic in the region $\text{Re}(s) > \frac{1}{2}$ and the zeros of an analytic function cannot cluster, implying that these cuts are manageable. For simplicity we will be assuming general RH and no such cuts will be discussed further except for the pole one at s=1 due to $\zeta(s)$.

1.2 Approximating $B(x)$

1.2.1 Perron's Formula

Perron's formula states that for an arithmetic function $b(n) : \mathbb{Z}^+ \to \mathbb{C}$ with a uniformly convergent Dirichlet series, $\beta(s) = \sum_{n=1}^{\infty} \frac{b(n)}{n^s}$, for $\text{Re}(s) > \sigma_0$, where the σ_0 is the abscissa of absolute convergence for the Dirichlet series, that

$$B'(x) := \frac{b(x)}{2} + \sum_{1\leq n<x} b(n) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \beta(s)\frac{x^s}{s}ds \tag{1.9}$$

where $c > 0$, $c > \sigma$ and $x > 0$. For the proof see [2]. One immediately sees the use of this formula. $B'(x)$ will closely correspond to the function $B(x)$ at the center of this paper. In fact the relative error as $n \to \infty$ will tend towards 0.

1.2.2 Revising the Integral

For simplicity we will assume the general Riemann Hypothesis. Then one can conclude that the function $\beta(s)$ is analytic, with a pole in 1 and without zeros in the region $R = \{s \in \mathbb{C} : \text{Re}(s) > \frac{1}{2}\}\backslash(-\infty, 1]$. R is a half-plane without the closed ray going from 1 to $-\infty$. The integral shown in figure 1.1 is the integral of Perron's formula ($c = 2$) with an extra enclosing integration path from $(1/2+\delta)+i\infty$ to $(1/2+\delta)-i\infty$ where $\delta > 0$ is small. Note also that the contour includes a keyhole around $s = 1$ to avoid the branch cut caused by the pole of the Riemann Zeta function here (note that the other factors in $\beta(s)$ are all clearly non-zero at s=1). This means that the shaded region in figure 1.1 is completely void of poles and zeros making this complete integral 0.

The pole of $\zeta(s)$ at $s = 1$ shows up in $\beta(s)$ as a pole of $\beta(s)$ on the form $\frac{1}{\sqrt{s-1}}$. [3] The residue of a pole on the form $\frac{1}{\sqrt{s}}$ is 0, see appendix B.3. Thus contour B contributes 0.

The contribution of contour C will become relatively small as x grows and can be neglected. This will be shown in section 1.2.3

Finally contours D and D' will give contributions in both directions and will not cancel out due to the branch cut present. In essence this implies that the integral over A almost equals the integral over $-(\mathrm{D}+\mathrm{D'})$.

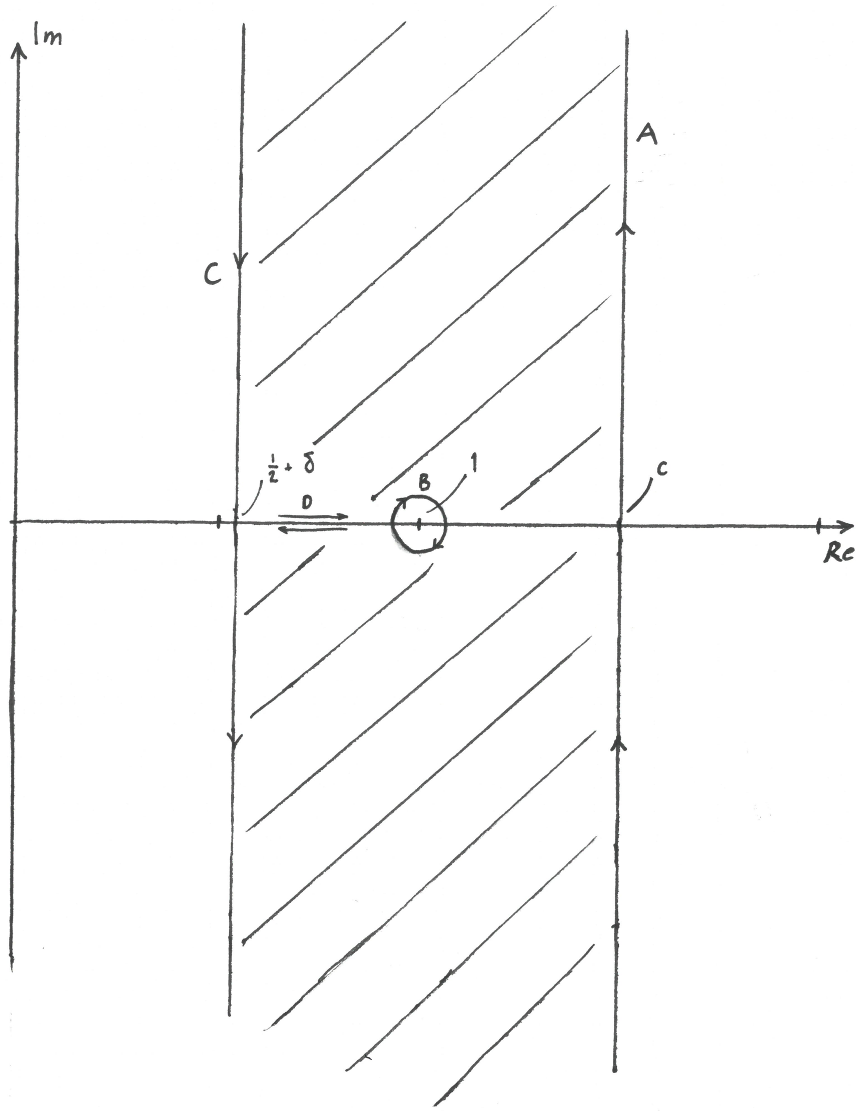

Figure 1.1: First contour.

1.2.3 Proving the Insignificance of C

The error that arises when neglecting the integration over C in figure 1.1 is small. We shall now show this and that there is no pathological behaviour for large imaginary parts. The proof will closely mimic that of Davenport's proof of the prime number theorem. [2] To start a result from [2] is used, if

$$I(y,T)=\frac{1}{2\pi i}\int_{c-iT}^{c+iT}\frac{y^s}{s}ds \tag{1.10}$$

and

$$\delta(y) = \begin{cases} 0 & if\ 0 < y < 1, \\ \frac{1}{2} & if\ y = 1, \\ 1 & if\ 1 < y \end{cases} \tag{1.11}$$

then

$$|I(y,T) - \delta(y)| < \begin{cases} y^c \min(1, T^{-1}|\ln(y)|^{-1}) & if\ y \neq 1 \\ cT^{-1} & if\ y = 1 \end{cases}. \tag{1.12}$$

Note that this gives us

$$\delta(y) = \lim_{T\to\infty} I(y,T). \tag{1.13}$$

Now introduce

$$J(x,T) = \frac{1}{2\pi i}\int_{c-iT}^{c+iT} \beta(s)\frac{x^s}{s}ds. \tag{1.14}$$

We can now deduce, using uniform convergence, that

$$|J(x,T) - B'(x)| = \sum_{n\geq 1} b(n)\left|I(\frac{x}{n},T) - \delta(\frac{x}{n})\right| < \sum_{\substack{1\leq n\\ n\neq x}} b(n)(\frac{x}{n})^c \min\left[1, T^{-1}|\ln(\frac{x}{n})|^{-1}\right] + cT^{-1}b(x) \tag{1.15}$$

$$|J(x,T) - B'(x)| < x^c \sum_{\substack{1\leq n\\ n\neq x}} (\frac{b(n)}{n^c}) \min\left[1, \frac{1}{T|\ln(\frac{x}{n})|}\right] + cT^{-1}b(x). \tag{1.16}$$

To facilitate the calculations we choose $c = 1 + \frac{1}{\ln(x)}$. Note that then we obtain $x^c = e^{\ln(x)c} = e^{1+\ln(x)} = ex$. Note also that the term $cT^{-1}b(x)$ is dominated by the rest of the expression and can be omitted from the following calculations. Let us first study the part of the error such that $|n-x| > \frac{x}{4}$. Then we have that an upper bound for $\frac{1}{|\ln(\frac{x}{n})|} < \frac{1}{|\ln(\frac{4}{3})|}$. We conclude that for $T > 4$

$$\sum_{\substack{1\leq n\\ |n-x|>\frac{x}{4}\\ n\neq x}} (\frac{b(n)}{n^c}) \min\left[1, \frac{1}{T|\ln(\frac{x}{n})|}\right] < \frac{1}{|\ln(\frac{4}{3})|}\sum_{\substack{1\leq n\\ n\neq x}} (\frac{b(n)}{n^c})\frac{1}{T} < \frac{1}{|\ln(\frac{4}{3})|}\beta(c)\frac{1}{T} \tag{1.17}$$

How does $\beta(c(x))$ behave as a function of x? We need a bound for this factor. c will converge to 1 as x grows. Recall the definition of $\beta(s)$, it has a pole due to $\sqrt{\zeta(s)}$ being one of its factors. So we can write

$$\beta(s) = \frac{1}{\sqrt{s-1}}A(s) \tag{1.18}$$

where $A(s)$ is analytic in a neighbourhood around $s = 1$. Close to 1 $A(s)$ is close to $A(1)$, a constant, so we can conclude that

$$\beta(c) = \mathcal{O}(\frac{1}{\sqrt{c-1}}) = \mathcal{O}(\sqrt{\ln(x)}) \tag{1.19}$$

In turn we obtain

$$\sum_{\substack{1\leq n\\ |n-x|>\frac{x}{4}\\ n\neq x}} b(n)(\frac{1}{n^c}) \min\left[1, \frac{1}{T|\ln(\frac{x}{n})|}\right] = \mathcal{O}(\frac{\sqrt{\ln(x)}}{T}) \tag{1.20}$$

This is a small term which will be dominated by the next one. We turn our attention to the rest of the error term. Now consider $n \in (\frac{3x}{4}, x)$ and treat the other case analogously. Let x_1 be the largest integer in this interval such that $b(x_1) = 1$. Then we have that the term contributes with a constant $\frac{1}{n^c} = \mathcal{O}(1)$. The rest of the terms in this interval can be written on the form $n = x_1 - \nu$ where $\nu \in (0, \frac{x}{4})$. Then can we write the following expression

$$|\ln(\frac{x}{n})| \geq |\ln(\frac{x_1}{n})| = |\ln(1 - \frac{\nu}{x_1})| \geq \frac{\nu}{x_1}. \tag{1.21}$$

This allows us to dominate the contribution of these terms to the error as follows using that $(\frac{x}{n})^c$ is bounded for these n

$$\sum_{n\in(\frac{3x}{4},x)} b(n)\ \min\left[1,\frac{1}{T|\ln(\frac{x}{n})|}\right] < \frac{1}{T}\sum_{\nu\in(0,\frac{x}{4})} b(n)\frac{x_1}{\nu} < \frac{x}{T}\sum_{\nu\in(0,\frac{x}{4})}\frac{1}{\nu} \sim \frac{x}{T}\int_1^{\frac{x}{4}}\frac{1}{\nu}d\nu = \frac{x}{T}\ln(x/4) = \mathcal{O}(\frac{x\ln(x)}{T}). \tag{1.22}$$

We will choose T to grow with x faster than $\ln(x)$ later and is what allows us say that $\min\left[1,\frac{1}{T|\ln(\frac{x}{n})|}\right] \neq 1$. Finally we may present the sought-after partial result

$$|J(x,T) - B'(x)| = \mathcal{O}(\frac{x\ln(x)}{T} + 1) \tag{1.23}$$

Now that we have shown that the infinite integral of (1.9) can be approximated by a finite integral from $c - iT$ to $c + iT$ we can consider the closed loop integral in figure 1.2. Since it is a closed loop integral over a space in which the integrand is void of poles the total integral is, as before, 0. We shall now show that the contribution of contour C in figure 1.2 is negligible.

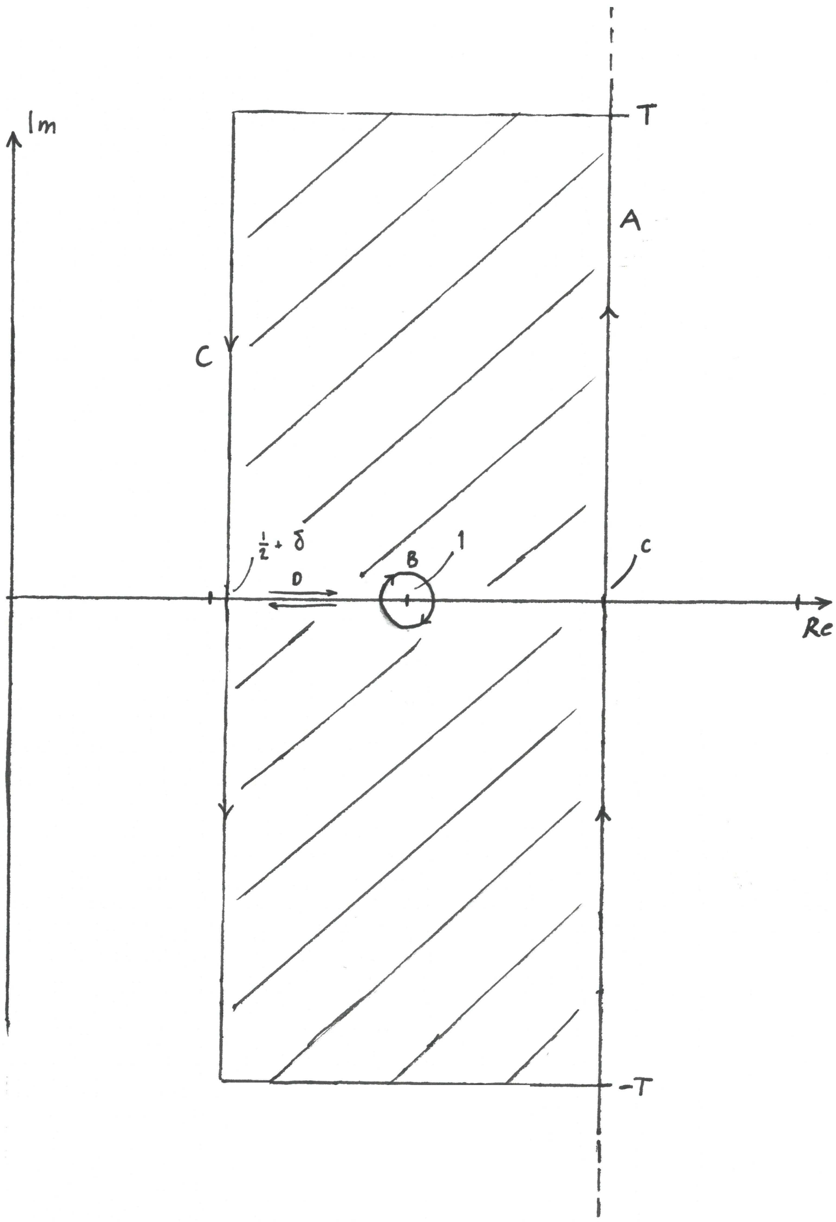

Figure 1.2: Second contour.

First it is known that in the half plane $\frac{1}{2} < \sigma$ (where $s = \sigma + it$) for sufficiently large t $|\beta(s)| = \mathcal{O}(t^{\epsilon})$ where ϵ is some real number. It is proved using convexity and a generalization of the maximum modules principle called the Phragmén-Lindelöf principle. For details see [4]. As β is symmetric in t we shall only consider the parts of C for which $t > 0$. We denote the horizontal line C_1 and the vertical line C_2.

For C_1 we have $s = \sigma + iT$ and thus for sufficiently large T the size of the contribution will be

$$\begin{aligned}
&\left|\int_{c+iT}^{\frac{1}{2}+\delta+iT} \beta(s)\frac{x^s}{s}ds\right| \leq \int_{\frac{1}{2}+\delta}^{c} |\beta(s)|\frac{|x^s|}{|\sqrt{\sigma^2+T^2}|}d\sigma \leq \\
&\int_{\frac{1}{2}+\delta}^{c} KT^{\epsilon}\frac{|e^{s\ln(x)}|}{T}d\sigma \leq \int_{\frac{1}{2}+\delta}^{c} KT^{\epsilon-1}e^{\sigma\ln(x)}d\sigma = \\
&KT^{\epsilon-1}\int_{\frac{1}{2}+\delta}^{c} e^{\sigma\ln(x)}d\sigma = KT^{\epsilon-1}\Big[\frac{x^{\sigma}}{\ln(x)}\Big]_{\frac{1}{2}+\delta}^{c} = KT^{\epsilon-1}(\frac{ex - x^{\frac{1}{2}+\delta}}{\ln(x)}) = \mathcal{O}(T^{\epsilon-1}\frac{x}{\ln(x)})
\end{aligned} \quad . \tag{1.24}$$

Where K is a suitable constant. For C_2 the size of the contribution will be

$$\begin{aligned}
&\left|\int_{\frac{1}{2}+\delta}^{\frac{1}{2}+\delta+iT} \beta(s)\frac{x^s}{s}ds\right| \leq \int_0^T |\beta(s)|\frac{|x^s|}{|\sqrt{(\frac{1}{2}+\delta)^2+t^2}|}dt \leq \\
&K\int_0^T t^{\epsilon}\frac{|e^{(\frac{1}{2}+\delta)\ln(x)}|}{t}dt \leq Kx^{(\frac{1}{2}+\delta)}\int_0^T t^{\epsilon-1}dt = \\
&Kx^{(\frac{1}{2}+\delta)}\Big[\frac{t^{\epsilon}}{\epsilon}\Big]_0^T = \mathcal{O}(x^{\frac{1}{2}+\delta}T^{\epsilon})
\end{aligned} \quad . \tag{1.25}$$

Now we will add the different contributions together to find the size of the error of our approximation. In the calculations below D is used to represent the sum of the integral over contours D and D'.

$$|\mathrm{D}-B'(x)| \leq |\mathrm{D}-J(x,T)|+|J(x,T)-B'(x)| \leq \mathcal{O}(T^{\epsilon-1}\frac{x}{\ln(x)})+\mathcal{O}(x^{\frac{1}{2}+\delta}T^{\epsilon})+\mathcal{O}(\frac{x\ln(x)}{T}+1) \tag{1.26}$$

If we now choose $T = x^{\frac{1}{2}}$ and $\delta = \frac{\epsilon}{2}$ we get

$$|\mathrm{D}-B'(x)| \leq \mathcal{O}(x^{\frac{\epsilon-1}{2}}\frac{x}{\ln(x)}) + \mathcal{O}(x^{\frac{1}{2}+\frac{\epsilon}{2}}x^{\frac{\epsilon}{2}}) + \mathcal{O}(\frac{x\ln(x)}{x^{\frac{1}{2}}}) = \mathcal{O}(x^{\frac{1}{2}+\epsilon}). \tag{1.27}$$

1.2.4 Logarithmic Taylor Expansion

Now we want study the integral with the greatest contribution to the integral more closely. It is of the form

$$B(x) \approx \frac{-1}{\pi i}\int_{1-L}^{1} \beta(s)\frac{x^s}{s}ds. \tag{1.28}$$

Here we are looking at contour D slightly above the real axis and $L = 1/2 - \delta$. This can be rewritten as

$$B(x) \approx \frac{1}{\pi i}\int_0^L \beta(1-t)\frac{x^{1-t}}{(1-t)}dt = \int_0^L x^{1-t}f(t)dt \tag{1.29}$$

where

$$f(t) = \frac{1}{\pi(1-t)}\frac{1}{\sqrt{t}}\sqrt{\frac{-t\zeta(1-t)L(1-t,\chi_4)}{(1-2^{t-1})}\prod_{q\equiv_4 3}(1-q^{2t-2})^{-1}}. \tag{1.30}$$

We introduce $g(t)$ and $h(t)$ to facilitate calculations later on.

$$f(t) = \frac{1}{\sqrt{t}}g(t) = \frac{1}{\sqrt{t}}\sqrt{-t\zeta(1-t)}h(t) \tag{1.31}$$

Now once the singularity of ζ has been factored out, the rest, $g(t)$ is analytic and we can Taylor expand g at $t = 0$ ($s = 1$). This lets us write

$$g(t) = \sum_{n=0}^{N}\frac{g^{(n)}(0)}{n!}\cdot t^n \quad + \mathcal{O}(t^{N+1}). \tag{1.32}$$

Now it is relevant to study the following integral

$$x\int_0^L x^{-t}t^{m-1/2}dt. \tag{1.33}$$

We will see it is very similar to the incomplete lower gamma function

$$\Gamma_l(a,x)=\int_0^x e^{-u}u^{a-1}du. \tag{1.34}$$

Here we can substitute $u = t\cdot \ln(x)$ to obtain

$$\begin{aligned} x\int_0^{L\ln(x)} e^{-u}\left(\frac{u}{\ln(x)}\right)^{m-1/2}\frac{du}{\ln(x)} = \frac{x}{\ln(x)^{m+\frac{1}{2}}}\int_0^{L\ln(x)} e^{-u}u^{m-1/2}du = \\ \frac{x}{\ln(x)^{m+\frac{1}{2}}}\Gamma_l(m+1/2, L\ln(x)) \end{aligned}. \tag{1.35}$$

This result along with uniform absolute convergence of the Taylor series allows us to interchange summation and integration and gives us a formula that can be tricky to calculate numerically but useful when trying to extend our theoretical results.

$$\begin{aligned} B(x) &= \frac{x}{\sqrt{\ln(x)}}\sum_{n=0}^{\infty}\frac{c_n(x)}{\ln(x)^n} \quad + \mathcal{O}\big(x^{1/2+\epsilon}\big) \\ c_n(x) &= \frac{g^{(n)}(0)\cdot\Gamma(n+\frac{1}{2}, L\ln(x))}{n!} \end{aligned} \tag{1.36}$$

For evaluating the expression a bit faster numerically we can approximate the lower incomplete function with the regular Γ for large x. Then an error term is introduced. It is of the form

$$\frac{x}{\ln(x)^{m+\frac{1}{2}}}\int_{L\ln(x)}^{\infty} e^{-u}u^{m-1/2}du. \tag{1.37}$$

Let us estimate the size of it. Clearly there is a constant C (depending on m) such that for any fix $\alpha > 0$ such that

$$\int_{L\ln(x)}^{\infty} e^{-u}u^{m-1/2}du < C\int_{L\ln(x)}^{\infty} e^{-(1-\alpha)u}du = \mathcal{O}(x^{-(1-\alpha)L}). \tag{1.38}$$

So as a conclusion we can write

$$\int_0^L x^{1-t}t^{m-1/2}dt = \frac{x}{\ln(x)^{m+\frac{1}{2}}}\Gamma(m+\frac{1}{2}) + \mathcal{O}\Big(\frac{x^{1-(1-\alpha)L}}{\ln(x)^{m+1/2}}\Big). \tag{1.39}$$

In hindsight this is actually a quite crude approximation, especially when languages like Matlab have an implementation of $\Gamma_l(a,x)$. To conclude this gives us the approximation formula for our numeric implementation.

$$\begin{aligned} B(x) &= \frac{x}{\sqrt{\ln(x)}}\sum_{n=0}^{N}\frac{c_n}{\ln(x)^n} + \mathcal{O}\Big(\frac{x}{\ln(x)^{N+3/2}}\Big) + \mathcal{O}\Big(\frac{x^{1-(1-\alpha)L}}{\sqrt{\ln(x)}}\Big) + \mathcal{O}\big(x^{1/2+\epsilon}\big) \\ c_n &= \frac{g^{(n)}(0)\cdot\Gamma(n+\frac{1}{2})}{n!} \end{aligned} \tag{1.40}$$

The good thing about this formula is that all we need to evaluate it at x, except for calculating $\ln(x)$, is the derivatives of $g(t)$ at 0. This will be discussed in 2. Here the first error term is due to us truncating the Taylor series of g(t). The second error term is due to simplifying the integral in (1.28) and the third is due to us changing and disregarding parts of the contour.

Note that we will be discussing yet another contour shift which might reduce the error from neglecting parts of the contour into $\sim \mathcal{O}(x^{1/4+\epsilon})$. Then we can no longer approximate $\Gamma_l(a, L\ln(x))$ with ordinary Γ because it introduces an error comparable to $\sqrt{x}$ and the formula from (1.36) must be used in order for the shift to be meaningful.

1.2.5 Calculating $g^{(n)}(0)$

The constants $g^{(n)}(0)$ of the previous section are derivatives in the complex plane. These are best treated with Cauchy's Integral formula. We recall that

$$g^{(n)}(a) = \frac{n!}{2\pi i}\int_C \frac{g(z)}{(z-a)^{n+1}}dz \tag{1.41}$$

where C is a closed loop around a. See section 2.2.6 for further details on how to do it numerically.

1.3 Analytic Extension

Now the Dirichlet series defining $\beta(s)$ only converges up the the line with real-part 1. In section 1.1.1 we concluded that $\beta(s)$ agrees with some other analytic expressions involving $\beta(s)^2$. If we find an analytic extension of $\beta(s)^2$ it will automatically produce an extension of $\beta(s)$ for us to use later. This extension demands branch cuts at each zero and pole of $\beta(s)^2$ as discussed previously. We are allowed to choose the branch cut to be a closed ray from the branch point stretching to the left.

In section 1.1.1 we found the following expression

$$\beta(s)^2 = (1-2^{-s})^{-1}\zeta(s)L(s,\chi_4)\prod_{q\equiv_4 3}(1-q^{-2s})^{-1}. \tag{1.42}$$

We want this to extend this function even further down to all of $\mathrm{Re}(s) > 1/4$. The method that will be described invites for recursively extending the function down to any line $\mathrm{Re}(s) > 2^{-n}$. However this has not been investigated further. We cannot do this unless we manipulate the factor $\prod_{q\equiv_4 3}(1-q^{-2s})^{-1}$. Now in the region $\mathrm{Re}(s) > 3$ we can manipulate it because of absolute convergence, small angles and the absence of zeros to turn it into something new.

$$\prod_{q\equiv_4 3}(1-q^{-2s})^{-1} = \frac{\prod_{q\equiv_4 3}(1-q^{-2s})^{-1}\prod_{p\equiv_4 1}(1-p^{-2s})^{-1}}{\prod_{p\equiv_4 1}(1-p^{-2s})^{-1}} = (1-2^{-2s})\zeta(2s)\prod_{p\equiv_4 1}(1-p^{-2s}) \tag{1.43}$$

$$\prod_{p\equiv_4 1}(1-p^{-2s}) = \prod_{p\equiv_4 1}(1-p^{-2s})\sqrt{\frac{\prod_{q\equiv_4 3}(1+q^{-4s})}{\prod_{q\equiv_4 3}(1+q^{-4s})}} = \sqrt{\frac{\prod_{p\equiv_4 1}(1-p^{-2s})^2\prod_{q\equiv_4 3}(1+q^{-4s})}{\prod_{q\equiv_4 3}(1+q^{-4s})}} \tag{1.44}$$

Recall from section 1.1.1 that in this region we can use

$$\zeta(s)L(s,\chi_4) = (1-2^{-s})^{-1}\prod_{p\equiv_4 1}(1-p^{-s})^{-2}\prod_{q\equiv_4 3}(1-q^{-2s})^{-1}. \tag{1.45}$$

Using this we obtain due to due well-behaved arguments

$$\prod_{p\equiv_4 1}(1-p^{-2s}) = \sqrt{\frac{1}{(1-2^{-2s})\zeta(2s)L(2s,\chi_4)\prod_{q\equiv_4 3}(1+q^{-4s})}} = \frac{1}{\sqrt{(1-2^{-2s})}\sqrt{\zeta(2s)}\sqrt{L(2s,\chi_4)\prod_{q\equiv_4 3}(1+q^{-4s})}}. \tag{1.46}$$

Using this we obtain in the domain $\mathrm{Re}(s) > 3$

$$\begin{aligned}
&\beta(s)^2 = \Phi(s)\sqrt{\Psi(s)}\\
&\Phi(s) := (1-2^{-s})^{-1}\zeta(s)L(s,\chi_4)\\
&\Psi(s) := (1-2^{-2s})\zeta(2s)L(2s,\chi_4)^{-1}\prod_{q\equiv_4 3}(1+q^{-4s})^{-1}
\end{aligned}. \tag{1.47}$$

Note that both Φ and Ψ are analytic on $\mathrm{Re}(s) > \frac{1}{4}$ except for Φ having a pole at $s = 1$. The monodromy theorem lets us extend $\beta(s)$ here as well except for branch cuts stretching to the left of each zero.

1.3.1 Assumptions

The form of $\beta(s)^2$ from (1.47) is what we want. Now we will make some very strong assumptions in order to get the results we want and extend this function beyond $\mathrm{Re}(s) > 1/2$. Essentially all branch cuts will to be due to the factors $(s-\rho)$ where $\beta(s)^2(\rho) = 0$. We assume

1. General Riemann Hypothesis
2. All zeros of $\zeta(s)$ and $L(s,\chi_4)$ on the critical line are simple.

Zeros of higher order can be handled in a similar way as we are about to but we do not know the order of the zeros of $\zeta(s)$. Finding ways to determine this numerically is out of the scope of this paper but is an interesting subject.

1.3.2 Second Revision of the Integral

Here we study what happens if the left side of the contour is shifted even further to the left, close to the line $\mathrm{Re}(s) = \frac{1}{4}$. Now that the existence of an analytic extension has been proven one can do this as long as one avoids the horizontal branch cuts caused by the zeros of $\beta(s)^2$.

The zeros of $\beta(s)^2$ arise only from the zeros of $\zeta(s)$ and $L(s,\chi_4)$ and they are simple. This let's us at each zero ρ study the function $\frac{\rho\beta(s)}{s\sqrt{s-\rho}} = \frac{\mathcal{O}(\beta(s))}{\sqrt{s-\rho}}$. Since the zeros are assumed to be simple the function does not have a branch point, since we factored out the zero of β, and is therefore analytic in a larger region than $\frac{\beta}{s}$, especially at ρ.

Just like at $s = 1$ we get a keyhole contour at each zero because of the square root that was factored out. At each keyhole contour around some zero ρ the integral's contribution will be very similar to that of the one around $s = 1$. The circle part will vanish and only the horizontal lines will contribute. The vertical lines connecting the keyholes will be our error term. The contribution of the integral along the keyholes of length L' around the horizontal branch cut at ρ will be

$$\frac{1}{\pi i}\int_{\rho-L'}^{\rho}\beta(s)\frac{x^s}{s}ds = \int_0^{L'}\frac{x^{\rho-t}}{\rho}\sqrt{t}g_\rho(t)dt \tag{1.48}$$

where g_ρ is the mentioned analytic function

$$g_\rho(t) = \frac{\rho}{\pi(\rho-t)}\sqrt{\frac{-\zeta(\rho-t)L(\rho-t,\chi_4)}{t(1-2^{t-\rho})}\sqrt{(1-2^{-2(\rho-t)})\zeta(2(\rho-t))L(2(\rho-t),\chi_4)^{-1}\prod_{q\equiv_4 3}(1+q^{-4(\rho-t)})^{-1}}}. \tag{1.49}$$

Because $g_\rho(t)$ has a Taylor expansion it is natural to try and study the following integral which we can manipulate just like in section 1.2.4

$$\int_0^{L'}x^{\rho-t}t^{m+1/2}dt = \Gamma_l(m+\frac{3}{2},L'\ln(x))\frac{x^\rho}{(\ln(x))^{m+3/2}}. \tag{1.50}$$

Now we will get a sum over all zeros of $\beta(s)$, for clarity we can use the expansion

$$g_\rho(t) = g_\rho(0) + \mathcal{O}(t). \tag{1.51}$$

Where

$$\zeta(\rho) = 0 \implies g_\rho(0) = \frac{1}{\pi}\sqrt{\frac{\zeta'(\rho)L(\rho,\chi_4)}{(1-2^{-\rho})}\sqrt{(1-2^{-2\rho})\zeta(2\rho)L(2\rho,\chi_4)^{-1}\prod_{q\equiv_4 3}(1+q^{-4\rho})^{-1}}} \tag{1.52}$$

$$L(\rho,\chi_4) = 0 \implies g_\rho(0) = \frac{1}{\pi}\sqrt{\frac{\zeta(\rho)L'(\rho,\chi_4)}{(1-2^{-\rho})}\sqrt{(1-2^{-2\rho})\zeta(2\rho)L(2\rho,\chi_4)^{-1}\prod_{q\equiv_4 3}(1+q^{-4\rho})^{-1}}}. \tag{1.53}$$

This gives us a picture of what the zeros do. Now we also have a pole due to $\zeta(2s)$ evaluated at $s = 1/2$. This will be handled just like all other branch points. The circle part of the keyhole contributes 0. Now however we factor out the fourth root of t. The point s=1/2 lies at the horizontal branch cut from $s = 1$ and we do not have to introduce a new one. We study the integral

$$\frac{1}{\pi i}\int_{1/2-L'}^{1/2}\beta(s)\frac{x^s}{s}ds = \int_0^{L'} x^{1/2-t}t^{-1/4}g_{\frac{1}{2}}(t)dt. \tag{1.54}$$

Here we define

$$g_{\frac{1}{2}}(t) = \frac{1}{i\pi(\frac{1}{2}-t)}\sqrt{\frac{-\zeta(\frac{1}{2}-t)L(\frac{1}{2}-t,\chi_4)}{(1-2^{t-\frac{1}{2}})}\sqrt{\frac{(1-2^{-2(\frac{1}{2}-t)})t\zeta(2(\frac{1}{2}-t))}{L(2(\frac{1}{2}-t),\chi_4)}\prod_{q\equiv_4 3}(1+q^{-4(\frac{1}{2}-t)})^{-1}}} \tag{1.55}$$

which is an analytic function at $s = \frac{1}{2}$ and has a uniformly and absolutely convergent Taylor series that converges for $t < 1/4$. Since $L' < 1/4$ the termwise integral of the Taylor series is well-defined.

$$g_{\frac{1}{2}}(t) = \sum_{k=0}^{\infty}\frac{g_{\frac{1}{2}}^{(k)}(\frac{1}{2})}{k!}t^k \tag{1.56}$$

So we can simplify the integral

$$\begin{aligned}\int_0^{L'} x^{1/2-t}t^{-1/4}g_{\frac{1}{2}}(t)dt &= \frac{x^{\frac{1}{2}}}{\ln(x)^{\frac{3}{4}}}\sum_{k=0}^{\infty}\frac{e_k(x)}{\ln(x)^k}.\\ e_k(x) &= \frac{g_{\frac{1}{2}}^{(k)}(\frac{1}{2})\Gamma_l(k+\frac{3}{4},L'\ln(x))}{k!}\end{aligned} \tag{1.57}$$

To conclude we have a new complete formula for $B(x)$, using the full taylor expansion of g_ρ at each zero

$$\begin{aligned}B(x) &= \frac{x}{\sqrt{\ln(x)}}\sum_{n=0}^{\infty}\frac{c_n(x)}{\ln(x)^n} + \frac{x^{\frac{1}{2}}}{\ln(x)^{\frac{3}{4}}}\sum_{k=0}^{\infty}\frac{e_k(x)}{\ln(x)^k} + \sum_{\substack{\rho\\ \mathrm{Im}(\rho)<T}}\frac{x^\rho}{\rho}\frac{1}{\ln(x)^{\frac{3}{2}}}\sum_{m=0}^{\infty}\frac{d_m(x)}{\ln(x)^m} + V + \mathcal{O}(\frac{x\ln(x)}{T}+1).\\ d_m(x) &= \frac{g_\rho^{(m)}(\rho)\Gamma_l(m+\frac{3}{2},L'\ln(x))}{m!}\end{aligned} \tag{1.58}$$

Here the first sum is due to the main term, the pole at $s = 1$. The second sum is due to the pole at $s = \frac{1}{2}$. The poles are of different order and contribute differently. The third term is due to the zeros of $\beta(s)$. V is the error from neglecting the vertical contour with real-part close to 1/4 and the lids connecting it to the contour on the right. V needs to be investigated but is hopefully small. The last term is due to the right side of the contour being finite. This is the result from equation (1.23) where T is the height of the contour.

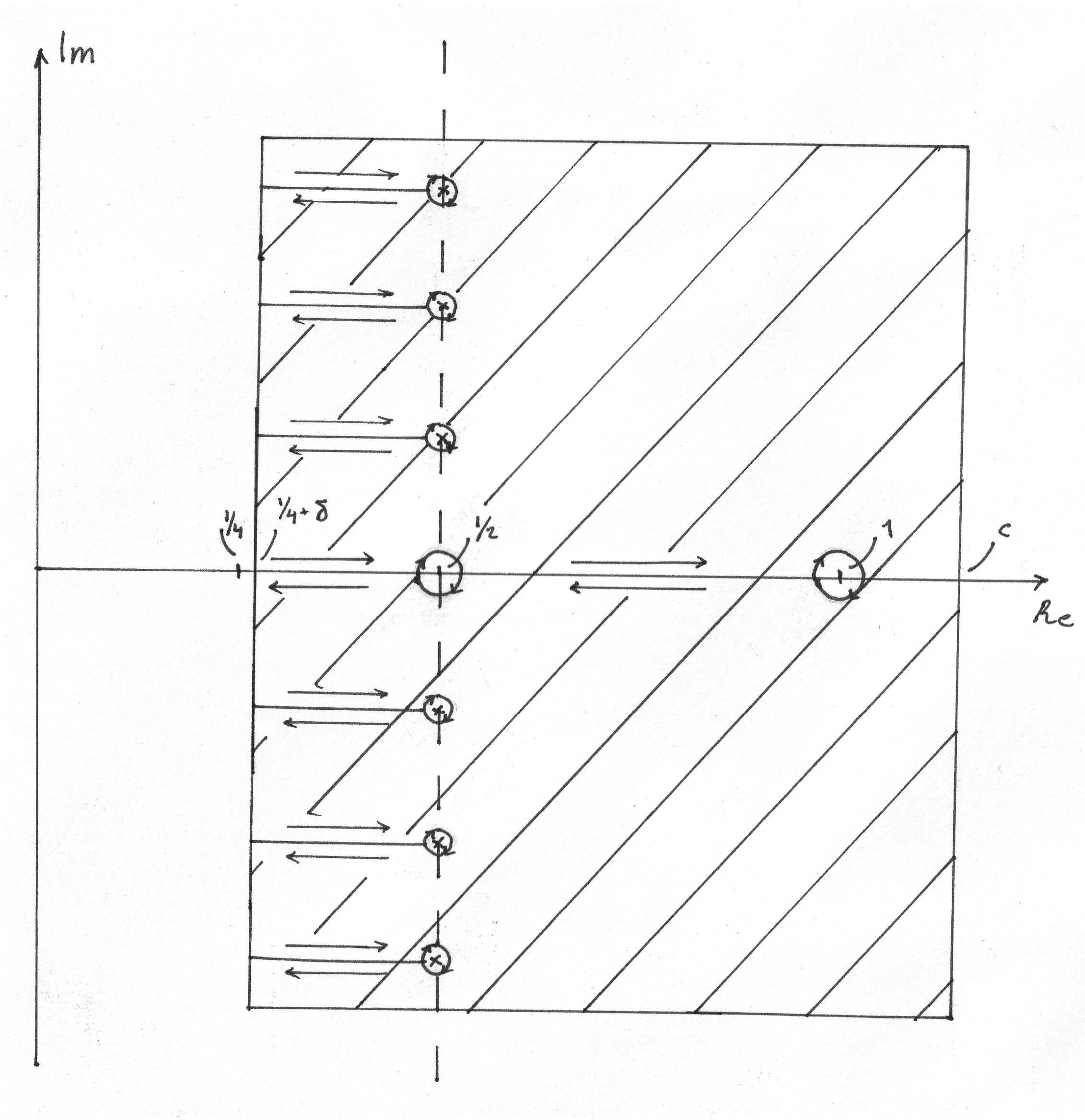

Figure 1.3: The contour shifted past $\mathrm{Re}(s) = 1/2$.

Chapter 2

Numerical Studies

2.1 SageMath

SageMath is a Python based computer programming language primarily used for performing numerical mathematical calculations. It has a vast mathematical library which is its main selling point. Because of the inclusion of such things as the Stieltje constants and the Riemann zeta function mainly Sage was used for the numerical portion of this report.

Due to the limited documentation of SageMath and its peculiarities most of the time spent on this project was spent on developing an understanding for this tool. During early stages of the project a lot of functions were implemented manually due to the lack of understanding for the many preprogrammed functions in SageMath. However in the finalized version as many of the already implemented methods as possible were used.

2.2 Calculating Higher Order Derivatives

Finding the constants $g^{(n)}(0)$ of section 1.2.4 is what is needed to evaluate our approximation. Two different methods were used.

2.2.1 Evaluating Riemann ζ close to $s = 1$

SageMath has an inbuilt implementation of Riemann zeta utilizing the MPFR library for real numbers and Pari C library for complex numbers. However this implementation did not behave well in a neighborhoods of 1, exactly where we are interested in studying the function. To work around this one can utilize the Laurent series of ζ at $s = 1$. From [3] this is known to be

$$\frac{1}{s-1} + \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \gamma_n (s-1)^n \tag{2.1}$$

Where γ_n are the Stieltje constants. Luckily these are available in the standard library of SageMath. Now, numerically, it is much easier to evaluate $(s-1)\zeta$ and this is what is used. It allows us to have the error in evaluation, denoted by $\mu(z)$, have an upper bound, μ, independent of how close we are to the pole.

2.2.2 Difference quotients

The first method that might come to mind for calculating derivatives numerically is difference quotients as per the Euler method. This is a rather crude method and quickly becomes problematic.

When restricted to the real line, $\beta(s)$ is a real-valued function and can be treated as such. We can find its derivatives by taking difference quotients. The proof of the two firs derivatives correctness is most easily shown by Taylor expanding as follows.

$$\begin{aligned}
f(x+h) &= f(x) + f'(x)h + f''(x)\frac{h^2}{2} + f^{(3)}(x)\frac{h^3}{3!} + f^{(4)}(x)\frac{h^4}{4!} + \mathcal{O}(h^5) \\
f(x-h) &= f(x) - f'(x)h + f''(x)\frac{h^2}{2} - f^{(3)}(x)\frac{h^3}{3!} + f^{(4)}(x)\frac{h^4}{4!} + \mathcal{O}(h^5) \\
f(x+2h) &= f(x) + 2f'(x)h + 2f''(x)h^2 + 4f^{(3)}(x)\frac{h^3}{3} + 2f^{(4)}(x)\frac{h^4}{3} + \mathcal{O}(h^5) \\
f(x-2h) &= f(x) - 2f'(x)h + 2f''(x)h^2 - 4f^{(3)}(x)\frac{h^3}{3} + 2f^{(4)}(x)\frac{h^4}{3} + \mathcal{O}(h^5)
\end{aligned} . \tag{2.2}$$

This lets us deduce that

$$\begin{aligned}
f(x+h) - f(x-h) &= 2f'(x)h + f^{(3)}(x)\frac{h^3}{3} + \mathcal{O}(h^5) \\
f(x+h) + f(x-h) &= 2f(x) + f''(x)h^2 + \mathcal{O}(h^4) \\
f(x+2h) - f(x-2h) &= 4f'(h) + 8f^{(3)}\frac{h^3}{3} + \mathcal{O}(h^5)
\end{aligned} . \tag{2.3}$$

Note that even higher order derivatives can be calculated with this method and the error continues to small assuming there is no error in evaluating f, which is wrong to assume.

These lets us obtain the following formulas first used to evaluate the derivatives of $\beta(s)$

$$\begin{aligned}
\frac{f(x+h) - f(x-h)}{2h} &= f'(x) + \mathcal{O}(h^2) \\
\frac{f(x+h) - 2f(x) + f(x-h)}{h^2} &= f''(x) + \mathcal{O}(h^2) \\
\frac{f(x+2h) - f(x-2h) - 2\cdot\Big[f(x+h) - f(x-h)\Big]}{2h^3} &= f^{(3)}(x) + \mathcal{O}(h^2)
\end{aligned} . \tag{2.4}$$

This gave us the estimates shown in table 2.1.

h	c_0	c_1	c_2	c_3
10^{-3}	0.7642228753	0.4447311944	0.9864563024	3.7223345586
10^{-6}	0.7642228753	0.4447299630	0.9867687981	-339.1159835
10^{-9}	0.7642228753	0.4447298812	-324.7689910	$1.537358655 \cdot 10^{11}$
10^{-12}	0.7642228753	0.4445708323	$-3.521692457 \cdot 10^{8}$	$2.459773844 \cdot 10^{20}$

Table 2.1: Derivatives of $g(s)$ for varying h by the Euler method.

Due to the limited precision of our numerical calculations the numerators of equation (2.4) cannot become arbitrarily small and errors are introduced here. Also as the denominator decreases (due to smaller h and larger powers of h) this error is magnified rendering the approximations of higher order derivatives extremely poor and in some cases completely unusable. Therefor this method is not at all recommended for calculating derivatives of high order and high precision. Other more numerically stable methods are used instead.

2.2.3 Evaluating the Euler Product

To use Cauchy's integral formula we need to evaluate β and especially the Euler product over primes congruent to 3 mod 4

$$\prod_{q\equiv_4 3} \frac{1}{(1-q^{-2s})}. \tag{2.5}$$

In section 1.3 we rewrite this as an expression that is now meromorphic on a larger set than the original expression, see equation (1.47). We can repeat this procedure inductively, as done in [5], and reach the form

$$\prod_{q\equiv_4 3} \frac{1}{(1-q^{-2s})} = \prod_{k=1}^{\infty} \left(\frac{\zeta(2^k s)(1-2^{-s\cdot 2^k})}{L(2^k s)} \right)^{\frac{1}{2^k}} \tag{2.6}$$

at least in the region $\text{Re}(s) > 1/2$. A quick look at the formula and inspecting the Dirichlet series of ζ and L will have the reader realize that the factors of this new product form converges much faster. This facilitates the evaluation of the Euler product when considering speed and accuracy.

2.2.4 Error of finite Cauchy's integral formula with Perfect Evaluation

The reasoning behind this way of extracting the derivatives is as follows. Choose a radius r for encircling the point a, then

$$\begin{aligned} g^{(n)}(a) &= \frac{n!}{2\pi i}\int_C \frac{g(z)}{(z-a)^{n+1}}dz = \frac{n!}{2\pi i}\sum_{k=0}^{\infty}\frac{g^{(k)}(a)}{k!}\int_C \frac{(z-a)^k}{(z-a)^{n+1}}dz = \\ &\frac{n!}{2\pi i}\sum_{k=0}^{\infty}\frac{g^{(k)}(a)}{k!}\int_0^1 (re^{2\pi i t})^{k-n-1} r 2\pi i e^{2\pi i t}dt = n!\sum_{k=0}^{\infty}\frac{g^{(k)}(a)}{k!}r^{k-n}\int_0^1 e^{2\pi i(k-n)t}dt \end{aligned} . \tag{2.7}$$

Now assuming we can evaluate functions perfectly, take a positive integer N. Then we approximate

$$g^{(n)}(a) \approx \frac{n!}{N}\sum_{k=0}^{\infty}\frac{g^{(k)}(a)}{k!}r^{k-n}\sum_{t=0}^{N-1} e^{\frac{2\pi i(k-n)t}{N}}. \tag{2.8}$$

Now we realize that the geometric sum $\sum_{t=0}^{N-1} e^{\frac{2\pi i(k-n)t}{N}} = \frac{1-e^{2\pi i(k-n)}}{1-e^{\frac{2\pi i(k-n)t}{N}}} = 0$ unless $(k-n)$ is multiple of N. So we have

$$g^{(n)}(a) \approx g^{(n)}(a) + n!\sum_{k=1}^{\infty}\frac{g^{(n+Nk)}(a)}{(n+Nk)!}r^{Nk-n}. \tag{2.9}$$

Evaluating the function in N points implies that only the Nth derivative will have an significant impact on the error for lower order derivatives! Of course this is not true when we have an error in evaluating g but it explains how 100 points give us 10 correct decimals for lower order derivatives in section 2.2.6.

2.2.5 Error of finite Cauchy's integral formula with Error in Evaluation

If we use the results from section 2.2.4 to mimic Cauchy's integral formula we see that our numerical integration gives us an accurate formula for the error in our coefficients. This must be modified a little because we have an error, $\mu(z)$, when evaluating the function. Let $\mu \in \mathbb{R}^+$ be a bound for the error. Using (2.9) we obtain a bound for the the total error E_n of our numerical integral when evaluating $g(z)$ along $z = re^{2\pi i\Delta t}$ at N equidistant points and gives us

$$\begin{aligned} E_n &= \left|\frac{n!}{N}\sum_{t=0}^{N-1}\frac{g(re^{\frac{2\pi i t}{N}})+\mu(z)}{(re^{\frac{2\pi i t}{N}})^n} - g^{(k)}(0)\right| = \left|n!\sum_{k=1}^{\infty}\frac{g^{(n+Nk)}(0)}{(n+Nk)!}r^{Nk-n} + \frac{n!}{N}\sum_{t=0}^{N-1}\frac{\mu(z)}{(re^{\frac{2\pi i t}{N}})^n}\right| \le \\ &n!\sum_{k=1}^{\infty}\left|\frac{g^{(n+Nk)}(0)}{(n+Nk)!}\right|r^{Nk-n} + \left|n!\frac{\mu}{r^n}\right| \le n!\sum_{k=1}^{\infty}\left|\frac{g^{(n+Nk)}(0)}{(n+Nk)!}\right|r^{Nk-n} + \frac{n!}{r^n}\mu \end{aligned} . \tag{2.10}$$

Note that this is the absolute error and not the relative error. It is the relative error which is the deciding factor for the number of correct significant decimals. We know from 2.2.3 that g has a pole dominated by the function $\frac{1}{(1/2-z)^{\frac{1}{4}}}$ close to $z = 1/2$. This in turn is dominated by $2\frac{2}{1-2z}$. This has a known Taylor series at $z = 0$.

$$\frac{1}{1-2z} = \sum_{n=0}^{\infty} 2^n z^n. \tag{2.11}$$

So the Taylor coefficients $\frac{g^{(n)}(1)}{n!}$ are bounded by 2^{n+2}. So for $n = 0$, $r = 1/4$ and N=100 we obtain that the error

$$E_0 < 0!\sum_{k=1}^{\infty} 2^{100k+2}2^{-2\cdot 100k} + \mu < 2^{-97} + \mu. \tag{2.12}$$

Now μ is clearly the limiting factor. This allows us to estimate the parameter μ to be about the same size as the error in the first derivative. We will see it is about 10^{-12} and this means that the main source of error $\frac{n!}{r^n}\mu$ should remain small relative to the coefficients themselves for $n \leq 10$ and hence we calculate these.

2.2.6 Cauchy's Integral Formula

As mentioned in section 1.2.5 Cauchy's Integral formula can be used to evaluate derivatives of analytic functions. This method does not at all have the same issues as the Euler method. There are no problems with differences between small numbers or division of small numbers. With the Cauchy Integral formula derivatives of high orders are attainable. This means that more terms of (1.40) can be calculated and the approximation is improved. The constants can be seen in table 2.2.

$c_i \backslash n$	10^2	10^3	10^4
c_0	0.7642236535892	0.7642236535892	0.7642236535892
c_1	0.4447389306251	0.4447389306251	0.4447389306251
c_2	0.9866106018490	0.986610601850	0.98661060185020
c_3	3.7253546472399	3.72535464723	3.725354647225
c_4	20.1862425191	20.1862425193	20.18624251933
c_5	144.9900524145	144.990052411	144.9900524098
c_6	1313.5045345	1313.50453459	1313.504534589
c_7	14477.286477	14477.286474	14477.2864745
c_8	188779.2160	188779.21610	188779.216094
c_9	2847988.186	2847988.1842	2847988.1840
c_{10}	48824018.02	48824018.1	48824018.06
c_{11}	937401747	937401745	937401745
c_{12}	19919500790	19919500900	19919500897
c_{13}	463960187000	463960184000	463960182900
c_{14}	11750211900000	11750212300000	11750212227000
c_{15}	321405170000000	321405165600000	321405167400000

Table 2.2: Constants c_n for varying the number of points n used for the integral in Cauchy's integral formula.

2.3 Numerical Results

We have now gathered all the essential parts to finally find an approximation of $B(x)$. The formula (1.40) uses the constants from section 2.2.6 and gives us the approximation.

Comparing our final approximation, $\mathfrak{B}(x)$, of $B(x)$ with the true values for some x gives the following table. Note that $\mathfrak{B}(x)$ was calculated using c_1 from [6], knowing that it is the Landau-Ramanujan constant and has previously been determined to very high precision. Here $S(x)$ denotes the approximation using the two first constants calculated by Shanks in [5]. The exact number of relevant digits that were used in the constants were 9.

x	$B(x)$	$S(x)$	$\mathfrak{B}(x)$	$B(x)/\mathfrak{B}(x)$	$B(x)/S(x)$
$1 \cdot 10^2$	43	40	787	0.0546	1.0720
$5 \cdot 10^2$	177	168	367	0.483	1.0559
$1 \cdot 10^3$	330	315	465	0.709	1.0467
$5 \cdot 10^3$	1443	1399	1532	0.9419	1.0316
$1 \cdot 10^4$	2749	2677	2832	0.9708	1.0268
$5 \cdot 10^4$	12460	12241	12547	0.99307	1.0179
$1 \cdot 10^5$	24028	23662	24117	0.99630	1.0155
$5 \cdot 10^5$	111379	110161	111499	0.99893	1.0111
$1 \cdot 10^6$	216341	214267	216488	0.999321	1.00968
$5 \cdot 10^6$	1017155	1009630	1017309	0.999849	1.00745
$1 \cdot 10^7$	1985459	1972275	1985644	0.9999067	1.00668
$5 \cdot 10^7$	9423222	9373333	9423396	0.9999815	1.00532
$1 \cdot 10^8$	18457847	18368583	18458002	0.99999162	1.00486
$5 \cdot 10^8$	88210025	87859100	88210129	0.99999882	1.00399
$1 \cdot 10^9$	173229058	172591375	173228787	1.00000156	1.00369
$5 \cdot 10^9$	832229729	829644038	832228161	1.00000188	1.00312
$1 \cdot 10^{10}$	1637624156	1632873167	1637621253	1.00000177	1.00291

Table 2.3: Approximation and true values of B for some values of x.

x	$B(x) - \mathfrak{B}(x)$	$(B(x) - \mathfrak{B}(x))/(\sqrt{x}/log(x))$
$1 \cdot 10^2$	-744	-343
$5 \cdot 10^2$	-190	-52.7
$1 \cdot 10^3$	-135	-29.6
$5 \cdot 10^3$	-89.0	-10.7
$1 \cdot 10^4$	-82.6	-7.61
$5 \cdot 10^4$	-87.0	-4.21
$1 \cdot 10^5$	-89.2	-3.25
$5 \cdot 10^5$	-120	-2.22
$1 \cdot 10^6$	-147	-2.03
$5 \cdot 10^6$	-154	-1.0620
$1 \cdot 10^7$	-185	-0.9443
$5 \cdot 10^7$	-174	-0.437
$1 \cdot 10^8$	-155	-0.285
$5 \cdot 10^8$	-104	-0.0931
$1 \cdot 10^9$	271	0.177
$5 \cdot 10^9$	1567	0.495
$1 \cdot 10^{10}$	2902	0.668

Table 2.4: Table of the absolute error and how it correlates to $\sqrt{x}/log(x)$

2.3.1 Approximation for Large Numbers

It is also possible to study the increase in error for intervals at higher values of x. That is we calculate $B(x_2) - B(x_1)$ and compare this to $\mathfrak{B}(x_2) - \mathfrak{B}(x_1)$. First we introduce a space saving measure in the form of some notation. We write $B(x_2, x_1) = B(x_2) - B(x_1)$ and similarly for the various approximations. Now, let us study intervals on the form $x_2 - x_1 = 10^l$ and $x_1 = 10^n$. The following results are procured.

l	n	$B(x_2, x_1)$	$S(x_2, x_1)$	$\mathfrak{B}(x_2, x_1)$	$S(x_2, x_1)/B(x_2, x_1)$	$\mathfrak{B}(x_2, x_1)/B(x_2, x_1)$
7	15	1303275	1302504	1303974	0.999408	1.000537
7	17	1224128	1223346	1224414	0.999361	1.000234
7	19	1159086	1157376	1157888	0.99852	0.99897
8	15	13037695	13025040	13039744	0.999029	1.000157
8	17	12244597	12233464	12244152	0.999091	0.9999637
8	19	11581362	11570432	11578624	0.999056	0.999764
9	15	130396995	130250396	130397443	0.99888	1.00000344
9	17	122439484	122334640	122441524	0.999144	1.0000167
9	19	115787287	115704832	115784960	0.999288	0.9999799
10	15	1401395794	1302503874	1303974345	0.99886	1.00000475
10	17	1224414229	1223346414	1224415260	0.999128	1.000000842
10	19	1157861020	1157046528	1157852416	0.999297	0.99999257

Table 2.5: Approximation and the true values of the increase in $B(x)$ for large x.

Chapter 3

Discussion

3.1 Discussion of numerical results

Specifications on the implementations of built-in functions of SageMath were hard to find and therefore the accuracy of the calculated constants can only be discussed by comparing them with ones that are already known. In [6] the constant c_1 has been calculated with high precision and we denote this value by c_1^*

$$c_1^* = 0.76422365358922066299... \tag{3.1}$$

The error of the calculated c_1 is

$$|c_1 - c_1^*| < 10^{-13}. \tag{3.2}$$

Moreover the quotient of the first and second constant is calculated by Shanks in [5] to

$$\left(\frac{c_2}{c_1}\right)^* = 0.581948659. \tag{3.3}$$

With the constants calculated here the first digits of the quotient are

$$\frac{c_2}{c_1} = 0.58194865931. \tag{3.4}$$

We see that all digits that Shanks calculated are the same. This should hopefully convince the reader that the higher order constants have decent accuracy as well. These approximate constants seem to be quite accurate but the authors still are not quite so sure of how an integral evaluation of 100 points gives just as good a value as 10000 points. The improved approximation for large x also hint at the correctness of the constants

3.2 Further studies

Studying the numerical results and obtaining quantitative information on how accurate the calculated values of c_n are exactly is a very interesting and relevant topic for future study. As previously mentioned priorities would lie elsewhere. Also using the lower incomplete Γ function to create $c_n(x)$ as described in equation (1.36) would yield some interesting results and should be implemented.

Another future continuation of this study would be to derive a proper error term when discussing the analytic extension of β and translating the left contour down to Re(s) = 1/4. After that calculating some of the correction terms from this shift, taken from eq 1.58. Calculating these terms and numerically checking if they give a better approximation would also be interesting to see.

One should try and remove the assumption that all zeros are simple. That would give us some other terms in the final formula but it will take some to determine to order of the zeros.

Discussing the possibility of extending $\beta(s)^2$ down to s=0 does not seem impossible with the formula from equation (2.6). If one were to succeed bounding the error of the vertical part of the contour close to $\mathrm{Re}(s) = 1/4$ by $\mathcal{O}(x^{1/4+\epsilon})$ the contour may again be shifted even further to the left!

Moreover the reader might have thought that maybe one could utilize that the function g is the square-root of a product where many of the individual factors have derivatives that can be calculated separately and then use the product rule on g. This would let us gain even more accurate results. Only the Euler product would have to be differentiated using Cauchy's integral formula and the rest can be done analytically, in fact they are implemented in SageMath.

Appendix A

Code

A.1 Code for Finding $B(x)$

The following code is written in C++ and made for calculating $B(x)$. The variable `length` needs to be defined in the same file and as a `const` of type `size_t`. It is x. The given `bitset` will be filled to match $b(n)$. Sum this up to get $B(x)$.

```
void make_b(std::unique_ptr<std::bitset<length>>& b)
{
   for (std::size_t x = 0; x < sqrtl(length/2) + 1; ++x)
   {
      for (std::size_t y = x; y < sqrtl(length) + 1; ++y)
      {
         std::size_t z = x * x + y * y;
         if (z < length)
         {
            b->set(z);
         }
         else {
            break;
         }
      }
   }
}
```

A.2 Code for Finding $B(x_2, x_1)$

The following code is written in C++ and made for calculating $B(x_2, x_1)$. It is a slight variation of the code from the previous section. The variables `begVal` and `endVal` need to be defined in the same file and as `const`s of type `size_t`. They are x_1 and x_2 respectively. The given `bitset` will be filled to match $b(n)$ in this interval. Sum this up to get $B(x_2, x_1)$.

```
void makeInterval_b(std::unique_ptr<std::bitset<endVal - begVal>>& b)
{
   for (std::size_t x = 0; x < sqrtl(endVal/2) + 1; ++x)
   {
      std::size_t num = sqrtl(begVal - x * x) - 1;
      num = std::max(num, x);
      for (std::size_t y = num; x*x + y*y < endVal + 1; ++y)
      {
         std::size_t z = x * x + y * y;
         if (z < endVal && z >= begVal)
         {
            b->set(z - begVal);
         }
      }
```

```
    }
}
```

A.3 Code for Finding $g^{(n)}(0)$

The following SageMath code is for finding the constants $g^{(n)}(0)$. Call the function `cauchy_deriv_g` with the argument n.

```
from sage.libs.lcalc.lcalc_Lfunction import *
from math import isnan
chi=DirichletGroup(4)[1]
L=Lfunction_from_character(chi, type="int")

def euler_product(t):
   s = 1-t
   ret = 1
   factors = log(125/abs(s.real()), 2)
   for i in range(1, factors + 1):
      temp = 1
      temp = (temp * zeta((2**i) * s))
      temp = (temp * (1 - 2**(-s * (2 ** i))))
      temp = (temp / L.value((2**i) * s))
      temp = (temp ** ((1/2) ** i))
      if(isnan(ComplexField(100)(temp).real()) or isnan(ComplexField(100)(temp).imag())):
         return ret
      ret = ret * temp

   return ret

def h(t):
   return sqrt(L.value(1-t) * euler_product(t))/(pi * (1-t) * sqrt(1-2**(t-1)))

def g(t):
   return sqrt(-t * zeta(1-t)) * h(t)

def cauchy_deriv_g(n, r=1/4, points=100):
   ret = factorial(n)/(2*pi)
   sum = 0
   for i in range(points):
      x = 2*pi*i/points
      width = 2*pi/points
      sum = sum + width * g(r*exp(x*I))/((r*exp(x*I))**n)
   ret = ret * sum
   return ret
```

A.4 Code for Approximating $B(x)$

This last section of code is written in Matlab for comparing $B(x)$ with its various approximations. The general form of the various approximations can be found in the following function. The input variables `x`, `c` and `gamma_inc` are x, a row vector with the constants c_n and a boolean specifying whether to use the incomplete gamma function or not.

```
function [ ret ] = f( x, vec, gamma_inc )
    logs = ones(length(x), length(vec));
    logaritms = 1./log(x);
    for i = 1:length(vec)
        logs(:, i) = logaritms.^(i-1);
    end
```

```
    ret = x.*log(x).^(-0.5);

    if gamma_inc
        gamma = zeros(length(vec), length(x));
        for i = 1:length(vec)
           gamma(i, :) = vec(i) * gammainc(log(x')/2, i-1/2);
        end
        ret = ret.*diag(logs*gamma);
    else
       ret = ret.*(logs*vec');
    end
end
```

The final code segment simply uses the previously defined function `f` to calculate the various approximations. The relative and absolute errors are also calculated. To run this code 7 vectors need to present in the workspace. Of these five are column vectors. These five are a vector with the values of x named `x`, one with the corresponding $B(x)$ and name `B`, one with l with name `l`, one with n with name `n` and one with the corresponding $B(x_2, x_1)$ with the name `B_diff`. The last two are row vectors containing the values of c_n with the name `c` and one with the values of Daniel Shanks constants, c_n, with the name `c_shanks`.

```
format long g

f_shanks = f(x, c_shanks, false);
f_normal = f(x, c, false);
f_incomplete = f(x, c, true);

results = [x B f_shanks f_normal f_incomplete];
relative = [x B./f_shanks B./f_normal B./f_incomplete];
absolute = [x B-f_shanks B-f_normal B-f_incomplete];
interesting = [x (B-f_normal).*log(x)./sqrt(x)];

f_shanks_diff = f(10.^n + 10.^l, c_shanks, false) - f(10.^n, c_shanks, false)
f_normal_diff = f(10.^n + 10.^l, c, false) - f(10.^n, c, false)
f_incomplete_diff = f(10.^n + 10.^l, c, true) - f(10.^n, c, true)

results_diff = [l n B_diff f_shanks_diff f_normal_diff f_incomplete_diff];
relative_diff = [l n B_diff./f_shanks_diff B_diff./f_normal_diff
    B_diff./f_incomplete_diff];
absolute_diff = [l n B_diff-f_shanks_diff B_diff-f_normal_diff B_diff-f_incomplete_diff];
```

Appendix B

Further Proofs

B.1 Uniform Absolute Convergence of $\beta(s)$ on any Closed Half Plane Defined by Re(s)$\geq c$>1

Let $s = \sigma + it$ be any complex number such that $\sigma \geq c$. Then first of all β(s) is absolutely convergent. This is because we can use integral convergence test on the sum of absolute values

$$\sum_{n\geq 1}^{\infty} |\frac{b(n)}{n^s}| \leq \sum_{n\geq 1}^{\infty} |\frac{1}{n^{\sigma}}| \leq 1 + \int_2^{\infty} (x-1)^{-\sigma} dx = 1 + [\frac{(x-1)^{1-\sigma}}{(1-\sigma)}]_2^{\infty} = 1 + \frac{1}{\sigma - 1}. \tag{B.1}$$

The series converges absolutely in the specified domain. Rearranging is now allowed. Now for proving uniform convergence we use a similar method. For any $\epsilon > 0$ there exists a N_ϵ such that $\sum_{n>N_\epsilon}^{\infty} |\frac{1}{n^c}| < \epsilon$ since c is a fix number greater than 1. Now one can use that for every s in our right half-plane has an even greater real part. This implies that for any such s

$$|(\sum_{n\geq 1}^{N_\epsilon} \frac{b(n)}{n^s}) - \beta(s)| = |\sum_{n>N_\epsilon}^{\infty} \frac{b(n)}{n^s}| \leq \sum_{n>N_\epsilon}^{\infty} |\frac{b(n)}{n^s}| \leq \sum_{n>N_\epsilon}^{\infty} |\frac{1}{n^s}| = \sum_{nN_\epsilon}^{\infty} |\frac{1}{n^{\sigma}}| \leq \sum_{nN_\epsilon}^{\infty} |\frac{1}{n^c}| < \epsilon. \tag{B.2}$$

Therefore the convergence is uniform. □

Note that each partial sum is a sum of analytic functions and is therefore analytic itself. $\beta(s)$ is the uniform limit of analytic functions and therefore analytic itself.

B.2 Rewriting β(s) in the Right Half Plane

Let $s = \sigma + it$ be any complex number such that $\sigma \geq c > 1$. For any given s in our half-plane of convergence we have that the series of partial sums converges absolutely and uniformly by appendix B.1. Now let q and p always denote some prime

$$\begin{aligned} S(N) &= \sum_{n=1}^{N} \frac{b(n)}{n^s} \\ P(N) &= (\sum_{n=0}^{N} 2^{-ns})(\prod_{\substack{q\equiv_4 3 \\ q\leq N}} \sum_{n=0}^{N} q^{-2ns})(\prod_{\substack{p\equiv_4 1 \\ p\leq N}} \sum_{n=0}^{N} p^{-ns}) \end{aligned} \tag{B.3}$$

The sum of two squares theorem and unique prime factorization implies that $P(N)$ is also a partial sum of $\beta(s)$. Given any n such that $b(n) = 1$, $\frac{1}{n^s}$ will be a term in the $P(N)$ for a large enough N. But it is clearly a reordering. Absolute convergence allows this kind of rearranging. Now we can choose $\epsilon > 0$, N_ϵ and M_ϵ such that $|S(N_\epsilon) - \beta(s)| < \epsilon$ and $S(N_\epsilon)$ is a partial sum of $P(M_\epsilon)$. In other words we have

$$|P(M_\epsilon) - \beta(s)| \leq |S(N_\epsilon) - \beta(s)| < \epsilon. \tag{B.4}$$

And therefore $P(N)$ converges to $\beta(s)$ absolutely and uniformly since we never specified anything depending on s.

Now we want to be able to manipulate each of the three factors independently. Let

$$\begin{aligned} X(N,s) &= (\sum_{n=0}^{N} 2^{-ns}) \quad \rightarrow \quad X(s) = (1-2^{-s})^{-1} \\ Y(N,s) &= \prod_{\substack{q\equiv_4 3 \\ q\leq N}} \sum_{n=0}^{N} q^{-2ns} \quad \rightarrow \quad Y(s) = \prod_{q\equiv_4 3} (1-q^{-2s})^{-1} \\ Z(N,s) &= \prod_{\substack{p\equiv_4 1 \\ p\leq N}} \sum_{n=0}^{N} p^{-ns} \quad \rightarrow \quad Z(s) = \prod_{p\equiv_4 1} (1-p^{-s})^{-1} \end{aligned}. \tag{B.5}$$

These are all clearly absolutely convergent to something. Note that the formula for geometric sums was used to simplify the expressions. It is clear that for each N all three are analytic. Repeat the procedure described in appendix B.1 to prove that the all three series converge absolutely and uniformly on any half-plane defined by $Re(s) \geq c > 1$ to some analytic function $X(s)$, $Y(s)$, $Z(s)$ respectively. Now it is well-known that as long as all limits are well-defined the product of limits is the limit of the product and therefore

$$\beta(s) = X(s)Y(s)Z(s). \tag{B.6}$$

B.3 Residue of $\frac{1}{\sqrt{s}}$

The residue of a pole $\frac{1}{\sqrt{s}}$ is

$$\int_C \frac{1}{\sqrt{s}} ds = \int_0^{2\pi} \frac{ire^{i\theta}}{r^{1/2}e^{i\theta/2}} d\theta = \int_0^{2\pi} ir^{1/2}e^{i\theta/2} d\theta = ir^{1/2} \int_0^{2\pi} e^{i\theta/2} d\theta = -2ir^{1/2}. \tag{B.7}$$

As $r \to 0$ this expression becomes 0. Thus the residue of this pole is 0.

Bibliography

[1] Underwood Dudley, *Elementary Number Theory*, W.H. Freeman and Company, 1969.

[2] Harold Davenport, *Multiplicative Number Theory*, Springer-Verlag, 1967.

[3] Yasushi Matsuoka, “On the power series coefficients of the riemann zeta function”, *TOKYO J. MATH.*, vol. 12, no. 1, pp. 49–58, 1989.

[4] Serge Lang, *Algebraic Number Theory*, Springer-Verlag, 1994.

[5] Daniel Shanks, “The second-order term in the asymptotic expansion of b(x)”, *Mathematics of Computation*, vol. 18, no. 85, pp. 75–86, 1964.

[6] The on-line encyclopedia of integer sequences, “Landau-ramanujan constant”, 2018.