



# Platt, D. J. (2017). Isolating some non-trivial zeros of Zeta. Mathematics of Computation. DOI: 10.1090/mcom/3198

Peer reviewed version

License (if available): Unspecified

Link to published version (if available): [10.1090/mcom/3198](http://dx.doi.org/10.1090/mcom/3198)

[Link to publication record in Explore Bristol Research](http://research-information.bristol.ac.uk/en/publications/isolating-some-nontrivial-zeros-of-zeta(2826fe29-b4d7-4911-964a-6aba9b0ce807).html) PDF-document

This is the author accepted manuscript (AAM). The final published version (version of record) is available online via American Mathematical Society at http://www.ams.org/journals/mcom/0000-000-00/S0025-5718-2017- 03198-7/home.html#Additional . Please refer to any applicable terms of use of the publisher.

## **University of Bristol - Explore Bristol Research General rights**

This document is made available in accordance with publisher policies. Please cite only the published version using the reference above. Full terms of use are available: http://www.bristol.ac.uk/pure/about/ebr-terms.html

#### ISOLATING SOME NON-TRIVIAL ZEROS OF ZETA

#### DAVID J. PLATT

ABSTRACT. We describe a rigorous algorithm to compute Riemann's zeta function on the half line and its use to isolate the non-trivial zeros of zeta with imaginary part  $\leq 30,610,046,000$  to an absolute precision of  $\pm 2^{-102}$ . In the process, we provide an independent verification of the Riemann Hypothesis to this height.

## 1. Introduction

Riemann's zeta function is defined initially for  $\Re s > 1$  by

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

It has analytic continuation to the entire complex plane with the exception of a simple pole at  $s = 1$  with residue 1 and we have the following functional equation

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

Since neither  $\zeta$  nor  $\Gamma$  have poles to the right of  $s = 1$ , the simple poles of  $\Gamma\left(\frac{s}{2}\right)$ for  $s \in \{-2, -4, \ldots\}$  correspond to simple zeros of  $\zeta$ . In addition to these "trivial" zeros,  $\zeta$  has an infinite number of zeros with real part in the interval  $(0, 1)$ . The conjecture that all of these non-trivial zeros have real part exactly  $\frac{1}{2}$  is the Riemann Hypothesis (RH).

1.1. Why isolate non-trivial zeros? Many applications in Number Theory involve sums over the non-trivial zeros of  $\zeta$ . Examples include computing  $\pi(x)$  via the Lagarias-Odlyzko analytic method [14][20] and locating sign changes for  $\pi(x)$ −li $(x)$ [26] and  $\theta(x) - x$  [23]. For our research, we determined we would need about  $10^{11}$ zeros, those to a height of  $t \approx 3 \times 10^{10}$ , isolated rigorously to an absolute precision of 100 bits or so. Tools such as Rubinstein's 'lcalc' [25] and Johansson et al's 'mpmath' package for Python [13] rely on the Riemann-Siegel algorithm (see below) and therefore become unwieldy as  $t$  increases. Some databases of pre-computed zeros do exist. For example, Odlyzko's web page [17] provides, inter alia, the first 2,001,052 zeros to  $\pm 4 \times 10^{-9}$  (about 30 bits), but again we required both more height and more precision. We therefore turned to isolating those zeros ourselves. This then requires an efficient method of computing  $\zeta$  on the half line, i.e. at points  $s = 1/2 + it$  with  $t \in \mathbb{R}$ .

<sup>2010</sup> Mathematics Subject Classification. Primary 11Y35 11M26.

This algorithm was developed during the author's Doctoral research under the patient supervision of Dr. Andrew Booker. The author would also like to thank the staff of the Advanced Computing Resource Centre at the University of Bristol for their invaluable support and the anonymous referees for their careful reading of and constructive comments on the original manuscript.

1.2. Existing methods. Many algorithms have been described for the evaluation of  $\zeta$  on the half line. These divide naturally into those for evaluating  $\zeta(1/2 + it)$ for single values of  $t$  and those which examine many values of  $t$  simultaneously.

Examples of the former include Euler-Maclaurin (see e.g. [3]), Riemann-Siegel [8] and Berry-Keating [4]. The algorithm exploiting Euler-Maclaurin has time complexity  $\mathcal{O}(t)$  whereas Riemann-Siegel achieves  $\mathcal{O}\left(t^{1/2}\right)$ . The distributed ZetaGrid computations of Wedeniwski were achieved using "vanilla" Riemann-Siegel [30]. Heath-Brown and Hiary have described ways to compute the main sum that bring the exponent down further to  $1/3 + o(1)$  and  $4/13 + o(1)$  respectively [12].

When one is interested in computing many values of  $\zeta$ , algorithms which amortise computations over many function evaluations become attractive. That due to Odlyzko and Schönhage [19] computes  $\mathcal{O}(t^{1/2+\epsilon})$  values in time  $\mathcal{O}(t^{1/2+\epsilon})$  and space  $\mathcal{O}(t^{1/2+\epsilon})$ . This algorithm has been used for the large scale computations of Odlyzko [18] and Gourdon [10]. Booker's algorithm for generic L-functions is described in [6]. When applied to  $\zeta$ , it has the same asymptotic time complexity as Odlyzko-Schönhage but requires space  $\mathcal{O}(t)$ . Its main advantage is that it is straightforward to make rigorous and in such a rigorous form, it has been applied by Booker to Artin L-functions and by the author to Dirichlet L-functions [21]. We will describe a windowed version of Booker's algorithm, specialised to  $\zeta$  that reduces its space requirement whilst retaining its rigorous numerics and efficiency.

We will proceed first with some notation, then we will describe how we compute  $\zeta(1/2 + it)$  at regularly spaced points up the half line. We will then discuss the techniques used to isolate zeros using these data points and the final section will provide some details on its implementation.

#### 2. NOTATION

We will write  $e(x)$  for  $exp(2\pi ix)$  and define the Fourier Transform of  $f(t)$  to be

$$
F(x) := \int_{-\infty}^{\infty} f(t)e(-tx) dt
$$

where this integral exists. The Discrete Fourier Transform of  $N \in \mathbb{Z}_{>0}$  complex values  $X_0 \ldots X_{N-1}$  results in N values  $Y_0 \ldots Y_{N-1}$  where

$$
Y_j = \sum_{k=0}^{N-1} X_k e\left(-\frac{jk}{N}\right).
$$

To obtain the inverse (Discrete) Fourier Transform we change the sign in the complex exponential.

## 3. The Algorithm

The algorithm we will now describe is essentially a windowed version of that of Booker, specialised to  $\zeta$ .

We start by defining

$$
\Lambda(t) = \pi^{-\frac{it}{2}} \Gamma\left(\frac{\frac{1}{2} + it}{2}\right) \zeta\left(\frac{1}{2} + it\right)
$$

which, by the functional equation for  $\zeta$ , is real-valued. We will work with a windowed version of  $\Lambda$  centred around  $t_0 > 0$  defined for  $h > 0$  by

(3.1) 
$$
f(t) := \Lambda(t + t_0) \exp\left(\frac{\pi(t + t_0)}{4} - \frac{t^2}{2h^2}\right).
$$

The  $\exp\left(\frac{\pi(t+t_0)}{4}\right)$  term is inserted for computational expedience and serves to counteract the decay of the Gamma function.

We proceed as follows:

(1) Select  $t_0, h > 0$ ,  $K \in \mathbb{Z}_{\geq 0}$  and  $A, B > 0$  such that  $N = AB \in 2\mathbb{Z}_{> 0}$ . For  $n = -\frac{N}{2} \dots \frac{N}{2} - 1$  and  $k = 0, 1, \dots, K$  compute  $g\left(\frac{n}{A}; k\right)$  where  $g(t; k)$  is defined by

$$
g(t; k) := \Gamma\left(\frac{\frac{1}{2} + i(t + t_0)}{2}\right) \exp\left(\frac{\pi(t + t_0)}{4} - \frac{t^2}{2h^2}\right) (-2\pi i t)^k.
$$

(2) Use each value of  $g\left(\frac{n}{A};k\right)$  to approximate

$$
\widetilde{g}(n;k) := \sum_{l \in \mathbb{Z}} g\left(\frac{n}{A} + lB; k\right).
$$

(3) Use discrete Fourier transforms to compute

$$
\widetilde{G}^{(k)}(m) := \sum_{l \in \mathbb{Z}} G^{(k)}\left(\frac{m}{B} + lA\right),\,
$$

where

$$
G(u) := \int_{-\infty}^{\infty} g(t; 0) e(-tu) dt.
$$

- (4) Use each value of  $\widetilde{G}^{(k)}(m)$  to approximate  $G^{(k)}\left(\frac{m}{B}\right)$ .
- (5) Use a series of convolutions to sum terms involving  $G\left(\frac{m}{B}\right)$  and its derivatives to approximate  $F\left(\frac{m}{B}\right)$ , where

$$
F(x) := \int_{-\infty}^{\infty} f(t)e(-tx) dt.
$$

(6) Use values of  $F\left(\frac{m}{B}\right)$  as an approximation to  $\widetilde{F}(m)$  where

$$
\widetilde{F}(m) := \sum_{l \in \mathbb{Z}} F\left(\frac{m}{B} + lA\right).
$$

(7) Now use another discrete Fourier transform to compute

$$
\widetilde{f}(n) := \sum_{l \in \mathbb{Z}} f\left(\frac{n}{A} + lB\right).
$$

(8) Finally, use  $\tilde{f}(n)$  as an approximation to  $f\left(\frac{n}{A}\right)$ .

The only issue in step (1) is the rigorous computation of  $\log \Gamma$  and we use Olver's bound (see (4.1) of [11]) for the error in truncating Stirling's approximation.

 $\overline{1}$ 

For steps  $(2)$ ,  $(4)$ ,  $(6)$  and  $(8)$  we need rigorous bounds for (respectively)

 $\mathbf{I}$ 

$$
\left| \sum_{l \in \mathbb{Z}_{\neq 0}} g\left(\frac{n}{A} + lB; k\right) \right|,
$$
  

$$
\left| \sum_{l \in \mathbb{Z}_{\neq 0}} G^{(k)}\left(\frac{m}{B} + lA\right) \right|,
$$
  

$$
\left| \sum_{l \in \mathbb{Z}_{\neq 0}} F\left(\frac{m}{B} + lA\right) \right|
$$
  

$$
\left| \sum_{l \in \mathbb{Z}_{\neq 0}} f\left(\frac{n}{A} + lB\right) \right|.
$$

and

Booker provides bounds for these quantities for the general (non-windowed) Lfunction case in [6]. However, we must accommodate the inclusion of the Gaussian and we can also exploit our knowledge of the specific analytic properties of  $\zeta$ . In the interests of readability, we defer the necessary Lemmas to appendix A.

Steps (3) and (7) rely on the following Lemma.

**Lemma 3.1.** Let  $f(t)$  be a function in the Schwartz space with Fourier transform  $F(x)$ . Let  $N = AB$  with  $A, B > 0$  and define

$$
\tilde{f}(n) := \sum_{l \in \mathbb{Z}} f\left(\frac{n}{A} + lB\right)
$$

and

$$
\tilde{F}(m) := \sum_{l \in \mathbb{Z}} F\left(\frac{m}{B} + lA\right).
$$

Then, up to a constant factor,  $\tilde{f}$  and  $\tilde{F}$  form a Discrete Fourier Transform pair of length N.

Proof. By Poisson summation we have

$$
\sum_{l \in \mathbb{Z}} f(t + lB) = \frac{1}{B} \sum_{l \in \mathbb{Z}} F\left(\frac{l}{B}\right) e\left(\frac{lt}{B}\right)
$$

$$
\tilde{f}(n) = \frac{1}{B} \sum_{l \in \mathbb{Z}} F\left(\frac{l}{B}\right) e\left(\frac{ln}{N}\right).
$$

We now write  $l = l'N + m$  to get

$$
\tilde{f}(n) = \frac{1}{B} \sum_{m=0}^{N-1} \sum_{l' \in \mathbb{Z}} F\left(\frac{l'N+m}{B}\right) e\left(\frac{(l'N+m)n}{N}\right)
$$

$$
= \frac{1}{B} \sum_{m=0}^{N-1} e\left(\frac{mn}{N}\right) \tilde{F}(m).
$$

This is, by definition, an inverse Discrete Fourier Transform.

We note that by choosing  $N = AB$  to be a power of two, the Discrete Fourier Transform can be computed with time complexity  $\mathcal{O}(N \log N)$  via any Fast Fourier Transform algorithm<sup>1</sup>.

The meat of step (5) is the following two Lemmas.

**Lemma 3.2.** Let  $F$  be the Fourier transform of  $f$ . Then

$$
\begin{vmatrix} F(x) & - \sum_{j=1}^{\infty} \frac{1}{\sqrt{j}} (j\sqrt{\pi})^{-it_0} G\left(x + \frac{\log (j\sqrt{\pi})}{2\pi}\right) \right] \\ & = 2\pi^{\frac{5}{4}} \exp\left(\frac{1}{8h^2} - \frac{t_0^2}{2h^2} - \pi x\right).
$$

*Proof.* We start with  $F(x) = \int_{0}^{\infty}$ −∞  $f(t)e(-tx) dt$  and substitute  $s = \frac{1}{2} + i(t+t_0)$ . We then shift the line of integration right to  $\Re(s) = \sigma > 1$  picking up the simple pole of  $\zeta(s)$  with residue 1 at  $s = 1$ . Now write  $\zeta(s)$  as a sum (over j), interchange the

sum and integral and move the line of integration back to  $\frac{1}{2}$ .

### Lemma 3.3.

(3.2) 
$$
F(x) = \sum_{k=0}^{\infty} \sum_{m} \frac{G^{(k)}(x + u_m)}{k!} S_m^{(k)}
$$

where  $S_m^{(k)}$  is defined for  $\xi = \frac{1}{2B}$  via

$$
S_m^{(k)} := \sum_{\frac{\log\left(j\sqrt{\pi}\right)}{2\pi} \in [u_m - \xi, u_m + \xi)} \frac{1}{\sqrt{j}} \left(j\sqrt{\pi}\right)^{-it_0} \left(\frac{\log\left(j\sqrt{\pi}\right)}{2\pi} - u_m\right)^k.
$$

*Proof.* This is a simple application of Taylor's theorem.  $\Box$ 

Now for each  $k$ ,  $(3.2)$  is a discrete convolution which we can evaluate with three DFT's. Computing  $F\left(\frac{m}{B}\right)$  is then achieved by summing the output of such convolutions.

Rigorous estimates for the error in truncating the Taylor expansion after  $K$  terms and the sum over  $j$  after  $J$  terms can both be found in Appendix B.

#### 4. Isolating Zeros

Armed with values of  $f(t_i)$  for regularly spaced  $t_i \in [T, T+h]$ , each change in sign between  $t_i$  and  $t_{i+1}$  indicates the presence of at least one non-trivial zero of  $\zeta$ . We now need to able to achieve three things:-

- We need to determine how many zeros there are in the rectangle  $\Re z \in (0,1)$ ,  $\Im z \in [T, T+h].$
- If we don't have enough sign changes to account for these expected zeros, we need a means of increasing our sample rate until we  $do^2$ .
- For each sign change, we need a way of "zooming in" to isolate the zero to high precision.

<sup>&</sup>lt;sup>1</sup>This complexity can actually be achieved for any  $N$ , even prime, but the implied constants are larger.

<sup>&</sup>lt;sup>2</sup>If RH does not hold, our algorithm will not halt.

#### 6 DAVID J. PLATT

In the (rare) event that we did not have enough sign changes, we simply re-ran the above algorithm having changed the parameters to achieve an increased sample rate. The other two requirements are the subject of the next two sub-sections.

4.1. Turing's Method. Providing a reference to confirm that all the non-trivial zeros have been accounted for was addressed in Turing's last publication [28] and subsequently corrected and improved by Lehman [15] and further improved by Trudgian [27]. Specifically, we have the following two Theorems.

**Theorem 4.1.** For t not the ordinate of a zero nor a pole of  $\zeta$ , define

(4.1) 
$$
S(t) := \frac{1}{\pi} \Im \int_{-\infty}^{\frac{1}{2}} \frac{\zeta'}{\zeta} (\sigma + it) d\sigma,
$$

and when t is a zero or a pole, define

$$
S(t) := \lim_{\epsilon \to 0+} S(t + \epsilon).
$$

Now for t not the ordinate of a zero of  $\zeta$ , define  $N(t)$  to be the number of zeros of  $\zeta(s)$  with  $\Re s \in (0,1)$  and  $\Im s \in [0,t]$ . Then

(4.2) 
$$
N(t) = \frac{1}{\pi} \left[ \Im \log \Gamma \left( \frac{\frac{1}{2} + it}{2} \right) - \frac{t \log \pi}{2} \right] + 1 + S(t).
$$

*Proof.* See, for example, page 128 of Edwards [9].  $\Box$ 

**Theorem 4.2** (Trudgian). For  $t_2 > t_1 > 168\pi$  with  $S(t)$  defined as above, we have

$$
\left| \int_{t_1}^{t_2} S(t) dt \right| \le 2.067 + 0.059 \log t_2.
$$

*Proof.* This is Theorem 2.2 of [27].

To exploit these results, assume we have  $168\pi < t_1 < t_2 < t_3$  and we have located some zeros in  $[t_1, t_3]$ . We use these zeros to estimate

$$
I_{comp} = \int_{t_1}^{t_3} N(t) dt = N(t_1)(t_3 - t_1) + \int_{t_1}^{t_3} N(t) - N(t_1) dt.
$$

Note that even though we do not know  $N(t_1)$  a priori, we know it to be an integer and Theorem 4.2 will allow us to determine which one.

We now compute

$$
I_{max} = 2.067 + 0.059 \log t_3 + \int_{t_1}^{t_3} \frac{1}{\pi} \left[ \Im \log \Gamma \left( \frac{\frac{1}{2} + it}{2} \right) - \frac{t \log \pi}{2} \right] + 1 dt
$$

and compare it with  $I_{comp}$ . Suppose  $I_{max} - I_{comp} = \Delta$  and  $\Delta < t_3 - t_2$ , then we have accounted for all the zeros in  $[t_1, t_2]$ . If not, we look again with a finer lattice of values.

4.2. Isolating Zeros. At this point, we have a lattice of values of f at points  $t_i$ and we have two adjacent points where  $f$  changes sign. We use a rigorous version of Whittaker-Shannon up-sampling to allow us to compute  $f$  at intermediate points.

**Theorem 4.3** (Whittaker-Shannon Sampling). Let  $f(t)$  be a continuous, real valued function with Fourier Transform  $F(x)$  such that  $F(x) = 0$  for  $|x| > B > 0$ (i.e.  $f(t)$  is band-limited with bandwidth B). Also, define

$$
\operatorname{sinc}(x) := \frac{\sin(\pi x)}{\pi x}.
$$

Then

$$
f(t) = \sum_{n \in \mathbb{Z}} f\left(\frac{n}{2B}\right) \operatorname{sinc}\left(2B\left(\frac{n}{2B} - t\right)\right),\,
$$

when this sum converges.

*Proof.* See [29].

Now, if our function is not strictly band-limited, all is not lost. We can appeal to the following Theorem due to Weiss.

**Theorem 4.4** (Weiss). Let  $f(t)$  be a real valued function with Fourier Transform  $F(x)$  such that

- $(1) \quad \int_{0}^{\infty}$  $-\infty$  $|F(x)|dx < \infty$
- (2)  $F(x)$  is of bounded variation on  $\mathbb R$
- (3) when F has a jump discontinuity at x, then  $F(x) = \lim_{\epsilon \to 0^+}$  $F(x-\epsilon)+F(x+\epsilon)$  $\frac{+F(x+\epsilon)}{2}$ .

Then

$$
\left| f(t) - \sum_{n \in \mathbb{Z}} f\left(\frac{n}{2B}\right) \operatorname{sinc}\left(2B\left(\frac{n}{2B} - t\right)\right) \right| \le 4 \int\limits_{B}^{\infty} |F(x)| dx.
$$

*Proof.* See for example [7].  $\Box$ 

We will work with the function

$$
W(t) = \Lambda(t) \exp\left(\frac{\pi t}{4} - \frac{(t - t_0)^2}{2H^2}\right)
$$

which is close enough to being band-limited for our purposes. Note that the H in the Gaussian here can be chosen independently of the  $h$  in 3.1. We defer the detailed error bounds which allow us to exploit the above Theorems to Appendix C. To apply them, we (non-rigorously) estimate the location of the zero by Newton-Raphson and do a final check with two rigorous computations, one either side of the conjectured sign change.

### 5. Implementing the Algorithm

We set out to isolate the non-trivial zeros of  $\zeta$  to a height of  $3 \times 10^{10}$  to an absolute precision of  $\pm 2^{-102}$ . This implies results accurate to more than 135 bits and a working precision significantly higher. Typical IEEE compliant hardware floating point uses a 53 bit mantissa so we are forced to use software multiple precision despite the performance penalty (perhaps a factor of 50 to 100) that implies. In addition, we chose to manage the accumulation of rounding error using

interval arithmetic (see, for example, [16]) and this introduces a further overhead, although much smaller in comparison (less than a factor of 4 in our experience). We used the 'C' programming language and for multiple precision interval arithmetic, the MPFI package [24]. We extended MPFI in the obvious way to handle complex valued intervals as rectangles and our working precision was 300 bits. For steps (1) to (6) we used  $N = 2^{15}$  with  $B = 5,476$  as the width of our window and  $A = N/B$ . However, by exploiting Whittaker-Shannon up-sampling once again we can increase  $N$  to  $2^{20}$  during the Discrete Fourier Transform at stage  $(6)$ , almost for free, keeping  $B$  the same. At this point our sampling rate  $A$  is a little over 190. The remaining parameters (determined largely empirically) were  $h = \frac{176,431}{2,048}$ ,  $J = 104,000^3$  and  $K = 44$  being the Gaussian width, the number of terms to sum when computing  $F(x)$  and the number of differentials of G to carry respectively.

When up-sampling, we set  $H = 2089.0/16384.0$  and used 70 points either side of  $t_0$  using every 5th one in the sum.

We used up to 32 nodes of the University of Bristol Bluecrystal II cluster [2] (each node comprising two 4 core Intel<sup>®</sup> Xeon<sup>®</sup> running at 2.8GHz) and we performed approximately  $6 \times 10^{12}$  high precision evaluations of  $\zeta$  and isolated 103, 800, 788, 359 zeros with  $0 <$  3s  $<$  30, 610, 046, 000 to  $\pm 2^{-102}$ . Turing's method confirms that these are the only zeros in that range, so we have;

**Theorem 5.1.** Let  $\rho$  be a non-trivial zero of the Riemann zeta function with  $|\Im \rho| \leq$  $3.0610046 \times 10^{10}$ . Then  $\rho$  is simple and  $\Re \rho = \frac{1}{2}$ .

The imaginary parts of these zeros (13 bytes each so occupying a total of 1.3 Tbytes) have been stored and made available by Bober via the LMFDB project [5]. Researchers are invited to contact the author if they require copies of some or all of this data for their own purposes.

Appendix A. Bounds for Steps 2, 4, 6 and 8.

We now give bounds for the error terms implicit in steps  $(2)$ ,  $(4)$ ,  $(6)$  and  $(8)$ . We will first state some preparatory Lemmas.

**Lemma A.1.** Define the incomplete Gamma function for  $\Re s > 0$  by [1]

$$
\Gamma(s,x) := \int\limits_x^\infty t^{s-1} \mathrm{e}^{-t} \,\mathrm{d}t.
$$

Then, given  $\kappa > -1$  and  $x, h > 0$ , we have

$$
\int\limits_x^\infty w^\kappa \exp\left(\frac{-w^2}{2h^2}\right)\mathrm{d}w = 2^{\frac{\kappa-1}{2}}h^{\kappa+1}\Gamma\left(\frac{\kappa+1}{2},\frac{x^2}{2h^2}\right).
$$

*Proof.* We use the substitution  $t = \frac{w^2}{2h^2}$  to get

$$
\int_{x}^{\infty} w^{\kappa} \exp\left(\frac{-w^2}{2h^2}\right) dw = \int_{\frac{x^2}{2h^2}}^{\infty} 2^{\frac{k-1}{2}} h^{k+1} t^{\frac{k-1}{2}} e^{-t} dt
$$

and the result follows from the definition.  $\hfill \Box$ 

<sup>&</sup>lt;sup>3</sup>Lemmas A.3 and B.1 below imply that we need  $J = \mathcal{O}(t_0^{\frac{1}{2}})$  and it is this that dictates the space required to implement the algorithm efficiently.

**Lemma A.2.** Let  $t \ge \sigma \ge 1$ . Then we have

$$
\left|\Gamma\left(\frac{\sigma+it}{2}\right)\right|\exp\left(\frac{\pi t}{4}\right) < 2^{\frac{3-\sigma}{4}}\sqrt{\pi}t^{\frac{\sigma-1}{2}}\exp\left(\frac{1+2\sqrt{2}}{6t}\right).
$$

Proof. By Stirling's approximation we have,

$$
\Re \log \Gamma \left( \frac{\sigma + it}{2} \right) =
$$
  

$$
\Re \left[ \frac{\sigma + it}{2} \log \left( \frac{\sigma + it}{2} \right) - \frac{\sigma}{2} + \frac{1}{2} \log \left( \frac{4\pi}{\sigma + it} \right) + \frac{1}{6(\sigma + it)} \right] + E
$$

where, since  $\sigma/2 + it/2$  is in the right half plane, Olver's bound [11] applies again, so √ √

$$
|E| < \frac{\sqrt{2}(\sigma + t)}{6(\sigma^2 + t^2)} < \frac{\sqrt{2}}{3t}
$$

.

We now write

$$
\Re \frac{\sigma + it}{2} \log \left( \frac{\sigma + it}{2} \right) = \frac{\sigma}{2} \log \left( \frac{\sqrt{\sigma^2 + t^2}}{2} \right) - \frac{t}{2} \arctan \left( \frac{t}{\sigma} \right)
$$

We now use  $t > \sigma > 1$  so that

$$
\frac{\pi t}{4} - \frac{t}{2}\arctan\left(\frac{t}{\sigma}\right) - \frac{\sigma}{2} < 0
$$

and this, together with

$$
\frac{\sigma}{2}\log\left(\frac{\sqrt{\sigma^2+t^2}}{2}\right) + \frac{1}{2}\log\left(\frac{4\pi}{\sqrt{\sigma^2+t^2}}\right) = \log\left(2^{1-\frac{\sigma}{2}}\sqrt{\pi}(\sigma^2+t^2)^{\frac{\sigma-1}{4}}\right) < \log\left(2^{1-\frac{\sigma}{2}+\frac{\sigma-1}{4}}\sqrt{\pi}t^{\frac{\sigma-1}{2}}\right)
$$

proves the proposition.  $\hfill \square$ 

**Lemma A.3.** For  $h > 0$ ,  $k \in \mathbb{Z}_{\geq 0}$ , and  $\sigma \in 2\mathbb{Z}_{>0} + 1$  with  $\sigma + \frac{1}{2} \leq t_0$  define

$$
C(\sigma, t_0, h, k) :=
$$
  

$$
(2\pi)^k \int_{-\infty}^{\infty} \left| \Gamma\left(\frac{\sigma + i(t + t_0)}{2}\right) \exp\left(\frac{\pi(t + t_0)}{4} - \frac{t^2}{2h^2}\right) \left(\frac{1}{2} + \sigma - it\right)^k \right| dt
$$

and

$$
X := \sum_{l=0}^{\frac{\sigma-1}{2}} {\frac{\sigma-1}{l}} 2^{\frac{k+l-1}{2}} h^{k+l+1} t_0^{\frac{\sigma-1}{2}-l} \Gamma\left(\frac{k+l+1}{2}, \frac{(\sigma+\frac{1}{2})^2}{2h^2}\right).
$$

Then

$$
C(\sigma, t_0, h, k) < 2^{\frac{6k+5-\sigma}{4}} \pi^k e^{\frac{1+2\sqrt{2}}{6t_0}} \left(\sigma + \frac{1}{2}\right)^k \left(\sigma + \frac{1}{2} + t_0\right)^{\frac{\sigma - 1}{2}} h
$$
  
+  $2^{\frac{6k+7-\sigma}{4}} \pi^{\frac{2k-1}{2}} e^{\frac{1+2\sqrt{2}}{6t_0}} X.$ 

*Proof.* Since  $\sigma \geq 3$  we have

$$
2^{k} \pi^{k} \int_{-\infty}^{\infty} \left| \Gamma\left(\frac{\sigma + i(t + t_{0})}{2}\right) \exp\left(\frac{\pi(t + t_{0})}{4} - \frac{t^{2}}{2h^{2}}\right) \left(\frac{1}{2} + \sigma - it\right)^{k} \right| dt
$$
  

$$
< 2^{k+1} \pi^{k} \int_{0}^{\infty} \left| \Gamma\left(\frac{\sigma + i(t + t_{0})}{2}\right) \exp\left(\frac{\pi(t + t_{0})}{4} - \frac{t^{2}}{2h^{2}}\right) \left(\frac{1}{2} + \sigma - it\right)^{k} \right| dt.
$$

We now split the integral into two parts.

For  $t \in [0, \sigma + \frac{1}{2}]$ , we apply Lemma A.2 to get

$$
2^{k+1}\pi^{k}\int_{0}^{\sigma+\frac{1}{2}}\left|\Gamma\left(\frac{\sigma+i(t+t_{0})}{2}\right)\exp\left(\frac{\pi(t+t_{0})}{4}-\frac{t^{2}}{2h^{2}}\right)\left(\frac{1}{2}+\sigma-it\right)^{k}\right|dt
$$
  

$$
<2^{\frac{4k+7-\sigma}{4}}\pi^{\frac{2k+1}{2}}\int_{0}^{\sigma+\frac{1}{2}}(t+t_{0})^{\frac{\sigma-1}{2}}\exp\left(\frac{1+2\sqrt{2}}{6(t+t_{0})}-\frac{t^{2}}{2h^{2}}\right)\left|\left(\frac{1}{2}+\sigma-it\right)\right|^{k}dt
$$
  

$$
<2^{\frac{6k+7-\sigma}{4}}\pi^{\frac{2k-1}{2}}\left(\sigma+\frac{1}{2}\right)^{k}\left(\sigma+\frac{1}{2}+t_{0}\right)^{\frac{\sigma-1}{2}}\exp\left(\frac{1+2\sqrt{2}}{6t_{0}}\right)\int_{0}^{\infty}e^{-\frac{t^{2}}{2h^{2}}}\mathrm{d}t
$$
  

$$
=2^{\frac{6k+5-\sigma}{4}}\pi^{k}\left(\sigma+\frac{1}{2}\right)^{k}\left(\sigma+\frac{1}{2}+t_{0}\right)^{\frac{\sigma-1}{2}}\exp\left(\frac{1+2\sqrt{2}}{6t_{0}}\right)h.
$$

Using Lemma A.2 again, we bound the integral for  $t \ge \sigma + \frac{1}{2}$  as follows

$$
2^{k+1}\pi^{k}\int_{\sigma+\frac{1}{2}}^{\infty} \left| \Gamma\left(\frac{\sigma+i(t+t_0)}{2}\right) \exp\left(\frac{\pi(t+t_0)}{4}-\frac{t^2}{2h^2}\right) \left(\sigma+\frac{1}{2}-it\right)^{k} \right| dt
$$
  

$$
< 2^{\frac{4k+7-\sigma}{4}}\pi^{\frac{2k+1}{2}}\int_{\sigma+\frac{1}{2}}^{\infty} (t+t_0)^{\frac{\sigma-1}{2}} \exp\left(\frac{1+2\sqrt{2}}{6(t+t_0)}-\frac{t^2}{2h^2}\right) \left| \left(\frac{1}{2}+\sigma-it\right) \right|^{k} dt
$$
  

$$
< 2^{\frac{6k+7-\sigma}{4}}\pi^{\frac{2k+1}{2}} \exp\left(\frac{1+2\sqrt{2}}{6t_0}\right) \int_{\sigma+\frac{1}{2}}^{\infty} (t+t_0)^{\frac{\sigma-1}{2}} t^{k} \exp\left(-\frac{t^2}{2h^2}\right) dt
$$
  

$$
= 2^{\frac{6k+7-\sigma}{4}}\pi^{\frac{2k+1}{2}} \exp\left(\frac{1+2\sqrt{2}}{6t_0}\right) \sum_{l=0}^{\frac{\sigma-1}{2}} \left(\frac{\sigma-1}{l}\right) t_0^{\frac{\sigma-1}{2}-l} \int_{\sigma+\frac{1}{2}}^{\infty} t^{k+l} \exp\left(-\frac{t^2}{2h^2}\right) dt
$$

and our result follows from Lemma A.1.

 $\Box$ 

We wish to bound the error introduced at step (2) by taking  $g\left(\frac{n}{A};k\right)$  as an approximation for  $\tilde{g}(n; k)$ . We start with a bound for  $|g(t; k)|$ .

**Lemma A.4.** For  $k \in \mathbb{Z}_{\geq 0}$ ,  $t \in \mathbb{R}$  and  $t_0, h > 0$ , recall that we define g by

$$
g(t; k) := \Gamma\left(\frac{\frac{1}{2} + i(t + t_0)}{2}\right) \exp\left(\frac{\pi(t + t_0)}{4} - \frac{t^2}{2h^2}\right) (-2\pi i t)^k.
$$

Then

$$
|g(t;k)| \le 4(2\pi|t|)^k \exp\left(\frac{-t^2}{2h^2}\right).
$$

Proof. We have

$$
\left| \Gamma \left( \frac{\frac{1}{2} + i(t + t_0)}{2} \right) \exp \left( \frac{\pi (t + t_0)}{4} - \frac{t^2}{2h^2} \right) (-2\pi i t)^k \right|
$$
  
< 
$$
< (2\pi |t|)^k \exp \left( -\frac{t^2}{2h^2} \right) \left| \Gamma \left( \frac{\frac{1}{2} + i(t + t_0)}{2} \right) \exp \left( \frac{\pi (t + t_0)}{4} \right) \right|
$$

and the result follows from the trivial bound  $\left| \right|$  $\Gamma\left(\frac{\frac{1}{2}+ix}{2}\right)$   $e^{\frac{\pi x}{4}}$  $< 4.$ 

 $\vert \cdot$ 

Now we can derive the following bound for the approximation implied at step (2).

**Lemma A.5.** Let 
$$
n \in \left[-\frac{N}{2}, \frac{N}{2} - 1\right]
$$
 and  $B > h\sqrt{k}$ . Then  

$$
\left|\sum_{l \in \mathbb{Z}_{\neq 0}} g\left(\frac{n}{A} + lB; k\right)\right| \le
$$

$$
8(\pi B)^k \left[\exp\left(\frac{-B^2}{8h^2}\right) + 2^{\frac{3k-1}{2}} \left(\frac{h}{B}\right)^{k+1} \Gamma\left(\frac{k+1}{2}, \frac{B^2}{8h^2}\right)\right]
$$

*Proof.* We consider the right tail from  $n = -\frac{N}{2}$ . The first term missing is  $g\left(\frac{B}{2};k\right)$ and  $\frac{B}{2}$  is sufficiently large that our bound for  $g(t; k)$  (Lemma A.4) is decreasing. Thus we can split off the first term and majorise the balance with an integral. This process results in

$$
2\left[ \left| g\left(\frac{B}{2};k\right) \right| + \int\limits_{1}^{\infty} 4(\pi B(2w-1))^{k} \exp\left(\frac{-(2w-1)^{2}B^{2}}{8h^{2}}\right) \mathrm{d}w \right].
$$

Now by Lemma A.4 we have

$$
\left| g\left(\frac{B}{2}; k\right) \right| < 4(\pi B)^k \exp\left(-\frac{B^2}{8h^2}\right).
$$

Using the substitution  $t = \frac{(2w-1)^2 B^2}{8h^2}$  the integral becomes

$$
\int_{\frac{B^2}{8h^2}}^{\infty} \frac{8\pi^k}{B} 8^{\frac{k-1}{2}} h^{k+1} t^{\frac{k-1}{2}} e^{-t} dt
$$

so we can apply Lemma A.1 and the result follows.

At step (4), we use  $G^{(k)}\left(\frac{m}{B}\right)$  as an approximation to  $\tilde{G}^{(k)}(m)$ . To enable us to bound the error this introduces, we first derive a bound for  $|G^{(k)}(u)|$ .

**Lemma A.6.** Let  $\sigma \in 2\mathbb{Z}_{>0} + 1$ . Then  $G^{(k)}(u)$  is bounded in absolute terms by

$$
C(\sigma, t_0, h, k) \exp\left(\frac{(2\sigma + 1)^2}{8h^2} - (2\sigma - 1)\pi |u|\right) +
$$
  

$$
2^{k+2} \pi^{k+1} \exp\left(\frac{-t_0^2}{2h^2}\right) \sum_{l=0}^{\frac{\sigma-1}{2}} \frac{((2l+1/2)^2 + t_0^2)^{\frac{k}{2}}}{l!} \exp\left(\frac{(4l+1)^2}{8h^2} - (4l+1)\pi |u|\right).
$$

*Proof.* First we consider  $u \geq 0$ . We write

$$
\left|G^{(k)}(u)\right| = \left|\int\limits_{-\infty}^{\infty} \Gamma\left(\frac{\frac{1}{2}+i(t+t_0)}{2}\right) \exp\left(\frac{\pi(t+t_0)}{4}-\frac{t^2}{2h^2}\right)(-2\pi i t)^k e(-tu) dt\right|.
$$

Substituting  $s = \frac{1}{2} + i(t+t_0)$ , we now move the line of integration right to  $\Re(s) = \sigma$ giving

(A.1)  

$$
\left| G^{(k)}(u) \right| \le \exp\left( \frac{(2\sigma - 1)^2}{8h^2} - \pi u (2\sigma - 1) \right) (2\pi)^k \times
$$
  
(A.1)  

$$
\int_{-\infty}^{\infty} \left| \Gamma\left( \frac{\sigma + i(t + t_0)}{2} \right) \exp\left( \frac{\pi (t + t_0)}{4} \right) \exp\left( \frac{-t^2}{2h^2} \right) \left( \frac{1}{2} - \sigma - it \right)^k \right| dt.
$$

For  $u < 0$ , we move the line of integration left to  $\Re(s) = -\sigma$ , picking up the poles of  $\Gamma\left(\frac{s}{2}\right)$  at  $s = 0, -2, \ldots, 1 - \sigma$ . These give a contribution bounded by

$$
2^{k+2}\pi^{k+1} \exp\left(\frac{-t_0^2}{2h^2}\right) \sum_{l=0}^{\frac{\sigma-1}{2}} \frac{((2l+1/2)^2+t_0^2)^{\frac{k}{2}}}{l!} \exp\left(\frac{(4l+1)^2}{8h^2}+(4l+1)\pi u\right).
$$

The integral which remains is now

$$
(2\pi)^k \exp\left(\frac{(2\sigma+1)^2}{8h^2} + (2\sigma+1)\pi u\right) \times
$$

$$
\int_{-\infty}^{\infty} \left| \Gamma\left(\frac{-\sigma + i(t+t_0)}{2}\right) \exp\left(\frac{\pi(t+t_0)}{4} - \frac{t^2}{2h^2}\right) (\sigma + \frac{1}{2} - it)^k \right| dt.
$$

Finally, for our range of  $\sigma$  and for  $t \in \mathbb{R}$ , we have  $|\Gamma(-\sigma/2 + it)| < |\Gamma(\sigma/2 + it)|$ and the result follows.  $\Box$ 

Now we can obtain a bound for the error introduced at step (4).

**Lemma A.7.** Let  $m \in [0, N/2]$  and  $\sigma \in 2\mathbb{Z}_{>0} + 1$ . Then we have

$$
\left| \sum_{l \in \mathbb{Z}_{\neq 0}} G^{(k)} \left( \frac{m}{B} + lA \right) \right| \leq 2^{k+3} \pi^{k+1} \exp\left( \frac{-t_0^2}{2h^2} \right) S +
$$
  
2\left( 1 + \frac{1}{A\pi(2\sigma - 1)} \right) C(\sigma, t\_0, h, k) \exp\left( \frac{(2\sigma + 1)^2}{8h^2} - \frac{A\pi(2\sigma - 1)}{2} \right)

where S is the sum

$$
\sum_{l=0}^{\frac{\sigma-1}{2}} \left(1 + \frac{1}{A\pi(4l+1)}\right) \frac{((2l+1/2)^2 + t_0^2)^{\frac{k}{2}}}{l!} \exp\left(\frac{(4l+1)^2}{8h^2} - \frac{A\pi(4l+1)}{2}\right).
$$

*Proof.* The left tail from  $m = \frac{N}{2}$  majorises every case. The first term missing is  $G^{(k)}\left(-\frac{A}{2}\right)$  which we can bound using Lemma A.6 by

$$
C(\sigma, t_0, h, k) \exp\left(\frac{(\sigma + 1)^2}{8h^2} - \frac{A\pi(2\sigma - 1)}{2}\right)
$$
  
+  $2^{k+2}\pi^{k+1} \exp\left(-\frac{t_0^2}{2h^2}\right) \sum_{l=0}^{\frac{\sigma-1}{2}} \frac{\left((2l + \frac{1}{2})^2 + t_0^2\right)^{\frac{k}{2}}}{l!} \exp\left(\frac{(4l + 1)^2}{8h^2} - \frac{A\pi(4l + 1)}{2}\right).$ 

Our bound for  $|G^{(k)}(u)|$  is decreasing over the remainder of the left tail so we can bound it with the integral

$$
\int_{1}^{\infty} \left[ C(\sigma, t_0, h, k) \exp \left( \frac{(2\sigma + 1)^2}{8h^2} - \frac{A\pi (2n - 1)(2\sigma - 1)}{2} \right) + \frac{2^{k+2}\pi^{k+1} \exp \left( \frac{-t_0^2}{2h^2} \right) \times \frac{\sum_{l=0}^{\frac{\sigma-1}{2}} \left( (2l + 1/2)^2 + t_0^2 \right)^{\frac{k}{2}}}{l!} \exp \left( \frac{(4l + 1)^2}{8h^2} - \frac{A\pi (2n - 1)(4l + 1)}{2} \right) \right] \, \mathrm{d}n
$$

and the result follows on evaluating this integral.  $\Box$ 

We now want to bound the error introduced at step (6) by approximating  $\tilde{F}(n)$ with  $F\left(\frac{n}{B}\right)$ . We will need a bound for F.

**Lemma A.8.** Let  $\sigma \in 2\mathbb{Z} + 1$  and  $1 < \sigma < t_0$ . Then we have

$$
|F(x)| \le \zeta(\sigma) \pi^{\frac{1-2\sigma}{4}} C(\sigma, t_0, h, 0) \exp\left(\frac{(2\sigma - 1)^2}{8h^2} - \pi |x|(2\sigma - 1)\right) + 2\pi^{\frac{5}{4}} \exp\left(\frac{1}{8h^2} - \pi |x| - \frac{t_0^2}{2h^2}\right).
$$

*Proof.* Since  $f(t)$  is real, its Fourier Transform  $F(x)$  has the property  $F(-x) = \overline{F(x)}$ so we need only consider  $x \geq 0$ . We write  $s = \frac{1}{2} + i(t + t_0)$  and shift the line of integration right to  $\Re(s) = \sigma$  encountering the pole of  $\zeta(s)$  at  $s = 1$ . This yields a residue smaller in absolute terms than

$$
2\pi^{\frac{5}{4}}\exp\left(\frac{1}{8h^2}-\pi x-\frac{t_0^2}{2h^2}\right).
$$

The remaining integral is then bounded in exactly the same fashion as in Lemma A.6 using  $|\zeta(\sigma + it)| \le |\zeta(\sigma)|$  for  $\sigma > 1$  and  $t \in \mathbb{R}$ .

Now we can deduce the following bound for step (6).

**Lemma A.9.** For  $n \in [0, \frac{N}{2}]$  we have

$$
\left| \tilde{F}(n) - F\left(\frac{n}{B}\right) \right| = \left| \sum_{l \in \mathbb{Z}_{\neq 0}} F\left(\frac{n}{B} + lA\right) \right| \le
$$
\n
$$
2\zeta(\sigma)\pi^{\frac{1-2\sigma}{4}} C(\sigma, t_0, h, 0) \exp\left(\frac{(2\sigma - 1)^2}{8h^2} - \frac{A\pi(2\sigma - 1)}{2}\right) \left(1 + \frac{1}{A\pi(2\sigma - 1)}\right)
$$
\n
$$
+ 4\pi^{\frac{5}{4}} \exp\left(\frac{1 - 4t_0^2}{8h^2} - \frac{A\pi}{2}\right) \left(1 + \frac{1}{A\pi}\right).
$$

*Proof.* The left tail from  $n = N/2$  majorises all other cases. The first term missing is  $F\left(\frac{-A}{2}\right)$  which we can bound in absolute terms using Lemma A.8 with

$$
\zeta(\sigma) \pi^{\frac{1-2\sigma}{4}} C(\sigma, t_0, h, 0) \exp\left(\frac{-\pi A (2\sigma - 1)}{2}\right) + 2\pi^{\frac{5}{4}} \exp\left(\frac{1 - 4t_0^2}{8h^2} - \frac{A\pi}{2}\right)
$$

The same bound gives a decreasing sequence for the remaining terms which we can therefore estimate with the integral

$$
\int_{1}^{\infty} \left[ \zeta(\sigma) \pi^{\frac{1-2\sigma}{4}} C(\sigma, t_0, h, 0) \exp\left(\frac{-\pi A(2\sigma - 1)(2n - 1)}{2}\right) + 2\pi^{\frac{5}{4}} \exp\left(\frac{1 - 4t_0^2}{8h^2} - \frac{A\pi(2n - 1)}{2}\right) \right] \, \mathrm{d}n.
$$

Again, our result follows on evaluating this integral.

Finally, we turn to the error introduced at step (8) by taking  $f\left(\frac{n}{A}\right)$  as an approximation to  $\tilde{f}(n)$ . We start with a bound for  $|f(t)|$ .

**Lemma A.10.** Let  $f(t)$  be as defined at 3.1, take  $t \geq 0$ ,  $t_0 > \exp(e)$  and set  $\beta = \frac{1}{6} + \frac{\log \log t_0}{\log t_0}$ . Then

$$
|f(t)| \le 3(t+t_0)^{\beta} \exp\left(-\frac{t^2}{2h^2}\right).
$$

Proof. From the definition, we have

$$
|f(t)| = \left| \pi^{\frac{-it}{2}} \Gamma\left(\frac{\frac{1}{2} + i(t + t_0)}{2}\right) \exp\left(\frac{\pi t}{4} - \frac{t^2}{2h^2}\right) \zeta\left(\frac{1}{2} + i(t + t_0)\right) \right|
$$
  
= 
$$
\left| \Gamma\left(\frac{\frac{1}{2} + i(t + t_0)}{2}\right) \exp\left(\frac{\pi t}{4}\right) \zeta\left(\frac{1}{2} + i(t + t_0)\right) \right| \exp\left(-\frac{t^2}{2h^2}\right).
$$

Now by [22] we have for  $t + t_0 > 2$ 

(A.2) 
$$
\left| \zeta \left( \frac{1}{2} + i(t + t_0) \right) \right| \leq 0.732(t + t_0)^{\frac{1}{6}} \log(t + t_0)
$$

and with  $(t + t_0) > \exp(e)$  and  $\beta$  defined as above

$$
(t+t_0)^{\frac{1}{6}}\log(t+t_0)\leq (t+t_0)^{\beta}.
$$

We bound the Gamma factor trivially again with 4 and round 2.928 up to 3.  $\Box$ 

Using the above, we can now bound the error implicit in step (8) of our algorithm.

**Lemma A.11.** For  $t \geq 0$  and  $t_0 > \exp(e)$  set  $\beta = \frac{1}{6} + \frac{\log \log t_0}{\log t_0}$ . Then providing  $\beta h^2$  $\frac{dh^2}{t_0} \leq \frac{B}{2} \leq t_0$  and  $n \in [0, N-1]$  we have

$$
\left| \sum_{l \in \mathbb{Z}_{\neq 0}} f\left(\frac{n - N/2}{A} + lB\right) \right| \le 6(X + \frac{2^{\beta}h}{B}(Y + Z)),
$$

where

$$
X = \left(\frac{B}{2} + t_0\right)^{\beta} \exp\left(-\frac{B^2}{8h^2}\right),
$$

$$
Y = 2^{-\frac{1}{2}}t_0^{\beta} \Gamma\left(\frac{1}{2}, \frac{B^2}{8h^2}\right)
$$

and

$$
Z = 2^{\frac{\beta-1}{2}} h^{\beta} \Gamma\left(\frac{\beta+1}{2}, \frac{t_0^2}{2h^2}\right).
$$

*Proof.* The lower bound on  $B$  ensures that the bound of Lemma A.10 is decreasing for  $t \geq \frac{B}{2}$ . The worst case is when  $n = 0$  and for any n, the right tail majorises the left. The first missing term to the right is  $f\left(\frac{B}{2}\right)$  and the remaining terms are majorised by

$$
\left|3\int\limits_{0}^{\infty}\left(\frac{(2w+1)B}{2}+t_0\right)^{\beta}\exp\left(-\frac{\left(\frac{(2w+1)B}{2}\right)^2}{2h^2}\right)\mathrm{d}w\right|\leq \frac{3}{B}\left|\int\limits_{\frac{B}{2}}^{t_0}(2t_0)^{\beta}\exp\left(\frac{-t^2}{2h^2}\right)\mathrm{d}t+\int\limits_{t_0}^{\infty}(2t)^{\beta}\exp\left(\frac{-t^2}{2h^2}\right)\mathrm{d}t\right|.
$$

The result follows from Lemma A.1.

APPENDIX B. BOUNDS FOR THE ERROR COMPUTING  $F(x)$  at step (5).

There are two sources of error in step (5). The following two Lemmas give us explicit bounds for both.

Lemma B.1. Let  $x \geq 0$ . Then

$$
\left| \sum_{j>J} \frac{1}{\sqrt{j}} \left( j \sqrt{\pi} \right)^{-it_0} G \left( x + \frac{\log \left( j \sqrt{\pi} \right)}{2\pi} \right) \right|
$$
  
 
$$
\leq C(\sigma, t_0, h, 0) \exp \left( \frac{(2\sigma - 1)^2}{8h^2} \right) \pi^{\frac{1-2\sigma}{4}} \frac{J^{1-\sigma}}{\sigma - 1}.
$$

*Proof.* Take  $x = 0$  and apply Equation A.1 of Lemma A.6.

**Lemma B.2.** Let  $w \in [-\xi, \xi]$ . Then we have

$$
\left|\sum_{k=K}^{\infty} \frac{G^{(k)}(u)w^k}{k!}\right| \le \frac{2^{\frac{K+5}{2}}\pi^{K+\frac{1}{2}}h^{K+1}\xi^K}{\Gamma\left(\frac{K+2}{2}\right)}.
$$

Proof.

$$
\left| \sum_{k=K}^{\infty} \frac{G^{(k)}(u)w^k}{k!} \right| \le \sup_{u' \in (u-\xi, u+\xi]} \left| \frac{G^{(K)}(u')\xi^K}{K!} \right|
$$
  

$$
\le \sup_{u' \in (u-\xi, u+\xi]} \left| \int_{-\infty}^{\infty} \frac{g(t;k)\xi^K e(-u't)}{K!} dt \right|
$$
  

$$
\le 8 \int_{0}^{\infty} \frac{(2\pi t\xi)^K}{K!} \exp\left(\frac{-t^2}{2h^2}\right) dt
$$
  

$$
= \frac{2^{\frac{3K+5}{2}} \pi^K \xi^K h^{K+1} \Gamma\left(\frac{K+1}{2}\right)}{\Gamma(K+1)}
$$

and the result follows from the duplication formula for Γ.  $\Box$ 

Since this error term occurs J times in Equation 3.2, weighted by  $\frac{1}{\sqrt{j}}$  each time, we multiply it by  $2\sqrt{J} - 1$ .

## Appendix C. Bounds Related to Up-sampling

Recall that we defined the function  $W : \mathbb{R} \to \mathbb{R}$ 

$$
W(t) := \Lambda(t) \exp\left(\frac{\pi t}{4} - \frac{(t - t_0)^2}{2H^2}\right).
$$

We aim to estimate  $W(t_0)$  from our samples using Theorems 4.3 (Whittaker-Shannon) and 4.4. The following Lemmas provide the necessary rigorous bounds.

Lemma C.1. Define I by

$$
I := 4 \int_{\frac{A}{2}}^{\infty} \left| \int_{-\infty}^{\infty} W(t) e(-xt) dt \right| dx.
$$

Then we have

$$
I \leq \frac{4\zeta(\sigma)}{2\sigma - 1} \pi^{\frac{-3 - 2\sigma}{4}} C(\sigma, t_0, H, 0) \exp\left(\frac{(2\sigma - 1)^2}{8H^2} - \frac{\pi A (2\sigma - 1)}{2}\right) + 8\pi^{\frac{1}{4}} \exp\left(\frac{1 - 4t_0^2}{8H^2} - \frac{\pi A}{2}\right).
$$

*Proof.* Using the substitution  $t \to t + t_0$  the inner integral looks exactly like the definition of  $F(x)$  with H taking the place of h. We bound this using Lemma A.8 and the outer integral is then trivial.  $\Box$ 

**Lemma C.2.** Let  $t \ge e$  and  $\beta = \frac{1}{6} + \frac{\log \log t}{\log t}$ . Then we have

$$
|W(t)| \le 3t^{\beta} \exp\left(\frac{-(t-t_0)^2}{2H^2}\right).
$$

*Proof.* The proof is almost identical to that of Lemma A.10.  $\Box$ 

**Lemma C.3.** Let  $t_0 > \exp(e)$  and  $\beta = \frac{1}{6} + \frac{\log \log t_0}{\log t_0}$ . Then given  $N_s \in \mathbb{Z}_{>0}$  with  $N_s \leq t_0 A$  we have

$$
\left| \sum_{\substack{n-\frac{t_0}{A} > N_s}} W\left(\frac{n}{A}\right) \operatorname{sinc}\left(A\left(\frac{n}{A} - t_0\right)\right) \right| \le \frac{6A}{\pi N_s} (X + Y + Z),
$$

where

$$
X = \left(t_0 + \frac{N_s}{A}\right)^{\beta} \exp\left(-\frac{N_s^2}{2A^2h^2}\right),
$$
  

$$
Y = 2^{\frac{2\beta-1}{2}}(t_0)^{\beta}A \cdot H \cdot \Gamma\left(\frac{1}{2}, \frac{N_s^2}{2A^2H^2}\right)
$$

and

$$
Z = 2^{\frac{3\beta-1}{2}} A \cdot H^{\beta+1} \Gamma\left(\frac{\beta+1}{2}, \frac{t_0^2}{2H^2}\right).
$$

Proof. The right tail majorises the left and the first term missing is less in absolute terms than

$$
\left| W\left(t_0 + \frac{N_s}{A}\right) \operatorname{sinc}\left(\frac{N_s}{A}\right) \right|
$$

which is less then

$$
\frac{3A}{\pi N_s} \left( t_0 + \frac{N_s}{A} \right)^{\beta} \exp \left( -\frac{N_s^2}{2A^2 H^2} \right).
$$

Now, since our bound for  $W$  is decreasing, we can majorise the rest of the tail with the integral

$$
\frac{3A}{\pi N_s} \int_{N_s}^{\infty} \left( t_0 + \frac{n}{A} \right)^{\beta} \exp\left( -\frac{n^2}{2A^2H^2} \right) \mathrm{d}n
$$
\n
$$
< \frac{3A}{\pi N_s} \int_{N_s}^{\infty} 2^{\beta} t_0^{\beta} \exp\left( -\frac{n^2}{2A^2H^2} \right) \mathrm{d}n + \frac{3A}{\pi N_s} \int_{t_0A}^{\infty} 2^{\beta} \left( \frac{n}{A} \right)^{\beta} \exp\left( -\frac{n^2}{2A^2H^2} \right) \mathrm{d}n
$$
\n
$$
= \frac{3A}{\pi N_s} \left[ 2^{\frac{2\beta - 1}{2}} t_0^{\beta} A \cdot H \cdot \Gamma \left( \frac{1}{2}, \frac{N_s^2}{2A^2H^2} \right) + 2^{\frac{3\beta - 1}{2}} A \cdot H^{\beta + 1} \Gamma \left( \frac{\beta + 1}{2}, \frac{t_0^2}{2H^2} \right) \right].
$$

#### 18 DAVID J. PLATT

#### **REFERENCES**

- 1. M. Abramowitz and I.A. Stegun, Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables, Dover publications, 1964.
- 2. ACRC, BlueCrystal Phase 2 User Guide, 2009.
- 3. T.M. Apostol, An elementary view of Euler's summation formula, American Mathematical Monthly 106 (1999), no. 5, 409–418.
- 4. M.V. Berry and J.P. Keating, A New Asymptotic Representation for  $\zeta(\frac{1}{2} + it)$  and Quantum Spectral Determinants, Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci. 437 (1992), no. 1899, 151–173.
- 5. Jonathan Bober, Zeros of  $\zeta(s)$ , 2014, http://www.lmfdb.org/zeros/zeta/.
- 6. Andrew R. Booker, Artin's conjecture, Turing's method and the Riemann hypothesis, Experiment. Math. 15 (2006), no. 4, 385–407.
- 7. J.L. Brown Jr., On the Error in Reconstructing a Non-Bandlimited Function by Means of the Bandpass Sampling Theorem, J. Math. Anal. Appl. 18 (1967), no. 1, 75–84.
- 8. J.A. de Reyna, High Precision Computation of Riemann's Zeta Function by the Riemann-Siegel Formula, I, Math. Comp 80 (2011), no. 274, 995–1009.
- 9. H.M. Edwards, Riemann's Zeta Function, Pure and applied mathematics, Academic Press Inc., 1974.
- 10. X. Gourdon, The  $10^{13}$  First Zeros of the Riemann Zeta Function, and Zeros Computation at Very Large Height, http://numbers.computation.free.fr/Constants/Miscellaneous/ zetazeros1e13-1e24.pdf, 2010.
- 11. D.E.G. Hare, Computing the principal branch of log-Gamma, J. Algorithms 25 (1997), no. 2, 221–236.
- 12. Ghaith Ayesh Hiary, Fast methods to compute the Riemann zeta function, Ann. of Math. (2) 174 (2011), no. 2, 891–946. MR 2831110 (2012g:11154)
- 13. Fredrik Johansson et al., mpmath: a Python library for arbitrary-precision floating-point arithmetic (version 0.19), 2014, http://www.mpmath.org/doc/0.19/index.html.
- 14. J. C. Lagarias and A. M. Odlyzko, Computing  $\pi(x)$ : an Analytic Method, J. Algorithms 8 (1987), no. 2, 173–191.
- 15. R. Sherman Lehman, On the distribution of zeros of the Riemann zeta-function, Proc. London Math. Soc. S3-20 (1970), no. 2, 303–320.
- 16. R.E. Moore, Interval analysis, vol. 60, Prentice-Hall Englewood Cliffs, New Jersey, 1966.
- 17. A.M. Odlyzko, Tables of zeros of the Riemann zeta function, http://www.dtc.umn.edu/ ~odlyzko/zeta\_tables/index.html.
- 18.  $\frac{1}{18}$ , The 10<sup>20</sup>-th zero of the Riemann zeta function and 175 million of its neighbors, http://www.dtc.umn.edu/~odlyzko/unpublished/index.html, 1992.
- 19. A.M. Odlyzko and A. Schönhage, Fast algorithms for multiple evaluations of the Riemann zeta function, Trans. Amer. Math. Soc. 309 (1988), no. 2, 797-809.
- 20. David J. Platt, Computing  $\pi(x)$  Analytically, Math. Comp. 84 (2015), 1521-1535.
- 21. Mumerical Computations Concerning the GRH, Math. Comp. (2015).
- 22. David J. Platt and T. Trudgian, An Improved Explicit Bound on  $\zeta\left(\frac{1}{2}+it\right)$ , J. Number Theory 147 (2015), 842–851.
- 23. , On the first sign change of  $\theta(x) x$ , Math. Comp. (2015).
- 24. N. Revol and F. Rouillier, A library for arbitrary precision interval arithmetic, 10th GAMM-IMACS International Symposium on Scientific Computing, Computer Arithmetic, and Validated Numerics, 2002.
- 25. Michael Rubinstein, lcalc The L-function calculator, http://code.google.com/p/l-calc/.
- 26. Y. Saouter, P. Demichel, and T.A. Trudgian, A still sharper region where  $\pi(x) \ell i(x)$  is positive, Math. Comp. (2015).
- 27. T. Trudgian, Improvements to Turing's method, Math. Comp 80 (2011), no. 276, 2259–2279. 28. Alan M. Turing, Some calculations of the Riemann zeta-function., Proc. Lond. Math. Soc. 3
	- (1953), no. 3, 99–117.
- 29. J.S. Walker, Fast Fourier Transforms, CRC press Boca Raton, 1991.
- 30. S. Wedeniwski, ZetaGrid–Computations connected with the Verification of the Riemann Hypothesis, Foundations of Computational Mathematics Conference, Minnesota, USA, 2002.

HEILBRONN INSTITUTE FOR MATHEMATICAL RESEARCH, UNIVERSITY OF BRISTOL, UNIVERSITY Walk, Bristol BS8 1TW

 $\it E\mbox{-}mail\;address:$ dave.platt@bris.ac.uk