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NUMERICAL COMPUTATIONS CONCERNING THE GRH

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ABSTRACT. We describe two new algorithms for the efficient and rigorous computation of Dirichlet L-functions and their use to verify the Generalised Riemann Hypothesis for all such L-functions associated with primitive characters of modulus $q \leq 400\,000$. We check, to height, $\max\left(\frac{10^8}{q}, \frac{A\cdot 10^7}{q} + 200\right)$ with $A = 7.5$ in the case of even characters and $A = 3.75$ for odd characters. In addition we confirm that no Dirichlet L-function with a modulus $q \leq 2\,000\,000$ vanishes at its central point.

1. INTRODUCTION

For a given modulus $q \in \mathbb{Z}_{>0}$ we define the Dirichlet characters $\chi : \mathbb{Z} \to \mathbb{C}$ axiomatically as follows:

- $\chi(n) = 0$ iff $(n, q) \neq 1$,
- $\chi(mn) = \chi(m)\chi(n)$ and
- $\chi(n + q) = \chi(n)$.

There are $\varphi(q)$ distinct characters of modulus q, where φ is Euler's totient function. The character $\chi(n) = 1$ for all n co-prime to q is known as the principal character. A character χ of modulus q is primitive if and only if for all d dividing q with $0 < d < q$ there exists an integer $a \equiv 1 \mod d$ with $(a, q) = 1$ and $\chi(a) \neq 1$; see [1]. Finally, we define the parity of a character by

$$a_\chi := \frac{1 - \chi(-1)}{2}.$$

The Dirichlet L-function of modulus q associated with a character χ is defined for $\Re s > 1$ by

$$L_\chi(s) = \sum_{n=1}^{\infty} \chi(n) n^{-s}$$

and has analytic continuation to $\mathbb{C}$ except (in the case of principal characters) a simple pole at $s = 1$.

Given ϵ_χ such that $|\epsilon_\chi| = 1$, we form the completed L-function via

$$\Lambda_\chi(t) := \epsilon_\chi \left(\frac{q}{\pi}\right)^{\frac{it}{2}} \Gamma\left(\frac{\frac{1}{2} + a_\chi + it}{2}\right) \exp\left(\frac{\pi t}{4}\right) L_\chi\left(\frac{1}{2} + it\right).$$

For suitably chosen ϵ_χ, Λ_χ is real valued and has the same zeros as $L_\chi\left(\frac{1}{2} + it\right)$. The exponential factor is introduced (for computational expedience) to counteract the decay of the gamma function as t increases.

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In the case $q = 1$, we have only the principal character leading to a single L-function, namely Riemann's zeta function. Riemann's guess that all zeros of this function with real part in $[0, 1]$ lie on the half line and are simple is the Riemann Hypothesis (RH). Extensive calculations have been undertaken to test RH to ever increasing heights, with Gourdon having checked the lowest 10^{13} zeros [6].

In contrast, the equivalent hypothesis for Dirichlet L-functions of primitive character, which we will refer to as the Generalised Riemann Hypothesis (GRH), has received less attention. The last significant rigorous computation was that by Rumely [16] who confirmed that the GRH holds for primitive L-functions modulus $q \leq 13$ to height 10 000 and various other moduli to height 2 500.[1] The largest modulus tested was $q = 432$ and in total about 10^7 zeros were examined. We note that Rumely went on to isolate these zeros with some precision and to generate statistics on their locations, but in terms of simply the number of zeros confirmed to lie on the half line, there remained a factor of 10^6 in favour of zeta. If this weren't motivation enough, recent advances in the application of the Circle Method held out the tantalising prospect that ternary Goldbach might succumb to a combined numerical and analytic assault.

We will describe a computation using new algorithms and exploiting improvements in hardware in the 20 years since Rumely's paper that extend his result by about 6 orders of magnitude in terms of the number of zeros checked. Furthermore, the combination of moduli and heights checked is more than sufficient to support Helfgott's proof of ternary Goldbach [7], [8].

2. Structure of this paper

In Section 3 we will review some of the properties of the Discrete Fourier Transform (DFT) pertinent to this application and in Section 4 we will describe our use of interval arithmetic. We then move on to describe the method itself, which comprises:

- Determine the number of zeros of $L_\chi(\sigma + it)$ with $\sigma \in [0, 1]$ and $t \in [0, T]$ using a variant of Turing's method which we describe in Section 5.
- Compute values of the associated completed L-function $\Lambda_\chi(t)$ for t going from 0 to T in evenly spaced steps. We actually used two different methods depending on the height up the critical line we need to consider. Sections 6 and 7 explain these methods in more detail.
- Count the sign changes between successive values of Λ_χ. By the Intermediate Value Theorem, each sign change corresponds to an odd number of zeros of Λ_χ and therefore of L_χ.
- If the number of sign changes accounts for all the zeros predicted by Turing's method, we are done. If not, we presume that the rate at which we sampled Λ_χ was too coarse to isolate all its sign changes. Section 8 describes the method used to progressively increase our sampling rate when necessary.[2]

Section 9 describes how the various parameters were chosen and Section 10 gives some details of the computation itself.

[1] Rumely refers the Extended Riemann Hypothesis (ERH), rather than the GRH.

[2] We expect GRH to hold. If it fails in our domain of interest, our algorithm will not terminate.

3. The Discrete Fourier Transform (DFT)

We will make extensive use of the DFT in what follows. We adopt the following (un-normalised) definition.

Definition 3.1. Given $N \in \mathbb{Z}_{>0}$ complex values denoted X_0 through X_{N-1}, the forward DFT results in N new values Y_0 through Y_{N-1} where

$$Y_m = \sum_{n=0}^{N-1} X_n \mathrm{e}\left(\frac{-nm}{N}\right)$$

and as usual $\mathrm{e}(x) := \exp(2\pi i x)$.

The backward or inverse DFT (iDFT) results from changing the sign in the complex exponential. Performing a forward then backward DFT (or vice versa) multiplies each datum by N.

As written, computing a DFT of length N would appear to have time complexity $\mathcal{O}(N^2)$. The ubiquity of the DFT stems from the existence of $\mathcal{O}(N \log N)$ algorithms, known collectively as the Fast Fourier Transforms (FFTs). For detailed descriptions of suitable algorithms, we refer the reader to, for example, [4]. However we note that, significantly for our purposes, this asymptotic complexity can be achieved for arbitrary (even prime) N. One such FFT, and the one we employ, is that due to Bluestein [2].

Throughout this paper, we will define $\widehat{f}$, the (continuous) Fourier transform of a function f (when it exists), to be

$$\widehat{f}(x) := \frac{1}{2\pi} \int_{-\infty}^{\infty} f(t) \exp(-ixt) \mathrm{d}t.$$

Under suitable conditions, the Fourier Inversion Theorem gives us

$$f(t) = \int_{-\infty}^{\infty} \widehat{f}(x) \exp(ixt) \mathrm{d}x.$$

To make the transition from the discrete to the continuous, we use the following theorem.

Theorem 3.2. *Let f be a function in the Schwartz space with Fourier transform $\widehat{f}$ and $N = AB$ with $A, B > 0$. Define*

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

and

$$\widetilde{\widehat{f}}(m) := \sum_{l \in \mathbb{Z}} \widehat{f}\left(\frac{2\pi m}{B} + 2\pi l A\right).$$

Then, up to a constant factor, $\tilde{f}(n)$ and $\widetilde{\widehat{f}}(m)$ form a DFT pair of length N.

Proof. By Poisson summation we have

$$\sum_{l\in\mathbb{Z}} f(t+lB) = \frac{2\pi}{B}\sum_{l\in\mathbb{Z}} \widehat{f}\left(\frac{2\pi l}{B}\right) \mathrm{e}\left(\frac{lt}{B}\right),$$

$$\tilde{f}(n) = \frac{2\pi}{B}\sum_{l\in\mathbb{Z}} \widehat{f}\left(\frac{2\pi l}{B}\right) \mathrm{e}\left(\frac{ln}{N}\right).$$

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

$$\begin{aligned}\tilde{f}(n) &= \frac{2\pi}{B}\sum_{m=0}^{N-1}\sum_{l'\in\mathbb{Z}} \widehat{f}\left(\frac{2\pi(l'N+m)}{B}\right) \mathrm{e}\left(\frac{(l'N+m)n}{N}\right)\\ &= \frac{2\pi}{B}\sum_{m=0}^{N-1} \mathrm{e}\left(\frac{mn}{N}\right) \widetilde{\widehat{f}}(m).\end{aligned}$$

This is by definition an iDFT. □

The utility of this theorem will be apparent when f and $\widehat{f}$ both decay quickly enough to allow $\tilde{f}(n)$ and $\widetilde{\widehat{f}}(m)$ to be approximated by $f\left(\frac{n}{A}\right)$ and $\widehat{f}\left(\frac{2\pi m}{B}\right)$, respectively.

4. Interval arithmetic

Like Rumely, we chose to manage rounding and truncation errors throughout our computations using interval arithmetic. We refer the interested reader to the extensive literature on this subject (perhaps [12] is a good starting point) but we summarise our approach below.

Almost all real numbers cannot be represented by a floating point number of any given precision. Thus, whenever an operation is carried out on floating point numbers, unless we are very lucky, the answer will not be exactly representable. We typically attempt to round to the nearest real number that is exactly representable and thus incur a rounding error. Such errors will accumulate over time and, to quote Moore, "it is often prohibitively difficult to tell in advance of a computation how many places must be carried to guarantee results of required accuracy." [11].

Instead, we store our intermediate results as two exactly representable floating point numbers representing an interval that brackets the true result. The usual mathematical operators and functions are then abstracted to handle this new data type.

Wherever possible, we would like to exploit the hardware implementation of IEEE floating point [9] available on most modern processors. Simply swapping the rounding mode backwards and forwards to achieve the correct behaviour is very inefficient and we therefore exploit an idea due to Lambov [10] that avoids this. Written in C++ but using in-line assembler for the kernel, we define real intervals as a class "int_double" with operators $+$, $-$, $\times$ and $\div$ and a $\sqrt{}$ function. Unfortunately, the hardware implementations of the transcendental functions are not IEEE compliant, so for exp, log, sin, cos and atan we use Muller and de Dinechin's "Correctly Rounded Mathematical Library" [13].

For high precision work (more than the 53 bits of IEEE double precision) we are forced into a software based solution and we use Revol and Rouillier's MPFI package [15]. In both the high precision and double precision cases, we extend

the real interval data type to the complexes in the obvious (and very probably sub-optimal) way, representing complex intervals as rectangles whose corners are exactly representable.

5. Turing's method

Armed with the completed L-function, we have reduced the problem of locating simple zeros of L_χ on the half line to that of finding sign changes of Λ_χ. However, we still need a reference to confirm that all the expected zeros are accounted for. We use a variation on Turing's method [18], generalised by Booker.

Theorem 5.1 (Booker)**.** *Let $L(s)$ be an L-function given by an Euler product of degree r and absolutely convergent for $\Re s > 1$. Define*

$$\Gamma_{\Re}(s) := \pi^{-s/2}\Gamma\left(\frac{s}{2}\right),$$

$$\gamma(s) := \epsilon N^{\frac{1}{2}\left(s-\frac{1}{2}\right)} \prod_{j=1}^{r} \Gamma_{\Re}(s+\mu_j),$$

$$\Lambda(s) := \gamma(s)L(s),$$

where $|\epsilon| = 1$, $N \in \mathbb{Z}_{>0}$ and $\Re\mu_j \geq -\frac{1}{2}$ are chosen so that Λ satisfies the functional equation

$$\Lambda(s) = \overline{\Lambda(1-\overline{s})}.$$

Now define

$$\Phi(t) := \frac{1}{\pi}\left[\arg\epsilon + \frac{\log N}{2}t - \frac{\log\pi}{2}\left(rt + \Im\sum_{j=1}^{r}\mu_j\right) + \Im\sum_{j=1}^{r}\log\Gamma\left(\frac{1/2+it+\mu_j}{2}\right)\right]$$

and for t neither the ordinate of a zero nor pole of Λ define

$$S(t) := \frac{1}{\pi}\Im\int_{\infty}^{1/2}\frac{L'}{L}(\sigma+it)\mathrm{d}\sigma.$$

Where t is the ordinate of a zero or pole, set $S(t) = \lim_{\epsilon\to 0^+} S(t+\epsilon)$ (i.e., S is upper semi-continuous). Finally, define

$$N(t) := \Phi(t) + S(t).$$

Then for $t_1 < t_2$, the net number of zeros with imaginary part in $(t_1, t_2]$ counting multiplicity is $N(t_2) - N(t_1)$.

Proof. See §4 of [3]. □

Theorem 5.2. *Given $T, h > 0$ such that neither T nor $T+h$ is the imaginary part of a zero of $L_\chi(s)$, let $N_\chi(T)$ be the number of zeros, counted with multiplicity, of $L_\chi(s)$ with $|\Im(s)| \leq T$ and $\Re(s) \in (0,1)$. Let $\check{N}_{T,\chi}(t)$ count the zeros of $L_\chi(s)$ with $\Im(s) \in [T, t)$, starting at 0 at T and increasing by 1 at every zero.*

Now for t not the ordinate of a zero of L_χ, define $S_\chi(t)$ by

$$S_\chi(t) := \frac{1}{\pi}\Im\int_{\infty}^{\frac{1}{2}} \frac{L_\chi'}{L_\chi}(\sigma+it)\mathrm{d}\sigma$$

and take $S_\chi(t)$ to be upper semi-continuous. Then we have

$$\begin{aligned} N_\chi(T) =& \frac{1}{h\pi}\left[2h + \frac{2hT+h^2}{2}\log\left(\frac{q}{\pi}\right) + 2\int_T^{T+h} \Im\log\Gamma\left(\frac{1/2+a_\chi+it}{2}\right)dt \right. \\ & \left. - \int_T^{T+h} \breve{N}_{T,\chi}(t)\mathrm{d}t - \int_T^{T+h} \breve{N}_{T,\overline{\chi}}(t)dt + \int_T^{T+h} S_\chi(t)\mathrm{d}t + \int_T^{T+h} S_{\overline{\chi}}(t)\mathrm{d}t \right]. \end{aligned}$$

Proof. This is Theorem 5.1 specialised to Dirichlet L-functions. In the terminology of that theorem, we have $N = q$, $r = 1$ and $\mu_1 = a_\chi$. We treat conjugate characters in pairs to avoid problems with the arbitrary choice of ϵ_χ and to allow for the possibility that $S_\chi(0)$ isn't small. Finally, we integrate both sides from T to $T+h$. □

This leaves us with the problem of bounding $\int_T^{T+h} S_\chi(t)\mathrm{d}t$.

Theorem 5.3 (Rumely)**.** *For $T > 50$ and $h > 0$,*

$$\left|\int_T^{T+h} S_\chi(t)\mathrm{d}t\right| \le 1.8397 + 0.1242\log\left(\frac{q(T+h)}{2\pi}\right).$$

Proof. Theorem 2 of [16]. □

Trudgian considered this problem in [17]. Specifically, applying Theorem 3.8 of that paper with $c = 1.1$ and $d = 0.8$ we derive revised constants optimised for qT in the region of 10^8. We have

Theorem 5.4 (Trudgian)**.** *For $T > 50$ and $h > 0$,*

$$\left|\int_T^{T+h} S_\chi(t)\mathrm{d}t\right| \le 2.17618 + 0.0679956\log\left(\frac{q(T+h)}{2\pi}\right).$$

The two bounds agree near $qt = 2\,501$ and at $qt = 10^8$ Trudgian's is better by a little more than 0.5.

6. Algorithm 1

When the height to which we are hoping to confirm GRH remains modest[3], we compute the values of $L_\chi(s)$ simultaneously for all characters of a given modulus by expressing the calculations as a Discrete Fourier Transform. Specifically, we appeal to the following lemma:

[3]See Section 9 for how we determined what was "modest".

Lemma 6.1. *For $q \in \mathbb{Z} \geq 3$ and given $\varphi(q)$ complex values $a(n)$ for $n \in [1, q-1]$ and $(n, q) \neq 0$, we can compute*

$$\sum_{n=1}^{q-1} a(n)\chi(n)$$

for the $\varphi(q)$ characters χ in $\mathcal{O}(q\log(q))$ time and $\mathcal{O}(q)$ space.

Proof. For any ring R, let $U(R)$ be its group of units. Taking $R = \mathbb{Z}/q\mathbb{Z}$ for $q \in \mathbb{Z}_{>0}$ and using the prime decomposition $q = 2^\alpha \prod_{i=1}^m p_i^{\alpha_i}$, we consider four cases:

(1) $\alpha = 0$ (q is odd), then by the Chinese Remainder Theorem (CRT) we have the constructive, canonical group isomorphism

$$U(\mathbb{Z}/q\mathbb{Z}) \cong \prod_{i=1}^m U(\mathbb{Z}/p_i^{\alpha_i}\mathbb{Z}).$$

Each of these groups is cyclic so given a primitive root for each $p_i^{\alpha_i}$ we have our construction. We now take slices through the product of the $U(\mathbb{Z}/p_i^{\alpha_i}\mathbb{Z})$ one p_i at a time and for each such slice we need $\varphi(q)/\varphi(p_i^{\alpha_i})$ DFTs, each of length $\varphi(p_i^{\alpha_i})$. The existence of Fast Fourier Transform algorithms for arbitrary length vectors means that the overall cost is

$$\sum_{i\in[1,m]} \varphi(q)/\varphi(p_i^{\alpha_i})\mathcal{O}(\varphi(p_i^{\alpha_i})\log\varphi(p_i^{\alpha_i})) = \mathcal{O}(\varphi(q)\log\varphi(q)) = \mathcal{O}(q\log q).$$

This analysis of the computational cost holds equally for the other three cases below, so we will refrain from repeating it.

(2) $\alpha = 1$, then by the CRT we have the constructive group isomorphism

$$U(\mathbb{Z}/q\mathbb{Z}) \cong U(\mathbb{Z}/2p_1^{\alpha_1}\mathbb{Z}) \prod_{i=2}^m U(\mathbb{Z}/p_i^{\alpha_i}\mathbb{Z}).$$

Each of these groups is cyclic so given a primitive root for $2p_1^{\alpha_1}$ and each $p_i^{\alpha_i}$ $(i > 1)$ we have our construction. Thus this case reduces to performing $\varphi(q)/\varphi(2p_1^{\alpha_1})$ length $\varphi(2p_1^{\alpha_1})$ DFTs followed by $\varphi(q)/\varphi(p_i^{\alpha_i})$ length $\varphi(p_i^{\alpha_i})$ DFTs for $i = 2 \ldots m$.

(3) $\alpha = 2$, then by the CRT we have the constructive, canonical group isomorphism

$$U(\mathbb{Z}/q\mathbb{Z}) \cong U(\mathbb{Z}/4\mathbb{Z}) \prod_{i=1}^m U(\mathbb{Z}/p_i^{\alpha_i}\mathbb{Z}).$$

Each of these groups is cyclic so given a primitive root for each $p_i^{\alpha_i}$ $(i > 1)$ we have our construction. Thus this case reduces to performing $\varphi(q)/2$ length 2 DFTs followed by $\varphi(q)/\varphi(p_i^{\alpha_i})$ length $\varphi(p_i^{\alpha_i})$ DFTs for $i = 1 \ldots m$.

(4) $\alpha > 2$, then by the CRT we have the constructive, canonical group isomorphism

$$U(\mathbb{Z}/q\mathbb{Z}) \cong U(\mathbb{Z}/2^\alpha\mathbb{Z}) \prod_{i=1}^m U(\mathbb{Z}/p_i^{\alpha_i}\mathbb{Z}).$$

Now $U(\mathbb{Z}/2^\alpha\mathbb{Z})$ is the product of a cyclic group of order 2 and a cyclic group of order $2^{\alpha-2}$ with pseudo primitive roots -1 and 5, respectively. The remaining groups (if there are any) are cyclic so given a primitive root for each $p_i^{\alpha_i}$ $(i > 1)$ we have our construction. Thus this case reduces to

performing $\varphi(q)/2$ length 2 DFTs, $\varphi(q)/2^{\alpha-2}$ length $2^{\alpha-2}$ DFTs followed by $\varphi(q)/\varphi(p_i^{\alpha_i})$ length $\varphi(p_i^{\alpha_i})$ DFTs for $i = 1 \dots m$. □

We seek to apply Lemma 6.1 by way of the Hurwitz zeta function, defined for $\Re s > 1$ and $\alpha \in (0, 1]$ by

$$\zeta(s, \alpha) := \sum_{n=0}^{\infty} (n + \alpha)^{-s}.$$

This function has an analytic continuation to $\mathbb{C}$ with the exception of a simple pole at $s = 1$ and except at this pole it can be used to express any Dirichlet L-function of modulus q via

$$L_\chi(s) = q^{-s} \sum_{a=1}^{q} \chi(a) \zeta\left(s, \frac{a}{q}\right)$$

(see § 12 of [1]).

Thus, for a given q and s, if we can supply the $\varphi(q)$ values of $\zeta\left(s, \frac{a}{q}\right)$ for $a \in [1, q-1]$ with $(a, q) = 1$, we can apply Lemma 6.1 to compute each $L_\chi(s)$ in, on average, time $\mathcal{O}(\log q)$.

6.1. **Computing $\zeta(1/2 + it, a/q)$.** For a given $t \in \mathbb{R}_{\geq 0}$ and $q \geq 3$, we need to be able to rapidly compute $\zeta(1/2 + it, a/q)$ for $a \in [1, q)$ with $(a, q) = 1$. We achieve this by pre-computing a table of values of ζ for each t and then interpolating using the following Lemma:

Lemma 6.2. *For $s \notin \mathbb{Z}_{\leq 0}$, $\alpha \in (0, 1]$ and $|\delta| < \alpha$,*

$$\zeta(s, \alpha + \delta) = \sum_{k=0}^{\infty} \frac{(-\delta)^k \zeta(s + k, \alpha) \prod_{j=0}^{k-1} (s + j)}{k!}.$$

Proof. Starting with $\Re s > 1$ and differentiating term by term we have

$$\zeta^{(k)}(s, \alpha) = \sum_{n=0}^{\infty} (-1)^k s(s+1)(s+2) \dots (s+k-1)(n+\alpha)^{-s-k}$$

and the result follows for $\Re s > 1$ by Taylor's theorem. The Taylor expansion also gives us the analytic continuation to $\mathbb{C} \setminus \mathbb{Z}_{\leq 0}$. □

In practice, it is better to work with

$$\zeta_1(s, \alpha) = \zeta(s, \alpha) - \alpha^{-s}$$

and recover $\zeta(s, \alpha)$ by adding back the missing term.

To be able to rigorously bound the error in truncating the series definition and the Taylor approximation, we use the following lemma:

Lemma 6.3. *If we use the first τ terms of the Taylor approximation to $\zeta_1(s, \alpha+\delta)$, then the absolute error is bounded by*

$$\frac{(\tau + 1) \left| s(s+1) \dots (s+\tau-1) \zeta_1(s+\tau, \alpha) \right| \delta^\tau}{\tau!(\tau + 1 - (|s| + \tau)\delta)}$$

and the approximation is valid for

$$\frac{(|s| + \tau)\delta}{\tau + 1} < 1.$$

Proof. The first term dropped is

$$\frac{s(s+1)\dots(s+\tau-1)\zeta_1(s+\tau,\alpha)\delta^\tau}{\tau!}$$

and the result follows by considering the geometric sequence with this first term and with common ratio

$$\frac{(|s|+\tau)\delta}{\tau+1}.$$

□

We discuss the choice of parameters in Section 9.

7. Algorithm 2

As will be discussed in Section 9, Algorithm 1 becomes inefficient as the height up the critical line increases. As an alternative, we took Booker's rigorous algorithm for computing L-functions described in [3] and specialised it to Dirichlet L-functions as follows:

For $\eta \in (-1,1)$ and even primitive characters χ define

$$F_e(t,\chi) := \epsilon_\chi q^{\frac{it}{2}} \pi^{-\frac{1/2+it}{2}} \Gamma\left(\frac{1/2+it}{2}\right) \exp\left(\frac{\pi\eta t}{4}\right) L_\chi\left(\frac{1}{2}+it\right) \text{ and}$$

$$\widehat{F}_e(x,\chi) := \frac{1}{2\pi}\int_{-\infty}^{\infty} F_e(t,\chi)e^{-ixt}\mathrm{d}t.$$

For odd primitive characters χ define

$$F_o(t,\chi) := \epsilon_\chi q^{\frac{it}{2}} \pi^{-\frac{3/2+it}{2}} \Gamma\left(\frac{3/2+it}{2}\right) \exp\left(\frac{\pi\eta t}{4}\right) L_\chi\left(\frac{1}{2}+it\right) \text{ and}$$

$$\widehat{F}_o(x,\chi) := \frac{1}{2\pi}\int_{-\infty}^{\infty} F_o(t,\chi)e^{-ixt}\mathrm{d}t.$$

We chose the parameter η to control the decay of the gamma factor as t increases (see Section 9).

We now choose $A, B > 0$ with $N = AB \in 2^{\mathbb{Z}_{>0}}$ and define

$$\widetilde{\widehat{F}}_e(n,\chi) := \sum_{k\in\mathbb{Z}} \widehat{F}_e\left(\frac{2\pi n}{B} + 2\pi kA, \chi\right) \text{ and}$$

$$\widetilde{\widehat{F}}_o(n,\chi) := \sum_{k\in\mathbb{Z}} \widehat{F}_o\left(\frac{2\pi n}{B} + 2\pi kA, \chi\right).$$

Similarly, define

$$\widetilde{F}_e(m,\chi) := \sum_{k\in\mathbb{Z}} F_e\left(\frac{m}{A} + kB, \chi\right) \text{ and}$$

$$\widetilde{F}_o(m,\chi) := \sum_{k\in\mathbb{Z}} F_o\left(\frac{m}{A} + kB, \chi\right).$$

In outline, the method is:

(1) Compute $\widehat{F}_e\left(\frac{2\pi n}{B}\right)$ or $\widehat{F}_o\left(\frac{2\pi n}{B}\right)$ for $n = 0\dots N-1$.
(2) Use these values as an approximation to $\widetilde{\widehat{F}}_e(n,\chi)$ or $\widetilde{\widehat{F}}_o(n,\chi)$, respectively.
(3) Appealing to Theorem 3.2, perform a DFT to yield $\widetilde{F}_e(m,\chi)$ or $\widetilde{F}_o(m,\chi)$, respectively.

(4) Use $\widetilde{F}_e(m,\chi)$ or $\widetilde{F}_o(m,\chi)$ as an approximation to $F_e\left(\frac{m}{A},\chi\right)$ or $F_o\left(\frac{m}{A},\chi\right)$, respectively.

We now make the above outline rigorous.

7.1. Computing $\widehat{F}_e(t)$ and $\widehat{F}_o(t)$.

Lemma 7.1. *Let $x \in \mathbb{R}$, $\eta \in (-1,1)$ and $u(x) := \frac{\pi\eta i}{4} + x$. Then we have*

$$\widehat{F}_e(x,\chi) = \frac{2\epsilon_\chi \exp\left(\frac{u(x)}{2}\right)}{q^{\frac{1}{4}}} \sum_{n=1}^{\infty} \chi(n) \exp\left(-\frac{\pi n^2 \exp(2u(x))}{q}\right).$$

Proof. Writing $s = 1/2 + it$ we get

$$\begin{aligned}
\widehat{F}_e(x,\chi) =& \frac{\epsilon_\chi}{2\pi i} \int\limits_{\Re(s)=\frac{1}{2}} q^{\frac{s-1/2}{2}} \pi^{-\frac{s}{2}} \Gamma\left(\frac{s}{2}\right) \exp\left(\frac{-(\pi\eta i + 4x)(s-1/2)}{4}\right) L_\chi(s) \mathrm{d}s \\
=& \frac{\epsilon_\chi}{2\pi i} \int\limits_{\Re(s)=2} q^{\frac{s-1/2}{2}} \pi^{-\frac{s}{2}} \Gamma\left(\frac{s}{2}\right) \exp\left(-u(x)(s-1/2)\right) L_\chi(s) \mathrm{d}s \\
=& \frac{\epsilon_\chi \exp\left(\frac{u(x)}{2}\right)}{q^{\frac{1}{4}}} \frac{1}{2\pi i} \int\limits_{\Re(s)=2} \left(\frac{q}{\pi}\right)^{\frac{s}{2}} \Gamma\left(\frac{s}{2}\right) \exp\left(2u(x)\right)^{-\frac{s}{2}} \sum_{n=1}^{\infty} \chi(n) n^{-s} \mathrm{d}s \\
=& \frac{\epsilon_\chi \exp\left(\frac{u(x)}{2}\right)}{q^{\frac{1}{4}}} \sum_{n=1}^{\infty} \chi(n) \frac{1}{2\pi i} \int\limits_{\Re(s)=2} \left(\frac{\pi n^2}{q}\right)^{-\frac{s}{2}} \Gamma\left(\frac{s}{2}\right) \exp(2u(x))^{-\frac{s}{2}} \mathrm{d}s \\
=& \frac{2\epsilon_\chi \exp\left(\frac{u(x)}{2}\right)}{q^{\frac{1}{4}}} \sum_{n=1}^{\infty} \chi(n) \exp\left(-\frac{\pi n^2 \exp(2u(x))}{q}\right),
\end{aligned}$$

as required. □

We can rigorously bound the error in truncating the sum either by reference to Lemma 5.4 of [3] or by majorising the missing terms with the obvious geometric series.

Lemma 7.2. *Let x, η and $u(x)$ be as defined in Lemma 7.1. Then we have*

$$\widehat{F}_o(x,\chi) = \frac{2\epsilon_\chi \exp\left(\frac{3u(x)}{2}\right)}{q^{\frac{3}{4}}} \sum_{n=1}^{\infty} n\chi(n) \exp\left(-\frac{\pi n^2 \exp(2u(x))}{q}\right).$$

Proof. The proof follows the same lines as Lemma 7.1. □

Section 9 contains a discussion of how many terms of the sum are required in practice.

7.2. Approximating $\widetilde{\widehat{F}}_e$ and $\widetilde{\widehat{F}}_o$ with $\widehat{F}_e$ and $\widehat{F}_o$.

We intend to choose our parameters to allow us to use $\widehat{F}_e$ and $\widehat{F}_o$ as approximations to $\widetilde{\widehat{F}}_e$ and $\widetilde{\widehat{F}}_o$, respectively. We therefore need to bound the error introduced and we start with two lemmas.

Lemma 7.3. *For $t \in \mathbb{R}$ we have*

$$\left|L_\chi\left(\frac{1}{2}+it\right)\right| \le \zeta\left(\frac{9}{8}\right)\left(\frac{q}{2\pi}\right)^{5/16}\left(\frac{3}{2}+|t|\right)^{5/16}.$$

Proof. We evaluate Rademacher's bound [14]

$$|L_\chi(s)| \le \zeta(1+\nu)\left(\frac{q|1+s|}{2\pi}\right)^{\frac{1+\nu-\Re(s)}{2}}$$

with $\nu = 1/8$ and $s = 1/2 + it$. □

Lemma 7.4 (Booker)**.** *Let $\eta \in (-1,1)$, $\delta := \frac{\pi}{2}(1-|\eta|)$ and $X(x) := \pi\delta \mathrm{e}^{2x-\delta}/q > 1$. Then*

$$\left|\sum_{k=0}^{\infty} \widehat{F}_e(x+2\pi kA,\chi)\right| \le \frac{4\exp\left(\frac{x}{2}-X(x)\right)\left(1+\frac{1}{2X(x)}\right)}{\delta^{\frac{1}{2}}q^{\frac{1}{4}}\left(1-\mathrm{e}^{-\pi A}\right)}$$

and

$$\left|\sum_{k=0}^{\infty} \widehat{F}_o(x+2\pi kA,\chi)\right| \le \frac{4\exp\left(\frac{3x}{2}-X(x)\right)\left(1+\frac{1}{2X(x)}\right)^{\frac{3}{2}}}{\delta^{\frac{1}{2}}q^{\frac{3}{4}}\left(1-\mathrm{e}^{-\pi A}\right)}.$$

Proof. This is Lemma 5.6 of [3] specialised to Dirichlet L-functions. □

The key aspect of Lemma 7.4 is that the sum ranges only over $k \ge 0$. This allows us to formulate the following bound for the error in taking $\widehat{F}_{e,o}(2\pi n/B,\chi)$ as an approximation to $\widetilde{\widehat{F}}_{e,o}(n,\chi)$:

Lemma 7.5. *Let $A \ge \frac{1}{2\pi}$, $B > 0$, $w_1 = \frac{2\pi n}{B} + 2\pi A$, $w_2 = -\frac{2\pi n}{B} + 2\pi A$, with $X(x)$ and δ as defined in Lemma 7.4 and $X(w_1), X(w_2) > 1$. Then*

$$\left|\widetilde{\widehat{F}}_e(n,\chi) - \widehat{F}_e\left(\frac{2\pi n}{B},\chi\right)\right|$$
$$\le \frac{4\left(\exp\left(\frac{w_1}{2}-X(w_1)\right)\left(1+\frac{1}{2X(w_1)}\right)+\exp\left(\frac{w_2}{2}-X(w_2)\right)\left(1+\frac{1}{2X(w_2)}\right)\right)}{q^{1/4}\delta^{1/2}(1-e^{-\pi A})}$$

and

$$\left|\widetilde{\widehat{F}}_o(n,\chi) - \widehat{F}_o\left(\frac{2\pi n}{B},\chi\right)\right|$$
$$\le \frac{4\left(\exp\left(\frac{3w_1}{2}-X(w_1)\right)\left(1+\frac{1}{2X(w_1)}\right)^{\frac{3}{2}}+\exp\left(\frac{3w_2}{2}-X(w_2)\right)\left(1+\frac{1}{2X(w_2)}\right)^{\frac{3}{2}}\right)}{q^{3/4}\delta^{1/2}(1-e^{-\pi A})}.$$

Proof. We will consider the even case, the odd case being identical. We have

$$\widetilde{\widehat{F}}_e(n,\chi) = \widehat{F}_e\left(\frac{2\pi n}{B},\chi\right) + \sum_{k=1}^{\infty}\widehat{F}_e\left(\frac{2\pi n}{B}+2\pi kA,\chi\right) + \sum_{k=1}^{\infty}\widehat{F}_e\left(\frac{2\pi n}{B}-2\pi kA,\chi\right).$$

Now, $F_e(x,\chi)$ is real valued, so $\widehat{F}_e(x,\chi) = \overline{\widehat{F}_e(-x,\chi)}$ and we get

$$\widetilde{\widehat{F}}_e(n,\chi) = \widehat{F}_e\left(\frac{2\pi n}{B},\chi\right) + \sum_{k=1}^{\infty}\widehat{F}_e\left(\frac{2\pi n}{B}+2\pi kA,\chi\right) + \overline{\sum_{k=1}^{\infty}\widehat{F}_e\left(-\frac{2\pi n}{B}+2\pi kA,\chi\right)}$$

and the result follows using Lemma 7.4 with $x = \pm\frac{2\pi n}{B} + 2\pi A$. □

Lemma 7.6. *Given $t \in \mathbb{R}$ and $B > 0$, we define*

$$E_e(t) := \zeta\left(\frac{9}{8}\right)\pi^{-\frac{1}{4}}\left|\Gamma\left(\frac{1}{4}+\frac{it}{2}\right)\right| e^{\frac{\pi}{4}\eta t}\left(\frac{q}{2\pi}\left|\frac{3}{2}+t\right|\right)^{\frac{5}{16}},$$

$$\beta_e(t) := \frac{\pi}{4} - \frac{1}{2}\arctan\left(\frac{1}{2|t|}\right) - \frac{4}{\pi^2|t^2-\frac{1}{4}|},$$

$$E_o(t) := \zeta\left(\frac{9}{8}\right)\pi^{-\frac{3}{4}}\left|\Gamma\left(\frac{3}{4}+\frac{it}{2}\right)\right| e^{\frac{\pi}{4}\eta t}\left(\frac{q}{2\pi}\left|\frac{3}{2}+t\right|\right)^{\frac{5}{16}}$$

and

$$\beta_o(t) := \frac{\pi}{4} - \frac{3}{2}\arctan\left(\frac{1}{2|t|}\right) - \frac{4}{\pi^2|t^2-\frac{9}{4}|}.$$

Then for $\beta_{e,o}\left(\frac{m}{A}+B\right) > \frac{\pi}{4}\eta$ and $\beta_{e,o}\left(\frac{m}{A}-B\right) > -\frac{\pi}{4}\eta$ we have

$$\left|\widetilde{F}_e(m,\chi) - F_e\left(\frac{m}{A},\chi\right)\right|$$
$$\leq \frac{E_e\left(\frac{m}{A}+B\right)}{1-\exp(-B(\beta_e(m/A+B)-\frac{\pi}{4}\eta))} + \frac{E_e\left(\frac{m}{A}-B\right)}{1-\exp(-B(\beta_e(m/A-B)+\frac{\pi}{4}\eta))}$$

and

$$\left|\widetilde{F}_o(m,\chi) - F_o\left(\frac{m}{A},\chi\right)\right|$$
$$\leq \frac{E_o\left(\frac{m}{A}+B\right)}{1-\exp(-B(\beta_o(m/A+B)-\frac{\pi}{4}\eta))} + \frac{E_o\left(\frac{m}{A}-B\right)}{1-\exp(-B(\beta_o(m/A-B)+\frac{\pi}{4}\eta))}.$$

Proof. We apply Lemma 5.7 (i) of [3] with $t = \frac{m}{A}+B$ and 5.7 (ii) with $t = \frac{m}{A}-B$, replacing the bound for $L_\chi(s)$ with our Lemma 7.3. □

We note here that the condition on $\beta_{e,o}(t)$ will fail when t is small, i.e., when $\frac{m}{A} \approx B$. However, this only happens for m approaching AB, by which point the loss of precision through other factors has rendered these values useless for computational purposes anyway.

8. Rigorous up-sampling

The algorithms described in Sections 6 and 7 both result in a lattice of values of $\Lambda_\chi(t)$. At any reasonable sampling rate, we expect to miss sign changes of Λ_χ and thus pairs of zeros. We employ a rigorous up-sampling technique based on theorems of Whittaker-Shannon and Weiss to resolve such cases.

Theorem 8.1 (Whittaker-Shannon Sampling Theorem)**.** *Let $f(t)$ be a continuous, real-valued function with Fourier Transform $\widehat{f}(x)$ such that $\widehat{f}(x) = 0$ for $|x| > A/2 > 0$. Also, define*

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

Then

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

when this sum converges.

Proof. See [19]. □

To apply Theorem 8.1 rigorously, we need to examine two sources of error:

- the error introduced by truncating the sum and
- the error introduced if the function is only approximately band-limited.

The former will be dealt with on a case-by-case basis. The latter, referred to as aliasing in signal processing circles, is the subject of a theorem due to Weiss.

Theorem 8.2 (Weiss)**.** *Let $f(t)$ be a real-valued function with Fourier Transform $\widehat{f}(x) := \frac{1}{2\pi}\int_{-\infty}^{\infty} f(t)\exp(-itx)dt$ such that*

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

Then

$$\left| f(t) - \sum_{n\in\mathbb{Z}} f\left(\frac{n}{A}\right) \operatorname{sinc}(n\pi - \pi A t) \right| \leq 4 \int\limits_{\pi A}^{\infty} \left|\widehat{f}(x)\right| dx.$$

Proof. See, for example, [5]. □

To exploit Theorems 8.1 and 8.2, we window $\Lambda_\chi(t)$ with a Gaussian. This is by no means the only choice, but it will suffice for our purposes, in that it returns a function which is approximately band limited. For $t_0 \in \mathbb{R}$ and $h > 0$ define $W : \mathbb{R} \to \mathbb{R}$ by

$$W(t,\chi) := \Lambda_\chi(t) \exp\left(\frac{-(t-t_0)^2}{2h^2}\right)$$

so $W(t_0,\chi) = \Lambda_\chi(t_0)$ and the parameter h (see Section 9) controls the effective width of the window.

Before moving on to estimate the error from the fact that $W(t,\chi)$ is only approximately band limited, we require two preparatory lemmas.

Lemma 8.3. *For $a_\chi \in \{0,1\}$,*

$$\left|\Gamma\left(\frac{\frac{1}{2}+it+a_\chi}{2}\right)\right| e^{\frac{\pi t}{4}} \leq \max\left(\sqrt{\pi}\,(3+\max(2t,0))^{\frac{1}{4}}\,\mathrm{e}^{\frac{1}{6}}, \sqrt{2\pi}\exp\left(\frac{\pi}{8}+\frac{1}{4}\right)\right).$$

Proof. We use Stirling's approximation separately for $a_\chi = 0$ and $a_\chi = 1$. □

Lemma 8.4. *Let $t_0 \geq 0$, $h > 0$ and define*

$$P(t_0,h) := \int\limits_{-\infty}^{\infty} \left|\Gamma\left(\frac{3+it}{2}\right)\right| \exp\left(\frac{\pi t}{4}\right) \exp\left(-\frac{(t-t_0)^2}{2h^2}\right) \mathrm{d}t.$$

Then

$$P(t_0,h) \leq h\pi\left(t_0 + \frac{h}{\sqrt{2\pi}} + 1 + \frac{1}{2\sqrt{2}}\right).$$

Proof. We have

$$\begin{aligned}
P(t_0,h) \leq & \int_0^\infty \left|\Gamma\left(\frac{3+it}{2}\right)\right| \exp\left(\frac{\pi t}{4}\right) \exp\left(\frac{-(t-t_0)^2}{2h^2}\right) \mathrm{d}t \\
& + \int_{-\infty}^0 \left|\Gamma\left(\frac{3+it}{2}\right)\right| \exp\left(\frac{\pi t}{4}\right) \exp\left(\frac{-(t-t_0)^2}{2h^2}\right) \mathrm{d}t \\
\leq & \int_0^\infty \frac{(1+t)}{2} \left|\Gamma\left(\frac{1+it}{2}\right)\right| \exp\left(\frac{\pi t}{4}\right) \exp\left(\frac{-(t-t_0)^2}{2h^2}\right) \mathrm{d}t \\
& \qquad + \Gamma\left(\frac{3}{2}\right) \frac{h\sqrt{2\pi}}{2} \left(1 - \operatorname{erf}\left(\frac{\sqrt{2}t_0}{2}\right)\right) \\
\leq & \int_0^\infty \frac{(1+t)}{2} \sqrt{\frac{\pi}{\cosh(\pi t/2)}} \exp\left(\frac{\pi t}{4}\right) \exp\left(\frac{-(t-t_0)^2}{2h^2}\right) dt \\
& \qquad + \Gamma\left(\frac{3}{2}\right) \frac{h\sqrt{2\pi}}{2} \\
\leq & \int_0^\infty \frac{(1+t)}{2} \sqrt{2\pi} \exp\left(\frac{-(t-t_0)^2}{2h^2}\right) \mathrm{d}t + \frac{h\pi\sqrt{2}}{4} \\
\leq & h\pi\left(\frac{h}{\sqrt{2\pi}} + t_0 + 1\right) + \frac{h\pi\sqrt{2}}{4},
\end{aligned}$$

as claimed. □

Lemma 8.5. *Define $P_0(t,h)$ as in Lemma 8.4 and $I_\chi(A)$ for $A > 0$ by*

$$I_\chi(A) := 4 \int_{\pi A}^\infty \left| \frac{1}{2\pi} \int_{-\infty}^\infty W(t,\chi) \exp(-ixt) \mathrm{d}t \right| \mathrm{d}x.$$

Then, writing M in place of $\frac{5}{2} - a_\chi$ we have

$$I_\chi(A) \leq \frac{2\left(\frac{q}{\pi}\right)^{\frac{M}{2}} \zeta(M+1/2) \exp\left(\frac{M^2}{2h^2} - \pi A M\right) P(t_0,h)}{\pi M}.$$

Proof. Writing $s = 1/2 + it$ we get

$$\begin{aligned}
I_\chi(A) \leq & \frac{2}{\pi} \int_{\pi A}^\infty \left| \int_{\Re(s)=1/2} \left(\frac{q}{\pi}\right)^{\frac{s-1/2}{2}} \Gamma\left(\frac{s+a_\chi}{2}\right) \exp\left(\frac{\pi i(1/2-s)}{4}\right) L_\chi(s) \right. \\
& \left. \exp((1/2-s)x) \exp\left(\frac{-(i(1/2-s)-t_0)^2}{2h^2}\right) \mathrm{d}s \right| \mathrm{d}x.
\end{aligned}$$

We now shift the contour of integration to the right so that $\Re(s) = \sigma = 3 - a_\chi$ and write $s = M + 1/2 + it$ to get

$$I_\chi(A) \leq \frac{2}{\pi} \int_{\pi A}^{\infty} \int_{-\infty}^{\infty} \left| \left(\frac{q}{\pi}\right)^{\frac{M}{2}} \Gamma\left(\frac{3+it}{2}\right) \exp\left(\frac{\pi t}{4}\right) \zeta(M+1/2) \right.$$
$$\left. \exp(-Mx) \exp\left(\frac{M^2 - (t-t_0)^2}{2h^2}\right) \right| \mathrm{d}t \, \mathrm{d}x.$$

Integrating with respect to t gives us

$$I_\chi(A) \leq \frac{2}{\pi} \left(\frac{q}{\pi}\right)^{\frac{M}{2}} \zeta(M+1/2) \exp\left(\frac{M^2}{2h^2}\right) P(t_0, h) \int_{\pi A}^{\infty} \exp(-Mx) \mathrm{d}x$$

and the result follows after integrating with respect to x. □

Lemma 8.6. *Let $h, A > 0$, $t_0 = \frac{n_0}{A}$ for some $n_0 \in \mathbb{Z}_{>0}$ and $S \in \mathbb{Z}_{>0}$. Now define*

$$G(n) := \frac{\left(\frac{3}{2} + t_0 + \frac{S+n}{A}\right)^{9/16} \exp\left(\frac{-(S+n)^2}{2A^2h^2}\right)}{\pi(S+n)}.$$

Then

$$\sum_{n \geq At_0 + S} \left(\frac{3}{2} + \frac{n}{A}\right)^{9/16} \exp\left(\frac{-\left(\frac{n}{A} - t_0\right)^2}{2h^2}\right) \operatorname{sinc}(\pi n - \pi A t_0) \leq \frac{G(0)}{1 - \frac{G(1)}{G(0)}}.$$

Proof. $G(n)$ is at least as large as the corresponding term in the sum and the ratio $G(n+1)/G(n)$ is a decreasing function of n so the result follows as the sum of a geometric series. □

We can now combine Lemmas 7.3, 8.3 and 8.6.

Lemma 8.7. *Define*

$$E := \sum_{|n| \geq S} W\left(\frac{n}{A}\right) \operatorname{sinc}\left(\pi A \left(\frac{n}{A} - t_0\right)\right).$$

Then for large enough t_0 we have

$$|E| \leq \sqrt{\pi} \zeta\left(\frac{9}{8}\right) \exp(1/6) 2^{5/4} \left(\frac{q}{2\pi}\right)^{5/16} \frac{G(0)}{1 - G(1)/G(0)}.$$

9. Selecting parameters

Before turning to the computation itself, we briefly discuss how we determined suitable values for the various parameters.

9.1. **Parameter A.** $1/A$ determines the spacing between successive values of $\Lambda_\chi(t)$ we will compute and is common across both algorithms. If $1/A$ is too large, we will miss many sign changes of Λ_χ and have to perform a lot of up-sampling as a result. Conversely, too small a value for $1/A$ means we will spend more time computing the values of Λ_χ than necessary. We initially planned to examine all moduli $q \leq 100\,000$ to a height t up the critical line such that $qt \geq 10^8$. This implies that the mean density of zeros is about 2.5 and we found that a sampling rate of approximately 5 times that density was a reasonable compromise. We settled on $A = 64/5$ as

this has the added advantage that $1/A$ is exactly representable in an IEEE floating point.

9.2. **The cut-over from Algorithm 1 to Algorithm 2.** Continuing to use Algorithm 1 all the way up to $10^8/3$ (when $q = 3$) would have presented us with a number of problems:

- As t increases, Lemma 6.3 dictates that we need to increase the number of terms of the Taylor series we use and/or reduce the size of δ in order to control the error terms. This increases both the computational cost of constructing the tables and the storage space required to hold them.
- As t increases, the cost of computing each table is amortised over fewer and fewer q. In the extreme, the tables needed to handle $10^8/4 < t \leq 10^8/3$ would only get used once (for $q = 3$).

These factors meant that above some height t, Algorithm 1 would become unwieldy compared with Algorithm 2. Experimentally, we concluded that a suitable cross over was at $q = 10\,000$ where the height to which we wished to check GRH was $t = 10\,000$.

9.3. **Parameters specific to Algorithm 1.** We used $\tau = 15$ terms in the Taylor expansion and by pre-computing $\zeta_1(1/2 + k + it, a/2^{11})$ for $k \in [0, \tau - 1]$ and $a \in [1, 2^{11}]$ we had $\delta \leq 2^{-12}$ in Lemma 6.3. This gave us an absolute error of $< 6 \cdot 10^{-7}$ at height $t = 10\,000$. Accordingly, each pre-computed table consisted of $15 \cdot 2^{11} = 30\,720$ double precision interval entries (16 bytes each).[4]

Since each value of t required its own table, and we sampled the half line at intervals $1/A = 5/64$ apart, we needed 128 000 such tables to reach $T = 10\,000$ and these occupied about 63 Gbytes of disk.

Computing the tables parallelises trivially and required an insignificant amount of time.

9.4. **Parameters specific to Algorithm 2.**

9.4.1. *Parameter η.* The parameter η is chosen to resist the decay of the $\log\Gamma$ function as we move up the critical line. Defining T to be the maximum height to which we wanted to confirm GRH for a given q (including a small region to support Turing's method), then we set

$$\eta := 1 - \frac{\varpi}{T}$$

where $\varpi = 4.0$ for even characters and $\varpi = 7.03$ for odd characters. In practice this meant that η ranged from $0.999\,299\,10\ldots$ for odd characters of modulus 10 000 to $0.999\,999\,80\ldots$ for the even primitive character of modulus 5.

The value chosen for η also determines the number of terms we need to take in the sums referred to in Lemmas 7.1 and 7.2. The worst case is when $x = 0$ when the first term dropped is of absolute magnitude

$$\frac{2}{q^{1/4}} \exp\left(-\frac{\pi n^2 \cos\left(\frac{\pi\eta}{2}\right)}{q}\right)$$

and

$$\frac{2n}{q^{3/4}} \exp\left(-\frac{\pi n^2 \cos\left(\frac{\pi\eta}{2}\right)}{q}\right)$$

[4]We could have varied these parameters with t, but did not do so.

for even and odd characters, respectively. Specifically, for $x = 0$ and $q = 10\,000$ we used 14 541 terms in the sum for even characters and 11 560 terms for odd ones. The first term omitted was of absolute magnitude $< 2 \cdot 10^{-19}$ in each case.

The number of terms needed to approximate $\widehat{F}_e(x, \chi)$ and $\widehat{F}_o(x, \chi)$ decays rapidly as x increases. For example, more than 3/4 of the values required at $q = 10\,000$ can be adequately approximated with a single term of the sum.

9.4.2. *Parameters N and B.* The parameter N determines the number of sample points at which we will compute $\widehat{F}_{e,o}$ and ultimately $F_{e,o}$. Thus to achieve a height of T up the critical line, we need $N \geq AT$, i.e., $B \geq T$. However, to control the error term in Lemmas 7.5 and 7.6[5], we need to take B larger than this minimum, and a factor of 7.5 suffices. Further, we would like N to be a power of 2 so that we can exploit one of the Fast Fourier Transform Algorithms, so we set N to be the next power of 2 larger than $7.5T$. Thus N ranged from 2^{20} when $q = 10\,000$ up to 2^{32} when $q = 3, 4$.[6]

Using these parameters, the worst case error from Lemma 7.6 was $< 2.21 \cdot 10^{-8}$ at $q = 9\,183$ when $N = 2^{20}$.

9.5. **Up-sampling parameters.** When up-sampling, we set h, the width of the Gaussian window, to be 7/32 and S, the number of samples on either side of t_0 to be 20. This gave us an up-sampling error (Lemma 8.7) $|E| < 8.3 \cdot 10^{-8}$.

10. Results

We were fortunate to be given access to various clusters in the UK and France, all with Error Correcting Code memory. Both algorithms parallelise trivially. In the case of Algorithm 1, we assign different q to each node and then different ranges of t to each core within a node. For Algorithm 2, we assign either the odd or even characters for a given q to a node, and then individual cores compute the sum in Lemma 7.1 for different equivalence classes modulo q.

We routinely up-sampled the output by a factor of 8 and then if necessary by 32, 128 and ultimately 512. At this point, about 0.000 3% of the L-functions remained due to one or more of the following issues:

- The sign of $\Lambda_\chi(1/2)$ could not be determined. This was resolved using a double precision interval implementation of Euler-MacLaurin.
- The sign of Λ_χ was positive, became indeterminate and then became positive again (or negative, indeterminate, negative). Since a failure to cross the x axis here would, on its own, be enough to refute GRH, we fully expected to find that the indeterminate region was actually hiding a pair of zeros. In every case, using an interval arithmetic version of Euler-MacLaurin (first at double precision, but occasionally resorting to MPFI at 100 bits) located the expected sign changes.
- The sign of Λ_χ was positive, indeterminate and then negative (or vice versa). Rather than hiding a single sign change, closer inspection revealed three sign changes in the indeterminate region.

[5]It turns out that the former is insignificant.

[6]With $N = 2^{32}$ and each double precision interval consisting of 16 bytes, the FFT vector occupied 64Gbytes of memory.

- Occasionally, the estimate for the number of zeros to locate computed via Turing's method did not bracket an integer. This was caused by zeros being missed in the region used to compute the Turing estimate itself and these were resolved by shifting the region or locating the missing zeros using high precision.

A series of Unix scripts were used to determine which of these failure modes was present in each case and the appropriate high precision routine was then used to resolve it. The time for this part of the computation was insignificant.

In all, the computation consumed approximately 400 000 core hours.[7] We checked all the 29 565 923 837 Dirichlet L-functions with primitive modulus $q \leq 400\,000$, isolating approximately $3.8 \cdot 10^{13}$ zeros (not counting those used in Turing's method). Specifically, we have:

Theorem 10.1. *GRH holds for Dirichlet L-functions of primitive characters of modulus $q \leq 400\,000$ and to height $T = max\left(\frac{10^8}{q}, \frac{7.5 \cdot 10^7}{q} + 200\right)$ for even q and to height $T = max\left(\frac{10^8}{q}, \frac{3.75 \cdot 10^7}{q} + 200\right)$ for odd q.*

In addition, we explored the central point of the 739 151 526 102 primitive characters with $q \leq 2\,000\,000$ using Algorithm 1. In 438 152 cases, the computation returned a value for the completed L-function as a double precision interval that straddled zero. Recomputing these points, again using double precision intervals but this time via Euler-MacLaurin, resolved all but 20 and these were in turn eliminated using Euler-MacLaurin implemented in MPFI at 100 bits of precision. We can therefore state:

Theorem 10.2. *For every Dirichlet L-function of primitive character of modulus $q \leq 2\,000\,000$, we have*

$$L_\chi(1/2) \neq 0.$$

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